Nanopore ePNP-NS modelling

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SUMMARY

This report represents the full implementation of the ePNP-NS equations for a 2D-axisymmetric model of the ClyA-AS nanopore.

It includes all used parameters, variables, functions, geometries, solver settings and mesh settings needed to reproduce the results.

In addition, it includes plots of the wall distance corrections and concentration dependent corrections (500 mM salt, -150 mV bias).

Contents

1 Global Definitions

Author	Kherim Willems
Date	May 22, 2020 11:17:01 AM

GLOBAL SETTINGS

Name	Npgrid clya v8 NaCl report.mph
Path	D:\repos\comsol\clya\npgrid_clya_v8_NaCl_report.mph
Version	COMSOL Multiphysics 5.4 (Build: 388)
Unit system	SI

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

1.1 PARAMETERS

1.1.1 System

SYSTEM

Name	**Expression**	**Value**	**Description**
V_bias	-150[mV]	−0.15 V	Applied bias voltage
T_system	25[degC]	298.15 K	Global system temperature
c_salt	500[mM]	500 mol/m^3	Bulk salt concentration
c_cis	c_salt	500 mol/m^3	Salt concentration in the cis compartment
c_trans	c_salt	500 mol/m^3	Salt concentration in the trans compartment

1.1.2 Geometry

GEOMETRY

Name	**Expression**	**Value**	**Description**
r_reservoir	250[nm]	2.5E−7 m	Reservoir radius
d_membrane	2.8[nm]	2.8E−9 m	Membrane thickness

1.1.3 Enabled Physics

ENABLED PHYSICS

Name	**Expression**	**Value**	**Description**
enable_wdf	1	1	Switch to toggle wall distance dependent diffusion, mobility and viscosity on (1) or off (0)
enable_cdf	1	1	Switch to toggle concentration dependent effects on (1) or off (0)

Name	Expression	Value	Description
enable_smp	1	1	Switch to toggle size-modified PNP on (1) or off (0)
enable_cdf_rho	1	1	Switch to toggle concentration dependent density on (1) or off (0)
enable_cdf_epsr	1	1	Switch to toggle concentration dependent permittivity on (1) or off (0)
enable_cdf_eta	1	1	Switch to toggle concentration dependent viscosity on (1) or off (0)
enable_cdf_mob	1	1	Switch to toggle concentration dependent mobility and diffusion coefficientson (1) or off (0)

1.1.4 Electrolyte

ELECTROLYTE

Name	Expression	Value	Description
a_cpos	0.5[nm]	5E−10 m	Maximum steric diameter, cpos (13.284 M)
a_cneg	0.5[nm]	5E−10 m	Maximum steric diameter, cneg (13.284 M)
a_sol	0.311[nm]	3.11E−10 m	Maximum steric diameter, water (55.2M)
z_cpos	1	1	Charge number, cpos
z_cneg	-1	−1	Charge number, cneg
epsr0	78.15	78.15	Relative permittivity of pure water
epsr_alpha	11.5	11.5	Relative permittivity, total excess polarization
epsr_ms	30.08	30.08	Relative permittivity, limitting permittivity at saturation
rho0	0.997[g/cm^3]	997 kg/m^3	Density of pure water
rho1	4.047e-2	0.04047	Density, P1
rho2	-6.149e-4	−6.149E−4	Density, P2
eta0	8.904e-4[Pa*s]	8.904E−4 Pa·s	Viscosity of pure water
eta1	7.558e-3	0.007558	Viscosity, P1
eta2	7.769e-2	0.07769	Viscosity, P2
eta3	1.192e-2	0.01192	Viscosity, P3
eta4	5.951e-4	5.951E−4	Viscosity, P4
d0_cpos	1.334e-9[m^2/s]	1.334E−9 m^2/s	Diffusion coefficient at infinite dilution, cpos

Name	Expression	Value	Description
d0_cneg	2.032e-9[m^2/s]	2.032E−9 m^2/s	Diffusion coefficient at infinite dilution, cneg
l0_cpos	(e_const^2*N_A_const)/(k_B_const*T_system)*d0_cpos	0.0050097 $s^3 \cdot A^2/(kg \cdot mol)$	Specific molar conductivity at infinite dilutions, cpos
l0_cneg	(e_const^2*N_A_const)/(k_B_const*T_system)*d0_cneg	0.0076309 $s^3 \cdot A^2/(kg \cdot mol)$	Specific molar conductivity at infinite dilution, cneg
d1_cpos	2.020e-01	0.202	Diffusion coefficient, P1, cpos
d2_cpos	-3.048e-01	−0.3048	Diffusion coefficient, P2, cpos
d3_cpos	2.190e-01	0.219	Diffusion coefficient, P3, cpos
d4_cpos	-3.124e-02	−0.03124	Diffusion coefficient, P4, cpos
d1_cneg	1.490e-01	0.149	Diffusion coefficient, P1, cneg
d2_cneg	-4.933e-02	−0.04933	Diffusion coefficient, P2, cneg
d3_cneg	3.392e-02	0.03392	Diffusion coefficient, P3, cneg
d4_cneg	1.431e-02	0.01431	Diffusion coefficient, P4, cneg
l1_cpos	7.907e-1	0.7907	Specific molar conductivity, P1, cpos
l2_cpos	-3.529e-1	−0.3529	Specific molar conductivity, P2, cpos
l3_cpos	1.459e-1	0.1459	Specific molar conductivity, P3, cpos
l4_cpos	9.241e-3	0.009241	Specific molar conductivity, P4, cpos
l1_cneg	6.289e-1	0.6289	Specific molar conductivity, P1, cneg
l2_cneg	-4.286e-1	−0.4286	Specific molar conductivity, P2, cneg
l3_cneg	2.123e-1	0.2123	Specific molar conductivity, P3, cneg
l4_cneg	-1.068e-2	−0.01068	Specific molar conductivity, P4, cneg
cmax	5.3[M]	5300 mol/m^3	Maximum valid concentration concentration for the fitting functions

2 Component 1: ClyA-AS

Date	Dec 4, 2017 4:51:24 PM

SETTINGS

Description	Value
Unit system	Same as global system
Geometry shape order	Automatic

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

Local physics properties

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
D_cpos	d0_cpos*cdf.D_cpos*wdf.D_wd_cpos	m^2/s	Local diffusion coefficient, cpos
D_cneg	d0_cneg*cdf.D_cneg*wdf.D_wd_cneg	m^2/s	Local diffusion coefficient, cneg
mu_cpos	(1/F_const^2) * l0_cpos*cdf.L_cpos*wdf.mu_wd_cpos	s·mol/kg	Local mobility, cpos
mu_cneg	(1/F_const^2) * l0_cneg*cdf.L_cneg*wdf.mu_wd_cneg	s·mol/kg	Local mobility, cneg

Name	Expression	Unit	Description
epsr_water	epsr0*cdf.epsr_c		Relative permittivity, reservoir
epsr_nanopore	20		Relative permittivity, nanopore
epsr_membrane	3.2		Relative permittivity, membrane
eta	eta0*cdf.eta_c*wdf.eta_wd	Pa·s	Local viscosity
rho	rho0*cdf.rho_c*wdf.rho_wd	kg/m³	Local density
scd.cpos	if(cpos<0, 0, cpos)	mol/m³	Never use negative ion concentration for calculating charge density during solving, cpos
scd.cneg	if(cneg<0, 0, cneg)	mol/m³	Never use negative ion concentration for calculating charge density during solving, cneg
scd_ions	F_const*(scd.cpos*tds.z_cpos + scd.cneg*tds.z_cneg)	C/m³	Space charge density due to ions
scd_pore	if(r<0.01[nm], 0, e_const*rhoq_pore(r, z)/(2*pi*r))	C/m³	Space charge density due to fixed charged in pore

Initial values

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
V_init	if(is_inside_pore, V_init_pore, if(z<0, V_bias, 0[V]))	V	Initial guess, V
V_init_pore	(V_bias - 0[V])/(z_trans - z_cis)*(z - z_cis) + 0[V]	V	Initial guess inside pore, V

Name	Expression	Unit	Description
cpos_init	if(is_inside_pore, cpos_init_pore, if(z<0, c_trans, c_cis))	mol/m³	Initial guess, cpos
cneg_init	if(is_inside_pore, cpos_init_pore, if(z<0, c_trans, c_cis))	mol/m³	Initial guess, cneg
cpos_init_pore	(c_trans - c_cis)/(z_trans - z_cis)*(z - z_cis) + c_cis	mol/m³	Initial guess inside pore, cpos
cneg_init_pore	(c_trans - c_cis)/(z_trans - z_cis)*(z - z_cis) + c_cis	mol/m³	Initial guess inside pore, cneg

Logicals

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
z_cis	12.25[nm]	m	Pore cis entry z-position
z_trans	-1.85[nm]	m	Pore trans entry z-position
is_inside_pore	(z <= z_cis) && (z >= z_trans) && r <= pre(r)		Boolean that is true (1) inside the pore and false (0) outside
central_integral_logical	(is_inside_pore && (wdf.wd > 0.1[nm]) || ((z>=z_cis || z<=z_trans) && (r < 6[nm])))		Boolean for performing the integration along the z-axis
is_inside_pore_bulk	is_inside_pore && (wdf.wd > 0.5[nm])		Boolean for integrating a 0.5 nm layer around the surface of the pore
is_inside_pore_surface	is_inside_pore && (wdf.wd <= 0.5[nm])		Boolean for integrating a the 'bulk' of the pore, at least 0.5 nm away from the surface of the pore

Concentration dependent factor (cdf)

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
cdf.enable	if(enable_cdf == 0, 0, 1)		Switch for concentration dependent effects
cdf.dcpos	if(cpos<1e-6[M], 1e-6, if(cpos>cmax, cmax[L/mol], cpos[L/mol]))		Dimensionless safe ion concentration, cpos

Name	Expression	Unit	Description
cdf.dcneg	if(cneg<1e-6[M], 1e-6, if(cneg>cmax, cmax[L/mol], cneg[L/mol]))		Dimensionless safe ion concentration, cneg
cdf.dcav	(cdf.dcpos + cdf.dcneg)*0.5		Arithmetic mean of ion concentrations
cdf.D_cpos	if(enable_cdf_mob == 0, 1, 1/(1 + d1_cpos*cdf.dcav^0.5 + d2_cpos*cdf.dcav + d3_cpos*cdf.dcav^(3/2) + d4_cpos*cdf.dcav^2))		Salt concentration dependent factor for self-diffusion, cpos
cdf.D_cneg	if(enable_cdf_mob == 0, 1, 1/(1 + d1_cneg*cdf.dcav^0.5 + d2_cneg*cdf.dcav + d3_cneg*cdf.dcav^(3/2) + d4_cneg*cdf.dcav^2))		Salt concentration dependent factor for self-diffusion, cneg
cdf.L_cpos	if(enable_cdf_mob == 0, 1, 1/(1 + l1_cpos*cdf.dcav^0.5 + l2_cpos*cdf.dcav + l3_cpos*cdf.dcav^(3/2) + l4_cpos*cdf.dcav^2))		Salt concentration dependent factor for ion mobility, cpos
cdf.L_cneg	if(enable_cdf_mob == 0, 1, 1/(1 + l1_cneg*cdf.dcav^0.5 + l2_cneg*cdf.dcav + l3_cneg*cdf.dcav^(3/2) + l4_cneg*cdf.dcav^2))		Salt concentration dependent factor for ion mobility, cneg
cdf.rho_c	if(enable_cdf_rho == 0, 1, 1 + rho1*cdf.dcav + rho2*cdf.dcav^2)		Salt concentration dependent factor for density
cdf.eta_c	if(enable_cdf_eta== 0, 1, 1 + eta1*cdf.dcav^0.5 + eta2*cdf.dcav + eta3*cdf.dcav^2 + eta4*cdf.dcav^3.5)		Salt concentration dependent factor for viscosity
cdf.epsr_c	if(enable_cdf_epsr == 0, 1, 1 - (1 - epsr_ms/epsr0)*(coth((3*epsr_alpha*cdf.dcav)/(epsr0 - epsr_ms)) - (epsr0 - epsr_ms)/(3*epsr_alpha*cdf.dcav)))		Salt concentration dependent factor for relative permitivitty

Wall distance factor (wdf)

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
wdf.enable	if(enable_wdf == 0, 0, 1)		Switch for wall distance dependent effects
wdf.wd	sqrt((r - wde(r))^2 + (z - wde(z))^2)	m	Distance from the nanopore walls

Name	Expression	Unit	Description
wdf.dwd	wdf.wd[1/nm]		Dimensionless wall distance (scaled to nm)
wdf.D_wd_cpos	if(wdf.enable == 0, 1, 1 - exp(-0.62e1*(wdf.dwd + 0.01)))		Wall distance factor for diffusion, cpos
wdf.D_wd_cneg	if(wdf.enable == 0, 1, 1 - exp(-0.62e1*(wdf.dwd + 0.01)))		Wall distance factor for diffusion, cneg
wdf.mu_wd_cpos	wdf.D_wd_cpos		Wall distance factor for mobility, cpos
wdf.mu_wd_cneg	wdf.D_wd_cneg		Wall distance factor for mobility, cneg
wdf.eta_wd	if(wdf.enable == 0, 1, 1 + exp(-wdf.a*(wdf.dwd - wdf.r0)))		Wall distance factor for viscosity
wdf.rho_wd	if(wdf.enable == 0, 1, 1)		Wall distance factor for density (not implemented)
wdf.a	3.36096		Wall distance factor, sigmoid slope
wdf.r0	0.14716		Wall distance factor, sigmoid offset

Size-modified Poisson-Nernst-Planck (smp)

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
smp.enable	if(enable_smp == 0, 0, 1)		Switch to enable steric concentration effects
smp.conc_max_sol	1/smp.rad3_solvent	mol/m^3	Maximum concentration, solvent
smp.conc_max_cpos	1/smp.rad3_cpos	mol/m^3	Maximum concentration, cpos
smp.conc_max_cneg	1/smp.rad3_cneg	mol/m^3	Maximum concentration, cneg
smp.rad3_cpos	N_A_const*a_cpos^3	m^3/mol	Specific volume, cpos
smp.rad3_cneg	N_A_const*a_cneg^3	m^3/mol	Specific volume, cneg

Name	Expression	Unit	Description
smp.rad3_solvent	N_A_const*a_sol^3	m^3/mol	Specific volume, solvent
smp.k_cpos	smp.rad3_cpos/smp.rad3_solvent		Ratio of ion over solvent size, cpos
smp.k_cneg	smp.rad3_cneg/smp.rad3_solvent		Ratio of ion over solvent size, cneg
smp.conc_sum	cpos + cneg	mol/m^3	Total ion concentration
smp.conc_rad3_sum	cpos*smp.rad3_cpos + cneg*smp.rad3_cneg		Total local steric repulsion
smp.alpha_cpos	(smp.k_cpos)/(1 - smp.conc_rad3_sum)		Concentration factor, cpos
smp.alpha_cneg	(smp.k_cneg)/(1 - smp.conc_rad3_sum)		Concentration factor, cneg
smp.sflux_cposr	smp.enable*smp.alpha_cpos*cpos*(smp.rad3_cpos*(-tds.D_cposrr*cposr - tds.D_cposrz*cposz) + smp.rad3_cneg*(-tds.D_cposrr*cnegr - tds.D_cposrz*cnegz))	mol/(m^2·s)	Steric flux, r component
smp.sflux_cposphi	smp.enable*smp.alpha_cpos*cpos*(smp.rad3_cpos*(-tds.D_cposphir*cposr - tds.D_cposphiz*cposz) + smp.rad3_cneg*(-tds.D_cposphir*cnegr - tds.D_cposphiz*cnegz))	mol/(m^2·s)	Steric flux, phi component
smp.sflux_cposz	smp.enable*smp.alpha_cpos*cpos*(smp.rad3_cpos*(-tds.D_cposzr*cposr - tds.D_cposzz*cposz) + smp.rad3_cneg*(-tds.D_cposzr*cnegr - tds.D_cposzz*cnegz))	mol/(m^2·s)	Steric flux, z component
smp.sflux_cnegr	smp.enable*smp.alpha_cneg*cneg*(smp.rad3_cpos*(-tds.D_cnegrr*cposr - tds.D_cnegrz*cposz) + smp.rad3_cneg*(-tds.D_cnegrr*cnegr - tds.D_cnegrz*cnegz))	mol/(m^2·s)	Steric flux, r component
smp.sflux_cnegphi	smp.enable*smp.alpha_cneg*cneg*(smp.rad3_cpos*(-tds.D_cnegphir*cposr - tds.D_cnegphiz*cposz) + smp.rad3_cneg*(-tds.D_cnegphir*cnegr - tds.D_cnegphiz*cnegz))	mol/(m^2·s)	Steric flux, phi component
smp.sflux_cnegz	smp.enable*smp.alpha_cneg*cneg*(smp.rad3_cpos*(-tds.D_cnegzr*cposr - tds.D_cnegzz*cposz) + smp.rad3_cneg*(-tds.D_cnegzr*cnegr - tds.D_cnegzz*cnegz))	mol/(m^2·s)	Steric flux, z component
smp.nsflux_cpos	smp.enable*smp.sflux_cposr*tds.nrc +	mol/(m^2·s)	Normal steric flux

Name	Expression	Unit	Description
	smp.sflux_cposphi*tds.nphic + smp.sflux_cposz*tds.nzc		
smp.nsflux_cneg	smp.enable*smp.sflux_cnegr*tds.nrc + smp.sflux_cnegphi*tds.nphic + smp.sflux_cnegz*tds.nzc	mol/(m²·s)	Normal steric flux
smp.sfluxMag_cpos	sqrt(smp.sflux_cposr^2 + smp.sflux_cposphi^2 + smp.sflux_cposz^2)	mol/(m²·s)	Steric flux magnitude
smp.sfluxMag_cneg	sqrt(smp.sflux_cnegr^2 + smp.sflux_cnegphi^2 + smp.sflux_cnegz^2)	mol/(m²·s)	Steric flux magnitude
smp.sfluxRes_cpos	smp.enable*smp.alpha_cpos*(smp.rad3_cpos*(-tds.D_cposrr*cposr - tds.D_cposrz*cposz - tds.D_cposzr*cposr - tds.D_cposzz*cposz) + smp.rad3_cneg*(-tds.D_cposrr*cnegr - tds.D_cposrz*cnegz - tds.D_cposzr*cnegr - tds.D_cnegzz*cposz))	m/s	Residual contribution
smp.sfluxRes_cneg	smp.enable*smp.alpha_cneg*(smp.rad3_cpos*(-tds.D_cnegrr*cposr - tds.D_cnegrz*cposz - tds.D_cnegzr*cposr - tds.D_cnegzz*cposz) + smp.rad3_cneg*(-tds.D_cnegrr*cnegr - tds.D_cnegrz*cnegz - tds.D_cnegzr*cnegr - tds.D_cnegzz*cnegz))	m/s	Residual contribution

Chemical potential

SELECTION

Geometric entity level	Domain
Name	Reservoir
Selection	Domain 1

Name	Expression	Unit	Description
muchem_cpos	pot_es_cpos + pot_ch_cpos + pot_st_cpos	J	Total chemical potential, cpos
muchem_cneg	pot_es_cneg + pot_ch_cneg + pot_st_cneg	J	Total chemical potential, cneg
pot_es_cpos	tds.z_cpos*e_const*V	J	Chemical potential, electrostatic part, cpos
pot_es_cneg	tds.z_cneg*e_const*V	J	Chemical potential,

Name	Expression	Unit	Description
			electrostatic part, cneg
pot_ch_cpos	-k_B_const*T_system*log(cpos*smp.rad3_cpos)	J	Chemical potential, concentration part, cpos
pot_ch_cneg	-k_B_const*T_system*log(cneg*smp.rad3_cneg)	J	Chemical potential, concentration part, cneg
pot_st_cpos	-k_B_const*T_system*smp.k_cpos*log(1 - cpos*smp.rad3_cpos - cneg*smp.rad3_cneg)	J	Chemical potential, steric part, cpos
pot_st_cneg	-k_B_const*T_system*smp.k_cneg*log(1 - cpos*smp.rad3_cpos - cneg*smp.rad3_cneg)	J	Chemical potential, steric part, cneg

Centrally integrated values (ci)

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
ci.distance	0.1[nm]	m	Distance from the wall 1
ci.r	(r <= pre(r) - ci.distance)*r	m	Effective integration radius 1
ci.area	cip(2*pi*ci.r)	m^2	Area of integration 1
ci.distance2	0.5[nm]	m	Distance from the wall 2
ci.r2	(r <= pre(r) - ci.distance2)*r	m	Effective integration radius 2
ci.area2	cip(2*pi*ci.r2)	m^2	Area of integration 2
ci.distance3	1.6[nm]	m	Distance from the wall 3
ci.r3	(r <= ci.distance3)*r	m	Effective integration radius 3
ci.area3	cip(2*pi*ci.r3)	m^2	Area of

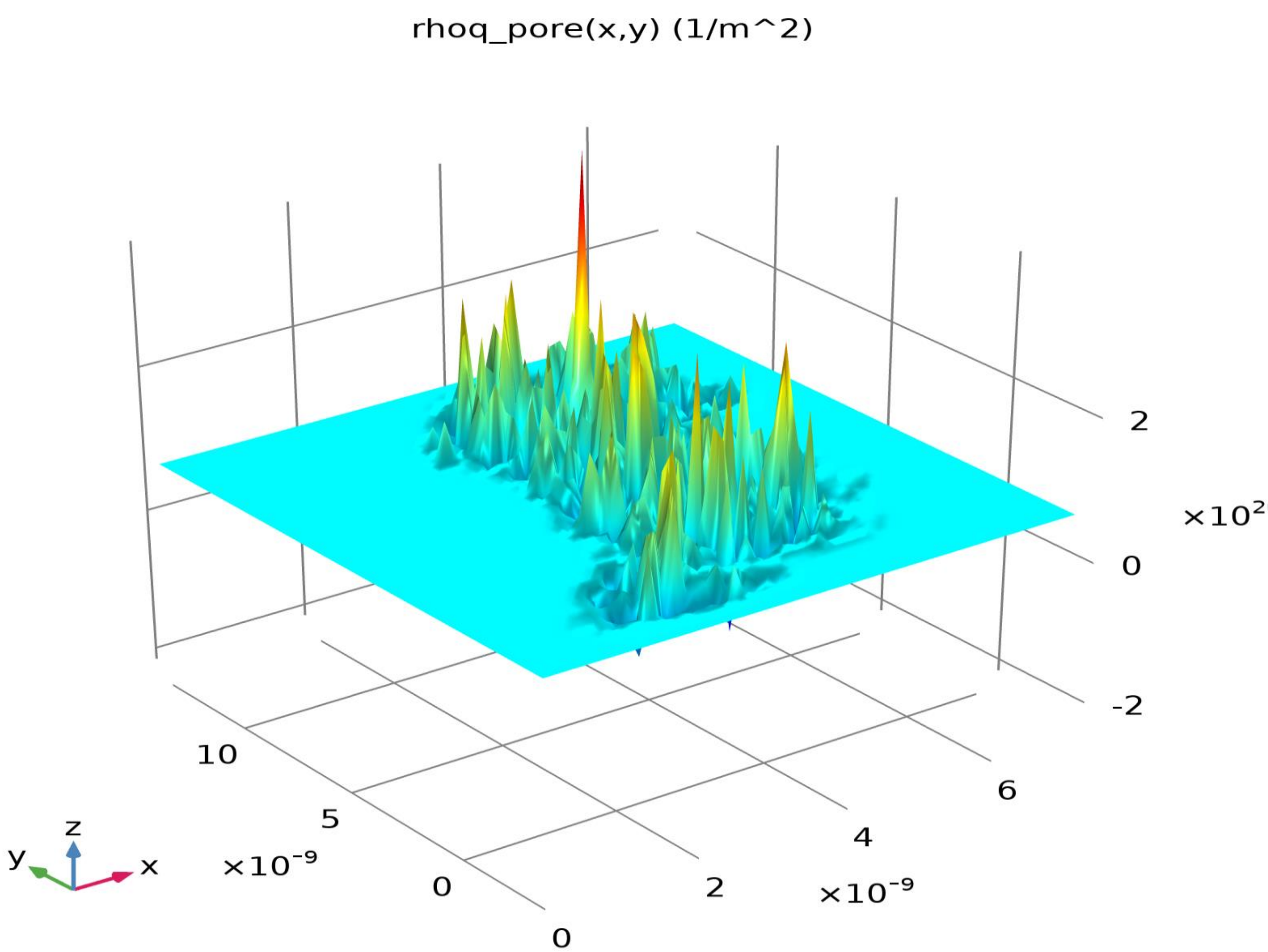
Name	Expression	Unit	Description
			integration 3
ci.cpos	cip(cpos*2*pi*ci.r)/ci.area	mol/m³	Centrally averaged concentration, cpos
ci.cneg	cip(cneg*2*pi*ci.r)/ci.area	mol/m³	Centrally averaged concentration, cneg
ci.scd_ions	cip(scd_ions*2*pi*ci.r)/ci.area	C/m³	Centrally averaged ion space charge density
ci.scd_ions2	cip(scd_ions*2*pi*ci.r2)/ci.area2	C/m³	Centrally averaged ion space charge density in the bulk of the pore
ci.V	cip(V*2*pi*ci.r)/ci.area	V	Centrally averaged potential
ci.u	cip(u*2*pi*ci.r)/ci.area	m/s	Centrally averaged velocity, r-component
ci.w	cip(w*2*pi*ci.r)/ci.area	m/s	Centrally averaged velocity, z-component
ci.U	cip(spf.U*2*pi*ci.r)/ci.area	m/s	Centrally averaged velocity magnitude
ci.p	cip(p*2*pi*ci.r)/ci.area	N/m²	Centrally averaged pressure, area 1
ci.p2	cip(p*2*pi*ci.r2)/ci.area2	N/m²	Centrally averaged pressure, area 2
ci.p3	cip(p*2*pi*ci.r3)/ci.area3	N/m²	Centrally averaged pressure, area 3
ci.D_cpos	cip(D_cpos*2*pi*ci.r)/ci.area	m²/s	Centrally averaged

Name	Expression	Unit	Description
			diffusion coefficient, cpos
ci.D_cneg	cip(D_cneg*2*pi*ci.r)/ci.area	m^2/s	Centrally averaged diffusion coefficient, cneg
ci.mu_cpos	cip(mu_cpos*2*pi*ci.r)/ci.area	s·mol/kg	Centrally averaged mobity, cpos
ci.mu_cneg	cip(mu_cneg*2*pi*ci.r)/ci.area	s·mol/kg	Centrally averaged mobity, cneg
ci.Fr	cip(spf.Fr*2*pi*ci.r)/ci.area	N/m^3	Centrally averaged body force, r component
ci.Fz	cip(spf.Fz*2*pi*ci.r)/ci.area	N/m^3	Centrally averaged body force, z component
Ci.Er	cip(es.Er*2*pi*ci.r)/ci.area	V/m	Centrally averaged electric field, r component
ci.Ez	cip(es.Ez*2*pi*ci.r)/ci.area	V/m	Centrally averaged electric field, z component
ci.normE	cip(es.normE*2*pi*ci.r)/ci.area	V/m	Centrally averaged electric field magnitude
ci.muchem_cpos	cip(muchem_cpos*2*pi*ci.r)/ci.area	J	Centrally averaged chemical potential, cpos
ci.muchem_cneg	cip(muchem_cneg*2*pi*ci.r)/ci.area	J	Centrally averaged chemical potential, cneg

2.1.2 Functions

Gridded charge of pore

Function names	rhoq_pore
Function type	Interpolation



Gridded charge of pore

INTERPOLATION AND EXTRAPOLATION

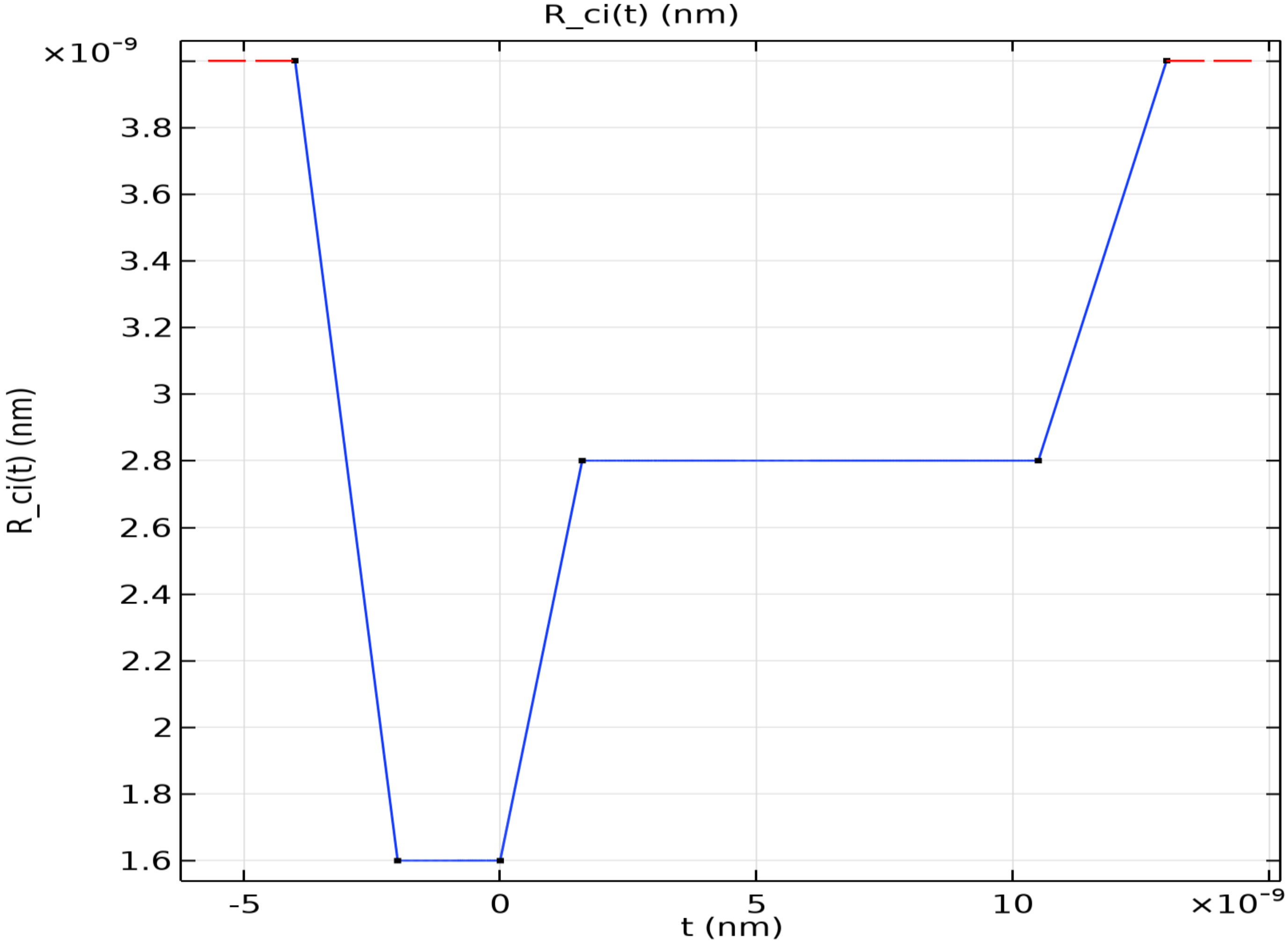
Description	Value
Extrapolation	Specific value

UNITS

Description	Value
Arguments	m, m
Function	1/m^2

Smooth central integration radius

Function names	R_ci
Function type	Interpolation



Smooth central integration radius

UNITS

Description	Value
Arguments	nm
Function	nm

2.1.3 Component Couplings

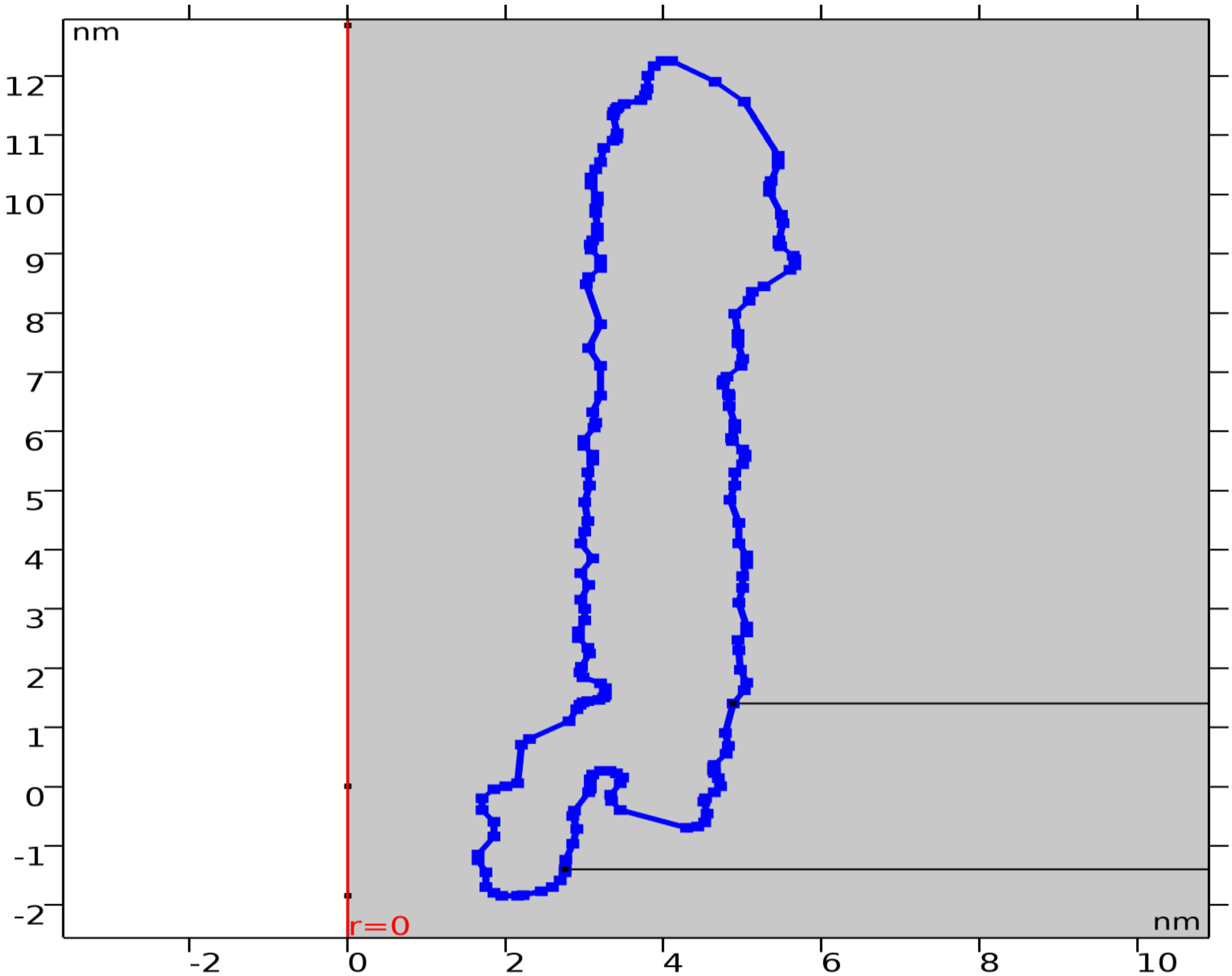
Wall distance extrusion

Coupling type	General extrusion

Operator name	wde

SELECTION

Geometric entity level	Boundary
Name	Wall distance boundary
Selection	Boundaries 7–29, 31–152, 154–194



Selection

DESTINATION MAP

Description	**Value**
Destination map	{r, z}

ADVANCED

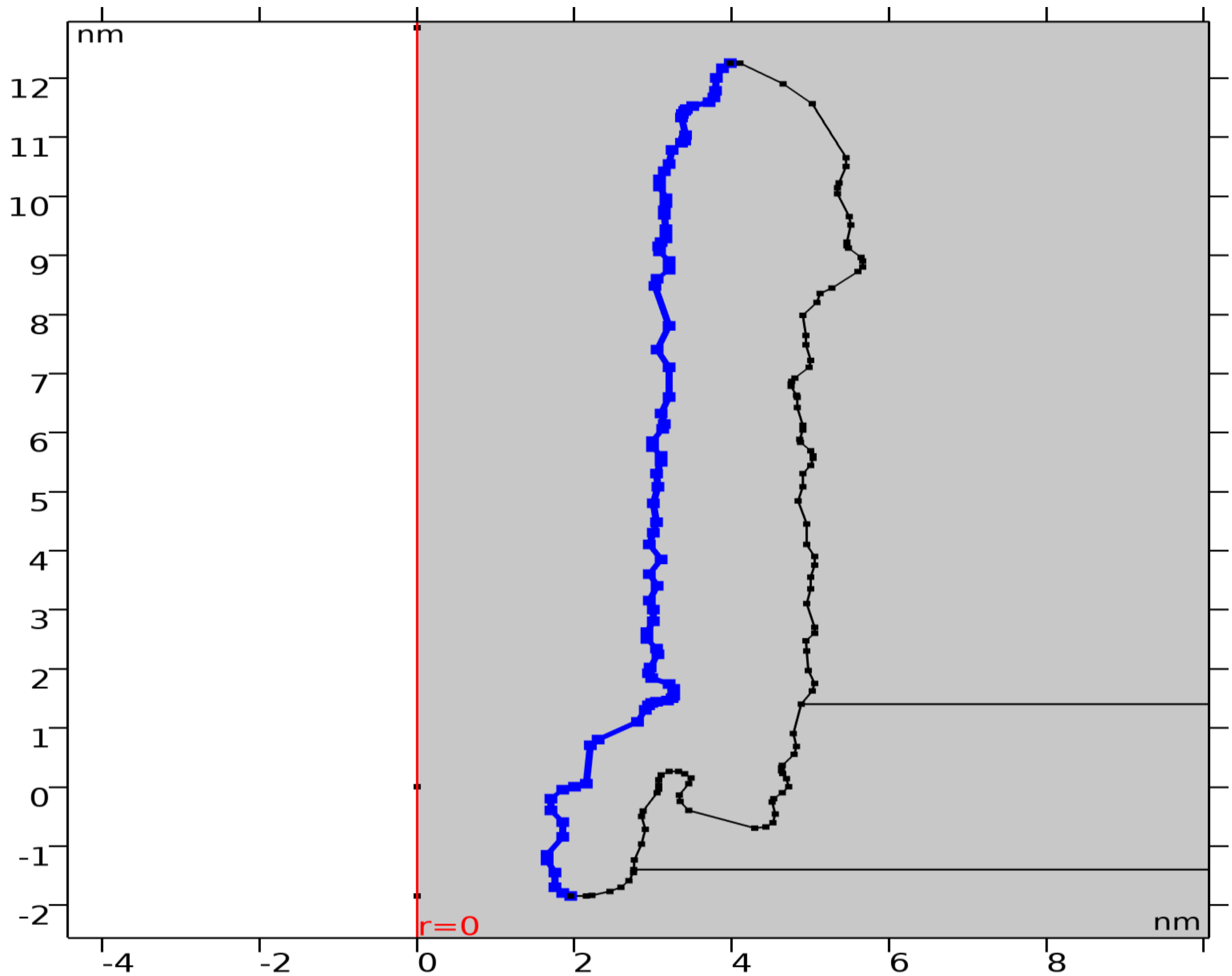
Description	**Value**
Mesh search method	Closest point

Pore radius extrusion

Coupling type	General extrusion
Operator name	pre

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 7–17, 19, 21–22, 24, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–119



Selection

DESTINATION MAP

Description	Value
Destination map	{z, }

SOURCE

Description	Value
Use source map	On
Source map	{z, }

ADVANCED

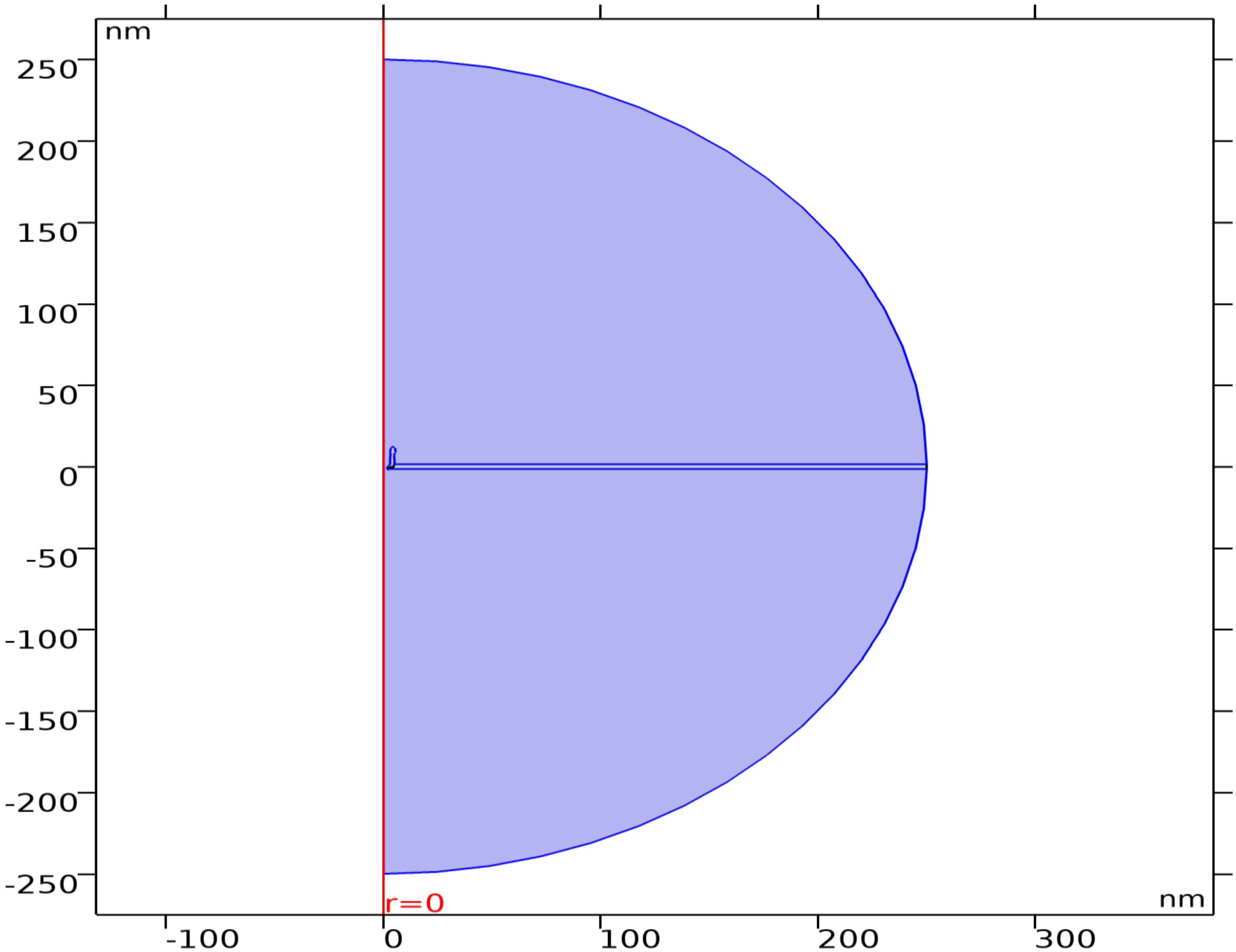
Description	Value
Mesh search method	Closest point

Central integration projection

Coupling type	General projection
Operator name	cip

SELECTION

Geometric entity level	Domain
Selection	Domain 1



Selection

DESTINATION MAP

Description	Value
Destination map	z

SOURCE MAP

Description	Value
Source map	{z, r}

2.1.4 Coordinate Systems

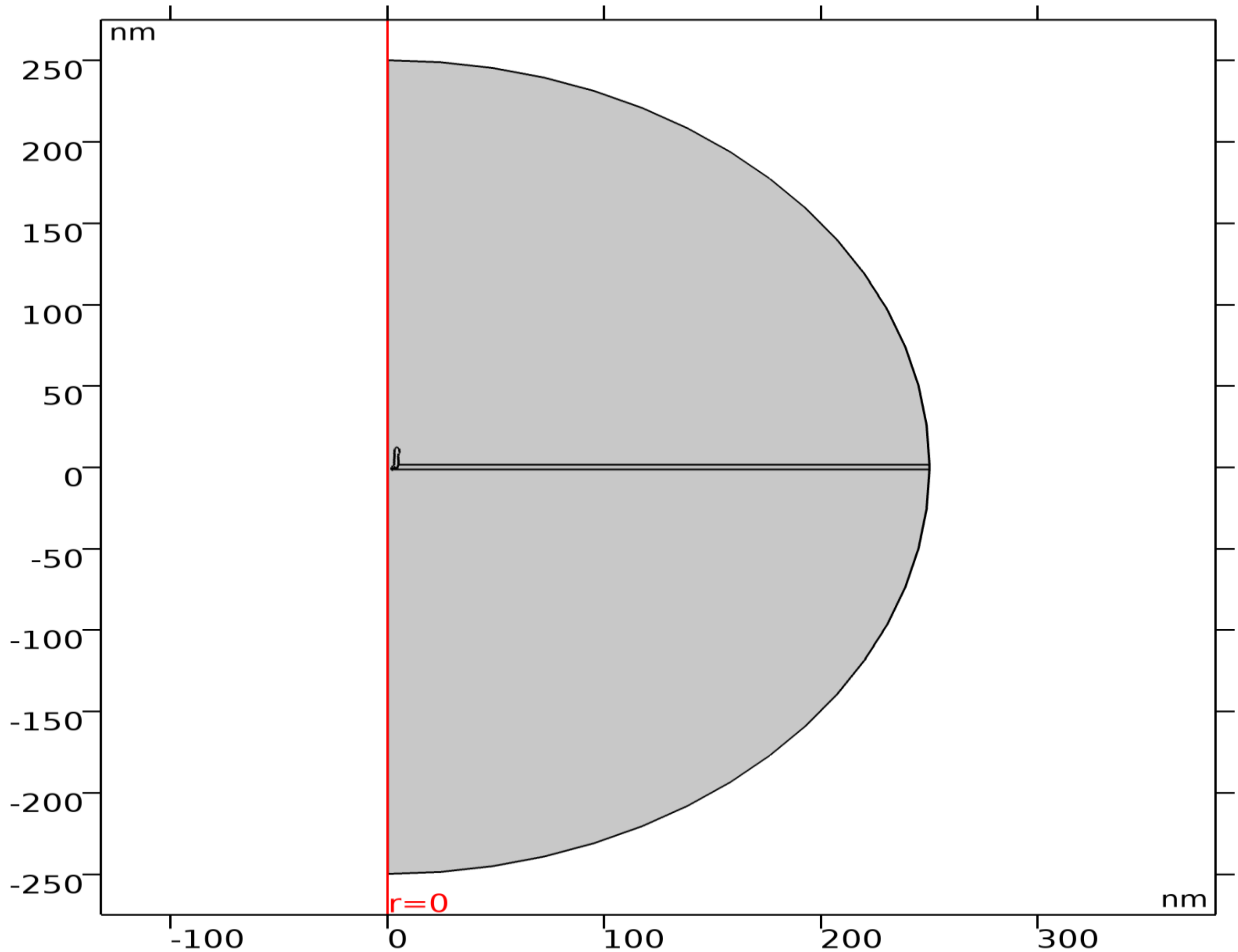
Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	to	n

2.2 GEOMETRY



Geometry

UNITS

Length unit	nm
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	2
Number of domains	3

Description	Value
Number of boundaries	198
Number of vertices	196

2.2.1 Circle 1 (c1)

POSITION

Description	Value
Position	{0, 0}

ROTATION ANGLE

Description	Value
Rotation	270

SIZE AND SHAPE

Description	Value
Radius	r_reservoir
Sector angle	180

2.2.2 Polygon 1 (pol1)

OBJECT TYPE

Description	Value
Type	Solid

COORDINATES

Description	Value
Data source	Table

COORDINATES

r (nm)	z (nm)
2.15	-1.85
1.95	-1.85
1.85	-1.8
1.75	-1.7
1.75	-1.45
1.65	-1.25
1.65	-1.15
1.85	-0.85
1.85	-0.6

r (nm)	z (nm)
1.7	-0.4
1.7	-0.2
1.85	-0.05
2	0
2.15	0.05
2.2	0.7
2.3	0.8
2.8	1.1
2.9	1.3
2.94	1.38
2.98	1.42
3.04	1.44
3.18	1.46
3.24	1.5
3.26	1.54
3.26	1.66
3.2	1.74
2.98	1.84
2.94	1.92
2.96	2.02
3.06	2.24
3.04	2.34
2.92	2.5
2.92	2.62
3	2.8
3	3
2.95	3.15
3.05	3.4
2.95	3.6
3.1	3.85
2.95	4.1
3	4.3
3.04	4.48
3	4.8
3.06	5.08

r (nm)	z (nm)
3.04	5.3
3.1	5.5
3.1	5.6
2.99	5.75
2.99	5.85
3.12	6.06
3.14	6.14
3.1	6.32
3.2	6.6
3.2	7.1
3.05	7.4
3.2	7.8
3.02	8.48
3.05	8.6
3.2	8.75
3.2	8.9
3.08	9.06
3.07	9.15
3.1	9.22
3.16	9.28
3.16	9.44
3.14	9.68
3.14	9.76
3.16	9.88
3.16	9.96
3.08	10.16
3.08	10.28
3.14	10.42
3.2	10.54
3.24	10.78
3.36	10.9
3.4	10.94
3.41	11.03
3.36	11.33
3.37	11.39

r (nm)	z (nm)
3.4	11.44
3.42	11.47
3.5	11.52
3.71	11.59
3.77	11.67
3.79	11.78
3.8	12
3.88	12.16
3.98	12.25
4.1	12.25
4.65	11.9
5.02	11.56
5.45	10.65
5.45	10.5
5.36	10.22
5.34	10.14
5.34	10.04
5.49	9.65
5.51	9.51
5.46	9.22
5.46	9.16
5.48	9.12
5.64	8.96
5.66	8.9
5.66	8.8
5.6	8.72
5.27	8.44
5.12	8.35
5.08	8.2
4.9	7.98
4.94	7.64
4.94	7.48
5	7.22
4.98	7.1
4.8	6.92

r (nm)	z (nm)
4.76	6.86
4.75	6.82
4.75	6.78
4.82	6.63
4.83	6.59
4.83	6.42
4.9	6.12
4.9	6.04
4.86	5.88
4.87	5.83
5	5.69
5.03	5.6
5.03	5.56
5	5.44
4.9	5.3
4.9	5.08
4.84	4.84
4.95	4.45
4.95	4.1
5.05	3.9
5.05	3.75
5	3.55
5	3.35
4.95	3.1
5.05	2.7
5.05	2.6
4.94	2.47
4.95	2.3
4.97	1.97
5.05	1.75
5.02	1.62
4.88	1.4
4.78	0.9
4.82	0.68
4.79	0.55

r (nm)	z (nm)
4.64	0.36
4.63	0.32
4.63	0.27
4.644	0.227
4.692	0.137
4.72	0
4.64	-0.1
4.53	-0.2
4.51	-0.26
4.55	-0.46
4.52	-0.61
4.43	-0.68
4.29	-0.7
3.45	-0.4
3.34	-0.25
3.33	-0.14
3.45	0.05
3.48	0.15
3.4	0.22
3.32	0.26
3.2	0.26
3.1	0.2
3.07	0.12
3.07	0.02
3.07	-0.04
3.05	-0.1
2.87	-0.41
2.85	-0.5
2.9	-0.72
2.85	-0.97
2.76	-1.24
2.75	-1.45
2.69	-1.59
2.59	-1.7
2.45	-1.77

r (nm)	z (nm)
2.22	-1.838

2.2.3 Polygon 2 (pol2)

OBJECT TYPE

Description	Value
Type	Solid

COORDINATES

Description	Value
Data source	Table

COORDINATES

r (nm)	z (nm)
2[nm]	-d_membrane/2
3.5[nm]	d_membrane/2
r_reservoir	d_membrane/2
r_reservoir	-d_membrane/2

2.2.4 Membrane+Pore (co4)

SETTINGS

Description	Value
Keep input objects	On

COMPOSE

Description	Value
Keep interior boundaries	Off
Set formula	(pol2 + pol1)*c1

2.2.5 Reservoir (co1)

SELECTIONS OF RESULTING ENTITIES

Description	Value
Resulting objects selection	On
Show in physics	All levels

SETTINGS

Description	Value
Keep input objects	On

COMPOSE

Description	Value
Set formula	c1 - co4

2.2.6 Membrane (co2)

SELECTIONS OF RESULTING ENTITIES

Description	Value
Resulting objects selection	On
Show in physics	All levels

SETTINGS

Description	Value
Keep input objects	On

COMPOSE

Description	Value
Keep interior boundaries	Off
Set formula	co4 - pol1

2.2.7 Nanopore (co3)

SELECTIONS OF RESULTING ENTITIES

Description	Value
Resulting objects selection	On
Show in physics	All levels

COMPOSE

Description	Value
Keep interior boundaries	Off
Set formula	pol1 + pol1*(c1 + pol2 + co4)

2.2.8 Wall distance boundary (unisel1)

GEOMETRIC ENTITY LEVEL

Description	Value
Level	Boundary

INPUT ENTITIES

Description	Value
Selections to add	Nanopore

2.2.9 Point 1 (pt1)

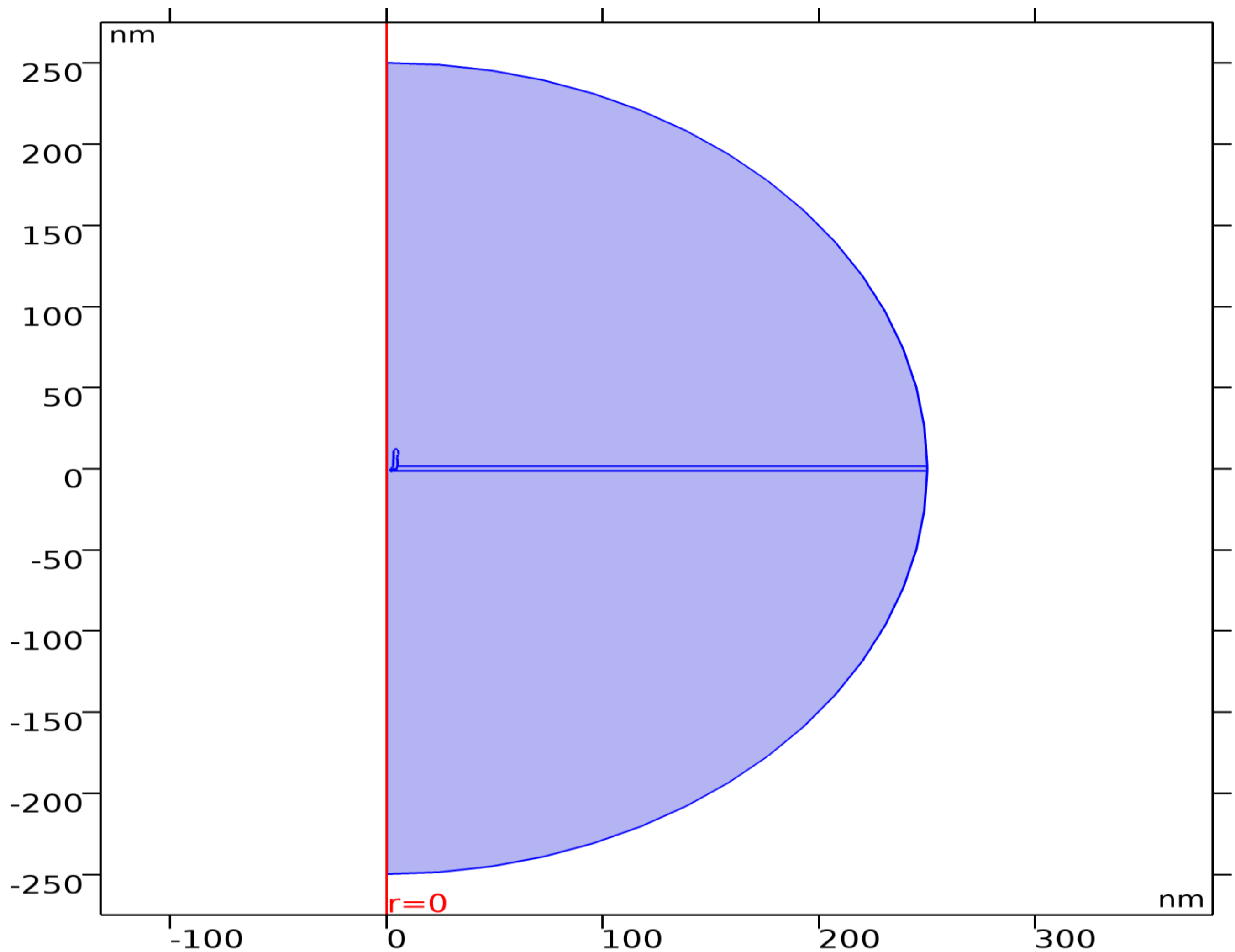
POINT

Description	Value
Point coordinate	{{0, 0, 0, 0}, {-50, -1.85, 12.85, 50}}

2.3 ELECTROSTATICS

USED PRODUCTS

COMSOL Multiphysics



Electrostatics

SELECTION

Geometric entity level	Domain
Selection	Domains 1–3

EQUATIONS

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

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

2.3.1 Interface settings

Discretization

SETTINGS

Description	Value
Electric potential	Quadratic

Manual terminal sweep settings

SETTINGS

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

2.3.2 Variables

Name	Expression	Unit	Description	Selection
es.d	1	1	Contribution	Domains 1–3
es.nr	nr		Normal vector, r component	Boundaries 7–194
es.nphi	0		Normal vector, phi component	Boundaries 7–194
es.nz	nz		Normal vector, z component	Boundaries 7–194
es.nr	dnr		Normal vector, r component	Boundaries 1–6, 195–198
es.nphi	0		Normal vector, phi component	Boundaries 1–6, 195–198
es.nz	dnz		Normal vector, z component	Boundaries 1–6, 195–198
es.nmeshr	nrmesh		Mesh normal vector, r component	Boundaries 7–194
es.nmeshphi	0		Mesh normal vector, phi component	Boundaries 7–194
es.nmeshz	nzmesh		Mesh normal vector, z component	Boundaries 7–194

Name	Expression	Unit	Description	Selection
es.nmeshr	dnrmesh		Mesh normal vector, r component	Boundaries 1–6, 195–198
es.nmeshphi	0		Mesh normal vector, phi component	Boundaries 1–6, 195–198
es.nmeshz	dnzmesh		Mesh normal vector, z component	Boundaries 1–6, 195–198
es.unmeshr	unrmesh		Mesh normal vector, upside, r component	Boundaries 1–198
es.unmeshphi	0		Mesh normal vector, upside, phi component	Boundaries 1–198
es.unmeshz	unzmesh		Mesh normal vector, upside, z component	Boundaries 1–198
es.dnmeshr	dnrmesh		Mesh normal vector, downside, r component	Boundaries 1–198
es.dnmeshphi	0		Mesh normal vector, downside, phi component	Boundaries 1–198
es.dnmeshz	dnzmesh		Mesh normal vector, downside, z component	Boundaries 1–198
es.unTr	es.unTer	Pa	Maxwell upward surface stress tensor, r component	Boundaries 1–198
es.unTphi	es.unTephi	Pa	Maxwell upward surface stress tensor, phi component	Boundaries 1–198
es.unTz	es.unTez	Pa	Maxwell upward surface stress tensor, z component	Boundaries 1–198
es.dnTr	es.dnTer	Pa	Maxwell	Boundaries 1–

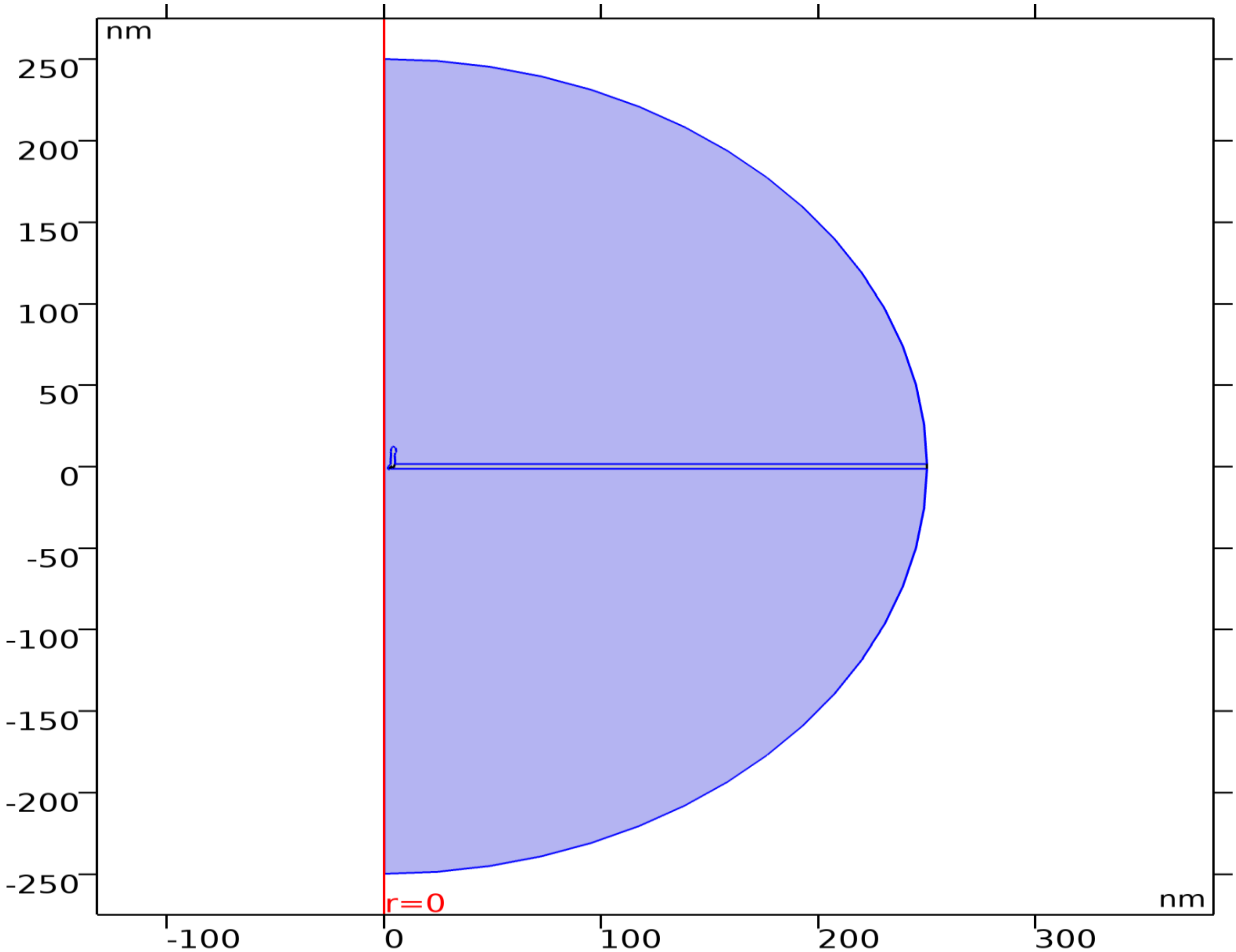
Name	Expression	Unit	Description	Selection
			downward surface stress tensor, r component	198
es.dnTphi	es.dnTephi	Pa	Maxwell downward surface stress tensor, phi component	Boundaries 1–198
es.dnTz	es.dnTez	Pa	Maxwell downward surface stress tensor, z component	Boundaries 1–198
es.unr	unr		Normal vector up direction, r component	Boundaries 1–198
es.unphi	0		Normal vector up direction, phi component	Boundaries 1–198
es.unz	unz		Normal vector up direction, z component	Boundaries 1–198
es.dnr	dnr		Normal vector down direction, r component	Boundaries 1–198
es.dnphi	0		Normal vector down direction, phi component	Boundaries 1–198
es.dnz	dnz		Normal vector down direction, z component	Boundaries 1–198
es.unTer	-0.5*epsilon0_const*es.dnr*(real(up(es.epsilonrrr))*real(up(es.Er))*real(up(es.Er))+real(up(es.epsilonrphiphi))*real(up(es.Ephi))*real(up(es.Ephi))+real(up(es.epsilonrzz))*real(up(es.Ez))*real(up(es.Ez)))+real(up(es.Er))*epsilon0_const*real(up(es.epsilonrrr))*(real(up(es.Er))*es.dnr+real(up(es.Ephi))*es.dnphi+real(up(es.Ez))*es.dnz)	Pa	Maxwell upward electric surface stress tensor, r component	Boundaries 7–194
es.unTephi	-0.5*epsilon0_const*es.dnphi*(real(up(es	Pa	Maxwell upward electric surface	Boundaries 7–194

Name	Expression	Unit	Description	Selection
	.epsilonrrr))*real(up(es.Er))*real(up(es.Er))+real(up(es.epsilonrphiphi))*real(up(es.Ephi))*real(up(es.Ephi))+real(up(es.epsilonrzz))*real(up(es.Ez))*real(up(es.Ez)))+real(up(es.Ephi))*epsilon0_const*real(up(es.epsilonrrr))*(real(up(es.Er))*es.dnr+real(up(es.Ephi))*es.dnphi+real(up(es.Ez))*es.dnz)		stress tensor, phi component	
es.unTez	-0.5*epsilon0_const*es.dnz*(real(up(es.epsilonrrr))*real(up(es.Er))*real(up(es.Er))+real(up(es.epsilonrphiphi))*real(up(es.Ephi))*real(up(es.Ephi))+real(up(es.epsilonrzz))*real(up(es.Ez))*real(up(es.Ez)))+real(up(es.Ez))*epsilon0_const*real(up(es.epsilonrrr))*(real(up(es.Er))*es.dnr+real(up(es.Ephi))*es.dnphi+real(up(es.Ez))*es.dnz)	Pa	Maxwell upward electric surface stress tensor, z component	Boundaries 7–194
es.unTer	0	Pa	Maxwell upward electric surface stress tensor, r component	Boundaries 1–6, 195–198
es.unTephi	0	Pa	Maxwell upward electric surface stress tensor, phi component	Boundaries 1–6, 195–198
es.unTez	0	Pa	Maxwell upward electric surface stress tensor, z component	Boundaries 1–6, 195–198
es.dnTer	-0.5*epsilon0_const*es.unr*(real(down(es.epsilonrrr))*real(down(es.Er))*real(down(es.Er))+real(down(es.epsilonrphiphi))*real(down(es.Ephi))*real(down(es.Ephi))+real(down(es.epsilonrzz))*real(down(es.Ez))*real(down(es.Ez)))+real(down(es.Er))*epsilon0_const*real(down(es.epsilonrrr))*(real(down(es.Er))*es.unr+real(down(es.Ephi))*es.unphi+real(down(es.Ez))*es.unz)	Pa	Maxwell downward electric surface stress tensor, r component	Boundaries 1–198
es.dnTephi	-0.5*epsilon0_const*es.unphi*(real(down(es.epsilonrrr))*real(down(es.Er))*real(down(es.Er))+real(down(es.epsilonrphiph	Pa	Maxwell downward electric surface stress tensor,	Boundaries 1–198

Name	Expression	Unit	Description	Selection
	i))*real(down(es.Ephi))*real(down(es.Ephi))+real(down(es.epsilonrzz))*real(down(es.Ez))*real(down(es.Ez)))+real(down(es.Ephi))*epsilon0_const*real(down(es.epsilonrrr))*(real(down(es.Er))*es.unr+real(down(es.Ephi))*es.unphi+real(down(es.Ez))*es.unz)		phi component	
es.dnTez	-0.5*epsilon0_const*es.unz*(real(down(es.epsilonrrr))*real(down(es.Er))*real(down(es.Er))+real(down(es.epsilonrphiphi))*real(down(es.Ephi))*real(down(es.Ephi))+real(down(es.epsilonrzz))*real(down(es.Ez))*real(down(es.Ez)))+real(down(es.Ez))*epsilon0_const*real(down(es.epsilonrrr))*(real(down(es.Er))*es.unr+real(down(es.Ephi))*es.unphi+real(down(es.Ez))*es.unz)	Pa	Maxwell downward electric surface stress tensor, z component	Boundaries 1–198
es.intWe	es.int_We(es.d*es.dWe)	J	Total electric energy	Global
es.I_srr	1	1	Spatial identity matrix, rr component	Domains 1–3
es.I_sphir	0	1	Spatial identity matrix, phir component	Domains 1–3
es.I_szr	0	1	Spatial identity matrix, zr component	Domains 1–3
es.I_srphi	0	1	Spatial identity matrix, rphi component	Domains 1–3
es.I_sphiphi	1	1	Spatial identity matrix, phiphi component	Domains 1–3
es.I_szphi	0	1	Spatial identity matrix, zphi component	Domains 1–3
es.I_srz	0	1	Spatial identity matrix, rz component	Domains 1–3
es.I_sphiz	0	1	Spatial identity matrix, phiz component	Domains 1–3

Name	Expression	Unit	Description	Selection
es.I_szz	1	1	Spatial identity matrix, zz component	Domains 1–3
es.I_sRR	(spatial.invF11*(spatial.invF11*es.I_srr+spatial.invF31*es.I_szr)+spatial.invF31*(spatial.invF11*es.I_srz+spatial.invF31*es.I_szz))*spatial.detF	1	Spatial identity matrix, RR component	Domains 1–3
es.I_sPHIR	if(Rg>0.001*h,R/r,Rr)*(spatial.invF11*es.I_sphir+spatial.invF31*es.I_sphiz)*spatial.detF	1	Spatial identity matrix, PHIR component	Domains 1–3
es.I_sZR	(spatial.invF11*(spatial.invF13*es.I_srr+spatial.invF33*es.I_szr)+spatial.invF31*(spatial.invF13*es.I_srz+spatial.invF33*es.I_szz))*spatial.detF	1	Spatial identity matrix, ZR component	Domains 1–3
es.I_sRPHI	if(Rg>0.001*h,R/r,Rr)*(spatial.invF11*es.I_srphi+spatial.invF31*es.I_szphi)*spatial.detF	1	Spatial identity matrix, RPHI component	Domains 1–3
es.I_sPHIPHI	if(Rg>0.001*h,R/r,Rr)^2*es.I_sphiphi*spatial.detF	1	Spatial identity matrix, PHIPHI component	Domains 1–3
es.I_sZPHI	if(Rg>0.001*h,R/r,Rr)*(spatial.invF13*es.I_srphi+spatial.invF33*es.I_szphi)*spatial.detF	1	Spatial identity matrix, ZPHI component	Domains 1–3
es.I_sRZ	(spatial.invF13*(spatial.invF11*es.I_srr+spatial.invF31*es.I_szr)+spatial.invF33*(spatial.invF11*es.I_srz+spatial.invF31*es.I_szz))*spatial.detF	1	Spatial identity matrix, RZ component	Domains 1–3
es.I_sPHIZ	if(Rg>0.001*h,R/r,Rr)*(spatial.invF13*es.I_sphir+spatial.invF33*es.I_sphiz)*spatial.detF	1	Spatial identity matrix, PHIZ component	Domains 1–3
es.I_sZZ	(spatial.invF13*(spatial.invF13*es.I_srr+spatial.invF33*es.I_szr)+spatial.invF33*(spatial.invF13*es.I_srz+spatial.invF33*es.I_szz))*spatial.detF	1	Spatial identity matrix, ZZ component	Domains 1–3
es.zref	50[ohm]	Ω	Reference impedance	Global

2.3.3 Charge Conservation (reservoir)



Charge Conservation (reservoir)

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

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

Electric field

SETTINGS

Description	**Value**
Constitutive relation	Relative permittivity

Description	Value
Relative permittivity	User defined
Relative permittivity	{{epsr_water, 0, 0}, {0, epsr_water, 0}, {0, 0, epsr_water}}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	0	C/m²	Surface charge density	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	+ operation
es.epsilonr_iso	epsr_water	1	Relative permittivity, isotropic value	Domain 1	
es.Dr	epsilon0_const*es.I_srr*es.Er+epsilon0_const*es.I_srphi*es.Ephi+epsilon0_const*es.I_srz*es.Ez+es.Pr	C/m²	Electric displacement field, r component	Domain 1	
es.Dphi	epsilon0_const*es.I_sphir*es.Er+epsilon0_const*es.I_sphiphi*es.Ephi+epsilon0_const*es.I_sphiz*es.Ez+es.Pphi	C/m²	Electric displacement field, phi component	Domain 1	
es.Dz	epsilon0_const*es.I_szr*es.Er+epsilon0_const*es.I_szphi*es.Ephi+epsilon0_const*es.I_szz*es.Ez+es.Pz	C/m²	Electric displacement field, z component	Domain 1	
es.Pr	epsilon0_const*(es.chirr*es.Er+es.chirphi*es.Ephi+es.chirz*es.Ez)	C/m²	Polarization, r component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
es.Pphi	epsilon0_const*(es.chiphir*es.Er+es.chiphiphi*es.Ephi+es.chiphiz*es.Ez)	C/m²	Polarization, phi component	Domain 1	
es.Pz	epsilon0_const*(es.chizr*es.Er+es.chizphi*es.Ephi+es.chizz*es.Ez)	C/m²	Polarization, z component	Domain 1	
es.normD	sqrt(realdot(es.Dr,es.Dr)+realdot(es.Dphi,es.Dphi)+realdot(es.Dz,es.Dz))	C/m²	Electric displacement field norm	Domain 1	
es.normP	sqrt(realdot(es.Pr,es.Pr)+realdot(es.Pphi,es.Pphi)+realdot(es.Pz,es.Pz))	C/m²	Polarization norm	Domain 1	
es.Er	-Vr	V/m	Electric field, r component	Domain 1	
es.Ephi	0	V/m	Electric field, phi component	Domain 1	
es.Ez	-Vz	V/m	Electric field, z component	Domain 1	
es.tEr	-VTr	V/m	Tangential electric field, r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
es.tEphi	0	V/m	Tangential electric field, phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
es.tEz	-VTz	V/m	Tangential electric field, z component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–	

Name	Expression	Unit	Description	Selection	Details
				99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
es.normE	sqrt(realdot(es.Er,es.Er)+realdot(es.Ephi,es.Ephi)+realdot(es.Ez,es.Ez))	V/m	Electric field norm	Domain 1	
es.normJ	sqrt(realdot(es.Jr,es.Jr)+realdot(es.Jphi,es.Jphi)+realdot(es.Jz,es.Jz))	A/m^2	Current density norm	Domain 1	
es.W	es.We	J/m^3	Energy density	Domain 1	+ operation
es.dWe	2*es.We*pi*r	J/m^2	Integrand for total electric energy	Domain 1	
es.We	0.5*epsilon0_const*(((es.I_srr+es.chirr)*es.Er+(es.I_srphi+es.chirphi)*es.Ephi+(es.I_srz+es.chirz)*es.Ez)*es.Er+((es.I_sphir+es.chiphir)*es.Er+(es.I_sphiphi+es.chiphiphi)*es.Ephi+(es.I_sphiz+es.chiphiz)*es.Ez)*es.Ephi+((es.I_szr+es.chizr)*es.Er+(es.I_szphi+es.chizphi)*es.Ephi+(es.I_szz+es.chizz)*es.Ez)*es.Ez)	J/m^3	Electric energy density	Domain 1	
es.epsilonrrr	epsr_water	1	Relative permittivity, rr component	Domain 1	
es.epsilonrphir	0	1	Relative permittivity, phir component	Domain 1	
es.epsilonrzr	0	1	Relative permittivity, zr component	Domain 1	
es.epsilonrrphi	0	1	Relative permittivity, rphi component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
es.epsilonrphiphi	epsr_water	1	Relative permittivity, phiphi component	Domain 1	
es.epsilonrzphi	0	1	Relative permittivity, zphi component	Domain 1	
es.epsilonrrz	0	1	Relative permittivity, rz component	Domain 1	
es.epsilonrphiz	0	1	Relative permittivity, phiz component	Domain 1	
es.epsilonrzz	epsr_water	1	Relative permittivity, zz component	Domain 1	
es.chirr	-1+es.epsilonrrr	1	Electric susceptibility, rr component	Domain 1	
es.chiphir	es.epsilonrphir	1	Electric susceptibility, phir component	Domain 1	
es.chizr	es.epsilonrzr	1	Electric susceptibility, zr component	Domain 1	
es.chirphi	es.epsilonrrphi	1	Electric susceptibility, rphi component	Domain 1	
es.chiphiphi	-1+es.epsilonrphiphi	1	Electric susceptibility, phiphi component	Domain 1	
es.chizphi	es.epsilonrzphi	1	Electric susceptibility, zphi component	Domain 1	
es.chirz	es.epsilonrrz	1	Electric susceptibility, rz component	Domain 1	
es.chiphiz	es.epsilonrphiz	1	Electric susceptibility, phiz component	Domain 1	
es.chizz	-1+es.epsilonrzz	1	Electric susceptibility, zz	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			component		
es.Jr	es.Jdr	A/m²	Current density, r component	Domain 1	+ operation
es.Jphi	es.Jdphi	A/m²	Current density, phi component	Domain 1	+ operation
es.Jz	es.Jdz	A/m²	Current density, z component	Domain 1	+ operation
es.Jdr	0	A/m²	Displacement current density, r component	Domain 1	
es.Jdphi	0	A/m²	Displacement current density, phi component	Domain 1	
es.Jdz	0	A/m²	Displacement current density, z component	Domain 1	
es.ccn1.nJ	es.unr*down(es.Jr)+es.unphi*down(es.Jphi)+es.unz*down(es.Jz)	A/m²	Inward current density	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	

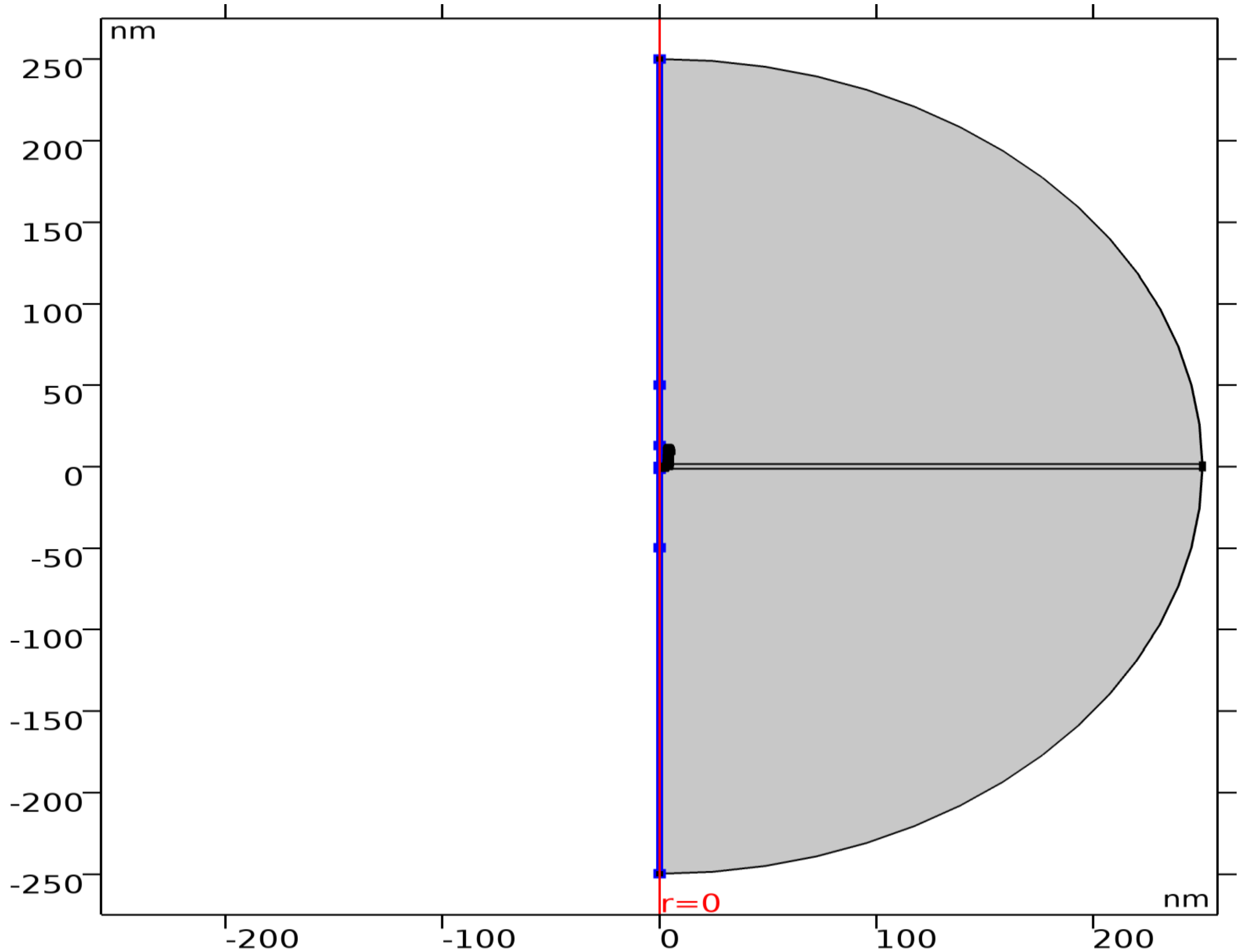
Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
V	Lagrange (Quadratic)	V	Electric potential	Spatial	Domain 1
V	Lagrange (Quadratic)	V	Electric potential	Material	Domain 1
V	Lagrange (Quadratic)	V	Electric potential	Geometry	Domain 1
V	Lagrange (Quadratic)	V	Electric potential	Mesh	Domain 1

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-2*(es.Dr*test(Vr)+es.Dz*test(Vz))*es.d*pi*r	4	Spatial	Domain 1

2.3.4 Axial Symmetry

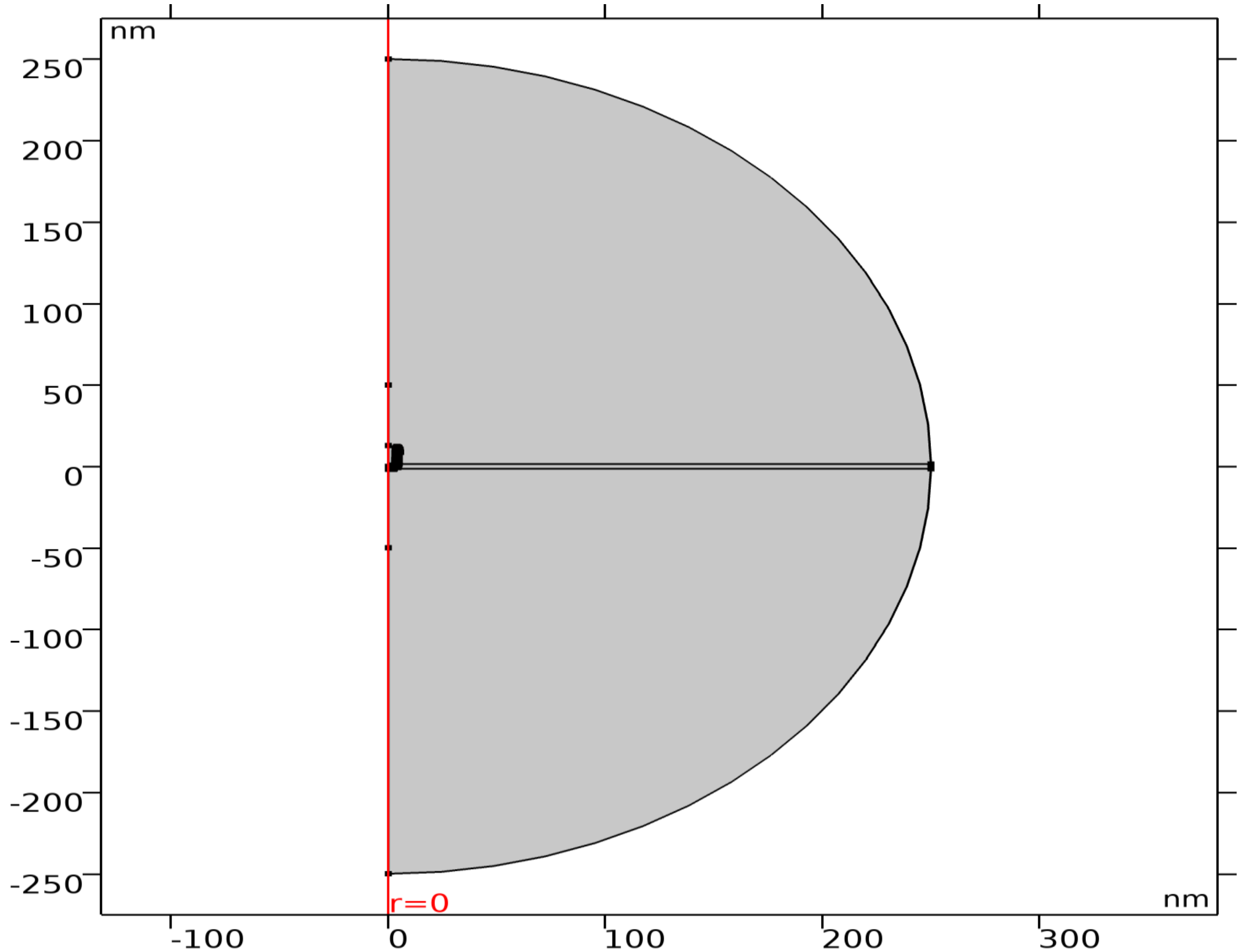


Axial Symmetry

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1–6

2.3.5 Zero Charge



Zero Charge

SELECTION

Geometric entity level	Boundary
Selection	No boundaries

EQUATIONS

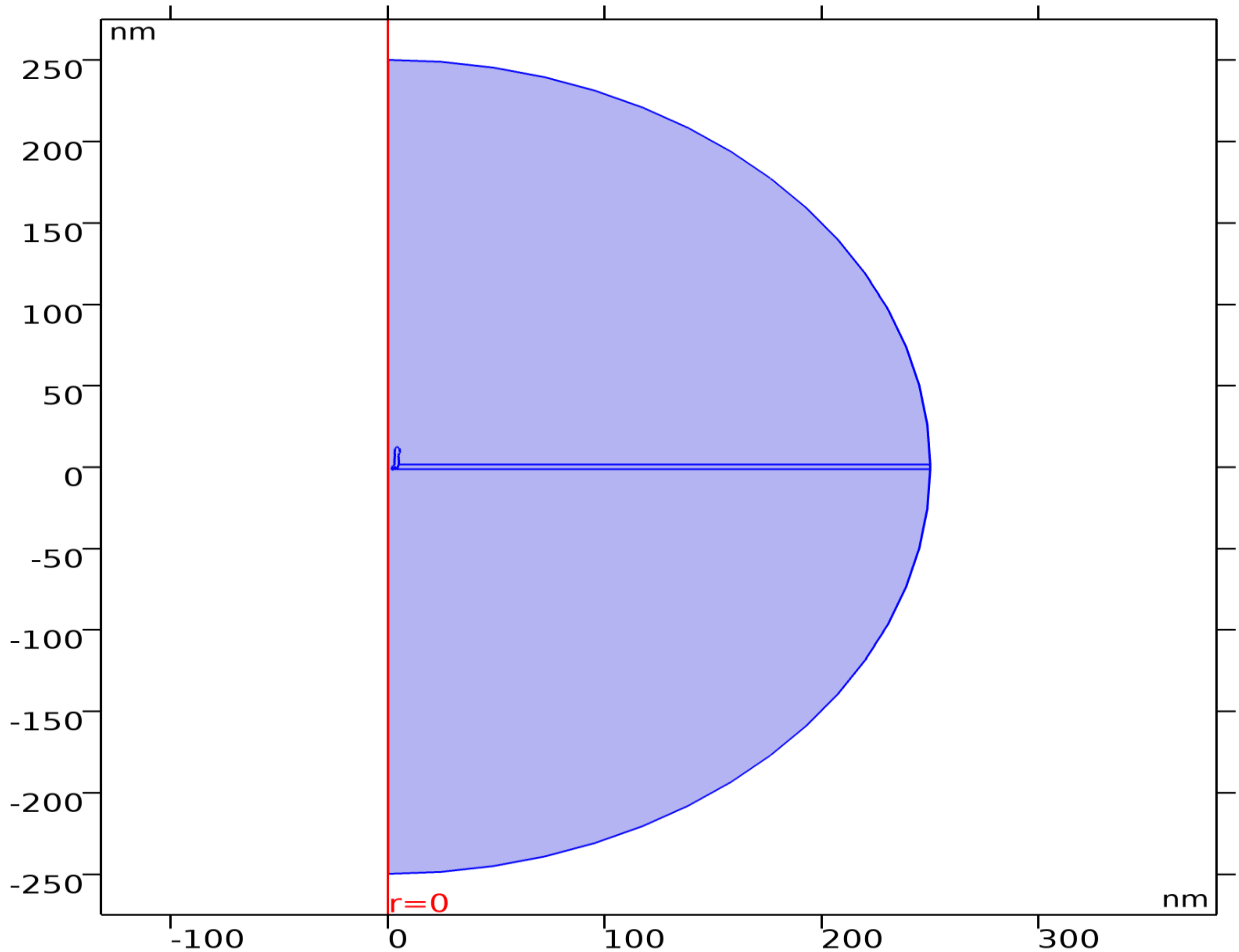
$$\mathbf{n} \cdot \mathbf{D} = 0$$

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection	Details
V	Lagrange (Quadratic)	V	Electric potential	Spatial	No boundaries	Slit
V	Lagrange	V	Electric	Material	No boundaries	Slit

Name	Shape function	Unit	Description	Shape frame	Selection	Details
	(Quadratic)		potential			
V	Lagrange (Quadratic)	V	Electric potential	Geometry	No boundaries	Slit
V	Lagrange (Quadratic)	V	Electric potential	Mesh	No boundaries	Slit

2.3.6 Initial Values



Initial Values

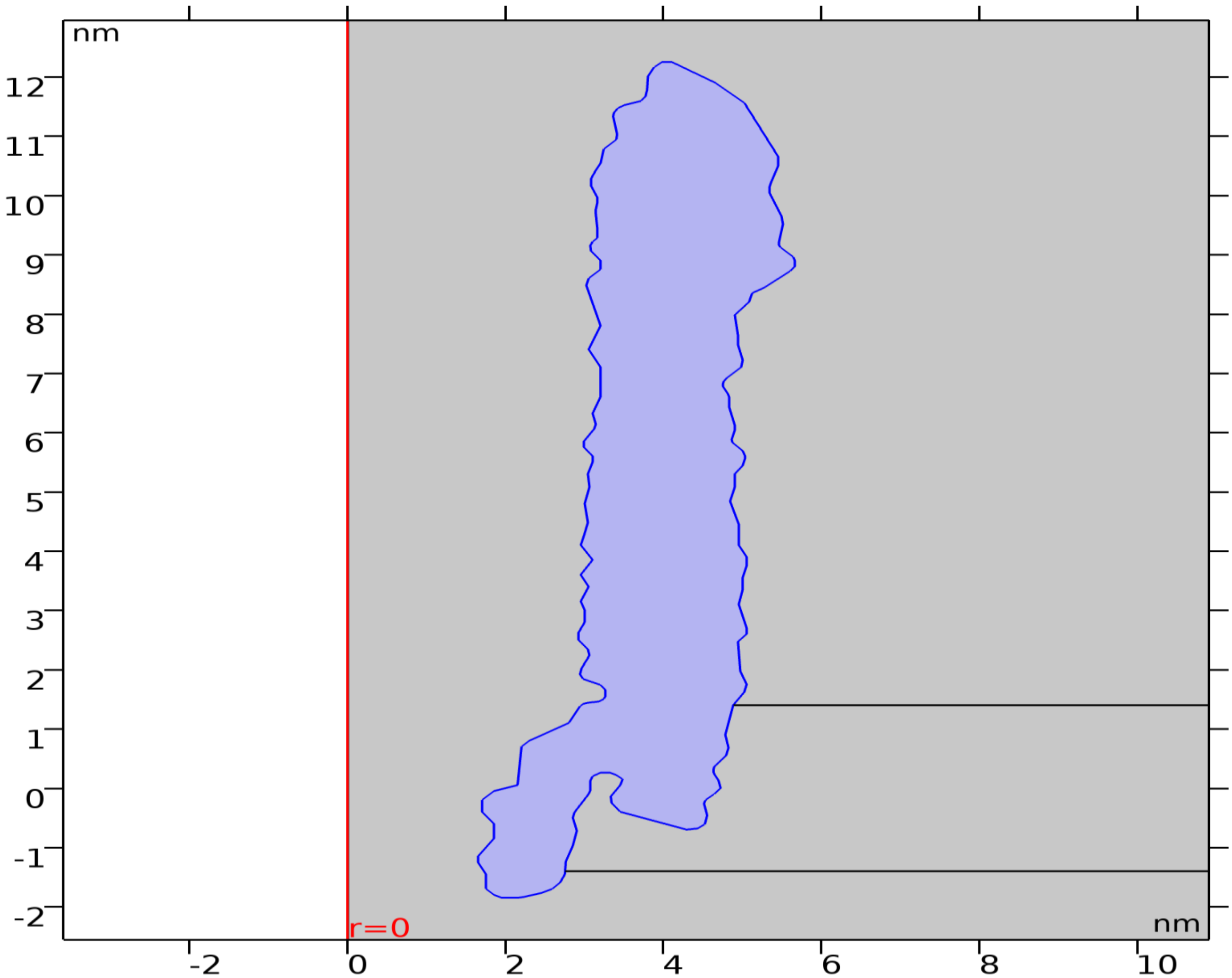
SELECTION

Geometric entity level	Domain
Selection	Domains 1–3

SETTINGS

Description	Value
Electric potential	V_init

2.3.7 Charge Conservation (nanopore)



Charge Conservation (nanopore)

SELECTION

Geometric entity level	Domain
Name	Nanopore
Selection	Domain 2

EQUATIONS

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

Electric field

SETTINGS

Description	Value
Constitutive relation	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{epsr_nanopore, 0, 0}, {0, epsr_nanopore, 0}, {0, 0, epsr_nanopore}}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	0	C/m²	Surface charge density	Boundaries 7–29, 31–152, 154–194	+ operation
es.epsilonr_iso	epsr_nanopore	1	Relative permittivity, isotropic value	Domain 2	
es.Dr	(spatial.F11*es.DR+spatial.F31*es.DZ)*spatial.detInvF	C/m²	Electric displacement field, r component	Domain 2	
es.Dphi	if(Rg>0.001*h,r/R,rR)*es.DPHI*spatial.detInvF	C/m²	Electric displacement field, phi component	Domain 2	
es.Dz	(spatial.F13*es.DR+spatial.F33*es.DZ)*spatial.detInvF	C/m²	Electric displacement field, z component	Domain 2	
es.Pr	(spatial.F11*es.PR+spatial.F31*es.PZ)*spatial.detInvF	C/m²	Polarization, r component	Domain 2	
es.Pphi	if(Rg>0.001*h,r/R,rR)*es.PPHI*spatial.detInvF	C/m²	Polarization, phi component	Domain 2	
es.Pz	(spatial.F13*es.PR+spatial.F33*es.PZ)*spatial.detInvF	C/m²	Polarization, z component	Domain 2	
es.normD	sqrt(realdot(es.Dr,es.	C/m²	Electric	Domain 2	

Name	Expression	Unit	Description	Selection	Details
	Dr)+realdot(es.Dphi,es.Dphi)+realdot(es.Dz,es.Dz))		displacement field norm		
es.normP	sqrt(realdot(es.Pr,es.Pr)+realdot(es.Pphi,es.Pphi)+realdot(es.Pz,es.Pz))	C/m^2	Polarization norm	Domain 2	
es.Er	spatial.invF11*es.ER+spatial.invF13*es.EZ	V/m	Electric field, r component	Domain 2	
es.Ephi	if(Rg>0.001*h,R/r,Rr)*es.EPHI	V/m	Electric field, phi component	Domain 2	
es.Ez	spatial.invF31*es.ER+spatial.invF33*es.EZ	V/m	Electric field, z component	Domain 2	
es.tEr	spatial.invF11*es.tER+spatial.invF13*es.tEZ	V/m	Tangential electric field, r component	Boundaries 7–29, 31–152, 154–194	
es.tEphi	if(Rg>0.001*h,R/r,Rr)*es.tEPHI	V/m	Tangential electric field, phi component	Boundaries 7–29, 31–152, 154–194	
es.tEz	spatial.invF31*es.tER+spatial.invF33*es.tEZ	V/m	Tangential electric field, z component	Boundaries 7–29, 31–152, 154–194	
es.normE	sqrt(realdot(es.Er,es.Er)+realdot(es.Ephi,es.Ephi)+realdot(es.Ez,es.Ez))	V/m	Electric field norm	Domain 2	
es.normJ	sqrt(realdot(es.JR,es.JR)+realdot(es.JPHI,es.JPHI)+realdot(es.JZ,es.JZ))*spatial.detInvF^2	A/m^2	Current density norm	Domain 2	
es.W	es.We	J/m^3	Energy density	Domain 2	+ operation
es.dWe	2*es.We*pi*R	J/m^2	Integrand for total electric energy	Domain 2	
es.We	0.5*epsilon0_const*(((es.I_sRR+es.chiRR)*es.ER+(es.I_sRPHI+es.chiRPHI)*es.EPHI+(es.I_sRZ+es.chiRZ)*es.EZ)*es.ER+((es.I_sPHIR+es.chiPHIR)*es.ER+(es.I_sPHIPHI+es.chiP	J/m^3	Electric energy density	Domain 2	

Name	Expression	Unit	Description	Selection	Details
	HIPHI)*es.EPHI+(es.I_sPHIZ+es.chiPHIZ)*es.EZ)*es.EPHI+((es.I_sZR+es.chiZR)*es.ER+(es.I_sZPHI+es.chiZPHI)*es.EPHI+(es.I_sZZ+es.chiZZ)*es.EZ)*es.EZ)*spatial.detInvF				
es.epsilonrRR	epsr_nanopore	1	Relative permittivity, RR component	Domain 2	
es.epsilonrPHIR	0	1	Relative permittivity, PHIR component	Domain 2	
es.epsilonrZR	0	1	Relative permittivity, ZR component	Domain 2	
es.epsilonrRPHI	0	1	Relative permittivity, RPHI component	Domain 2	
es.epsilonrPHIPHI	epsr_nanopore	1	Relative permittivity, PHIPHI component	Domain 2	
es.epsilonrZPHI	0	1	Relative permittivity, ZPHI component	Domain 2	
es.epsilonrRZ	0	1	Relative permittivity, RZ component	Domain 2	
es.epsilonrPHIZ	0	1	Relative permittivity, PHIZ component	Domain 2	
es.epsilonrZZ	epsr_nanopore	1	Relative permittivity, ZZ component	Domain 2	
es.DR	epsilon0_const*es.I_sRR*es.ER+epsilon0_const*es.I_sRPHI*es.EPHI+epsilon0_const*es.I_sRZ*es.EZ+es.PR	C/m²	Electric displacement field, R component	Domain 2	
es.DPHI	epsilon0_const*es.I_sPHIR*es.ER+epsilon0_const*es.I_sPHIPHI*	C/m²	Electric displacement field, PHI	Domain 2	

Name	Expression	Unit	Description	Selection	Details
	es.EPHI+epsilon0_const*es.I_sPHIZ*es.EZ+es.PPHI		component		
es.DZ	epsilon0_const*es.I_sZR*es.ER+epsilon0_const*es.I_sZPHI*es.EPHI+epsilon0_const*es.I_sZZ*es.EZ+es.PZ	C/m²	Electric displacement field, Z component	Domain 2	
es.PR	epsilon0_const*(es.chiRR*es.ER+es.chiRPHI*es.EPHI+es.chiRZ*es.EZ)	C/m²	Polarization, R component	Domain 2	+ operation
es.PPHI	epsilon0_const*(es.chiPHIR*es.ER+es.chiPHIPHI*es.EPHI+es.chiPHIZ*es.EZ)	C/m²	Polarization, PHI component	Domain 2	+ operation
es.PZ	epsilon0_const*(es.chiZR*es.ER+es.chiZPHI*es.EPHI+es.chiZZ*es.EZ)	C/m²	Polarization, Z component	Domain 2	+ operation
es.chiRR	-1+es.epsilonrRR	1	Electric susceptibility, RR component	Domain 2	
es.chiPHIR	es.epsilonrPHIR	1	Electric susceptibility, PHIR component	Domain 2	
es.chiZR	es.epsilonrZR	1	Electric susceptibility, ZR component	Domain 2	
es.chiRPHI	es.epsilonrRPHI	1	Electric susceptibility, RPHI component	Domain 2	
es.chiPHIPHI	-1+es.epsilonrPHIPHI	1	Electric susceptibility, PHIPHI component	Domain 2	
es.chiZPHI	es.epsilonrZPHI	1	Electric susceptibility, ZPHI component	Domain 2	
es.chiRZ	es.epsilonrRZ	1	Electric susceptibility, RZ component	Domain 2	
es.chiPHIZ	es.epsilonrPHIZ	1	Electric	Domain 2	

Name	Expression	Unit	Description	Selection	Details
			susceptibility, PHIZ component		
es.chiZZ	-1+es.epsilonrZZ	1	Electric susceptibility, ZZ component	Domain 2	
es.ER	-VR	V/m	Electric field, R component	Domain 2	+ operation
es.EPHI	0	V/m	Electric field, PHI component	Domain 2	+ operation
es.EZ	-VZ	V/m	Electric field, Z component	Domain 2	+ operation
es.tER	-VTR	V/m	Tangential electric field, R component	Boundaries 7–29, 31–152, 154–194	
es.tEPHI	0	V/m	Tangential electric field, PHI component	Boundaries 7–29, 31–152, 154–194	
es.tEZ	-VTZ	V/m	Tangential electric field, Z component	Boundaries 7–29, 31–152, 154–194	
es.JR	es.JdR	A/m²	Current density, R component	Domain 2	+ operation
es.JPHI	es.JdPHI	A/m²	Current density, PHI component	Domain 2	+ operation
es.JZ	es.JdZ	A/m²	Current density, Z component	Domain 2	+ operation
es.JdR	0	A/m²	Displacement current density, R component	Domain 2	
es.JdPHI	0	A/m²	Displacement current density, PHI component	Domain 2	
es.JdZ	0	A/m²	Displacement current density, Z component	Domain 2	
es.ccn2.nJ	es.dnr*(spatial.invF11*up(es.JR)+spatial.invF13*up(es.JZ))+es.dnphi*if(Rg>0.001*h,R/r,Rr)*up(es.JPHI)+es.dnz*(spatial.invF31*up(es.JR)+spatial.invF33*up(es.JZ))	A/m²	Inward current density	Boundaries 7–29, 31–152, 154–194	

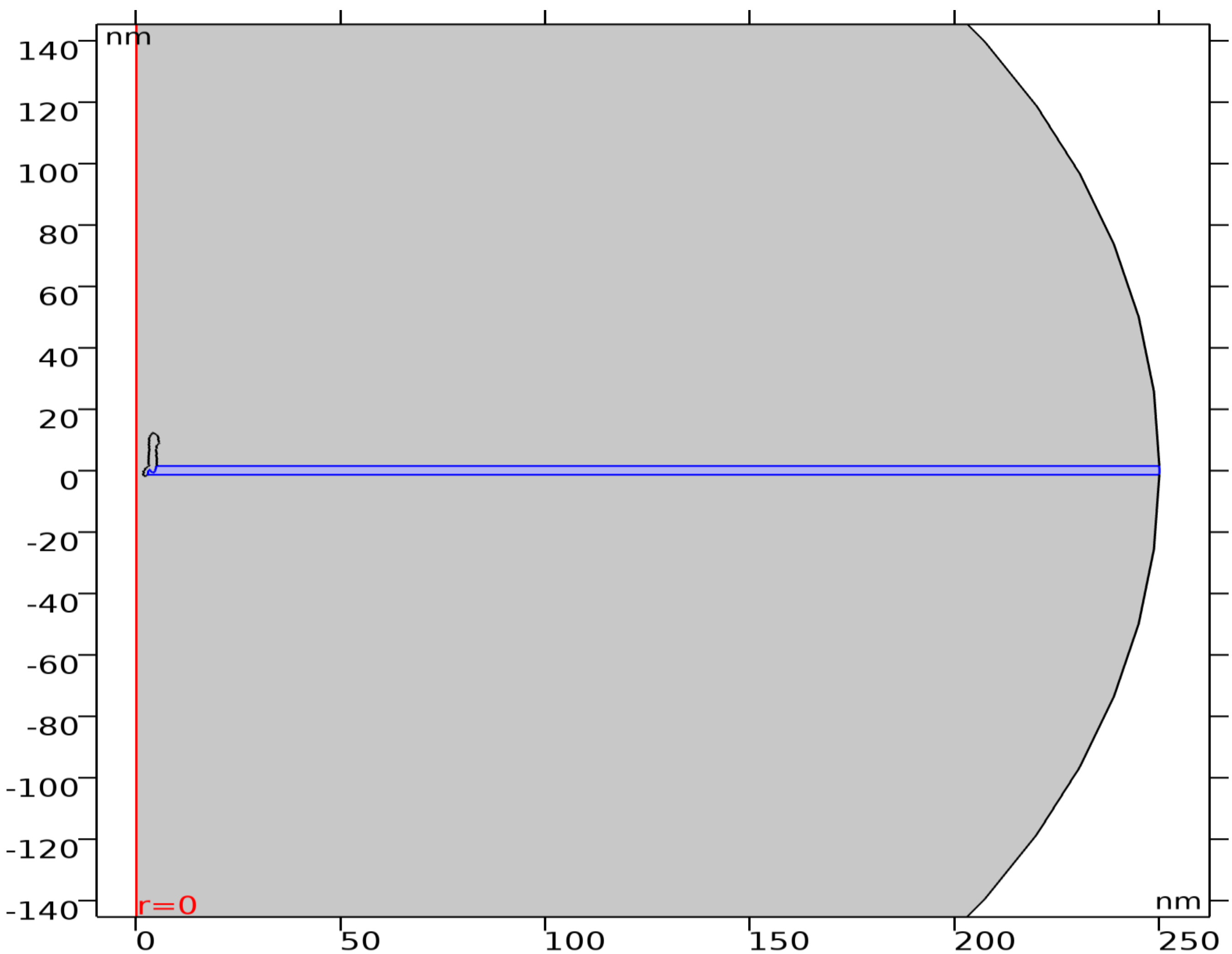
Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
V	Lagrange (Quadratic)	V	Electric potential	Material	Domain 2
V	Lagrange (Quadratic)	V	Electric potential	Spatial	Domain 2
V	Lagrange (Quadratic)	V	Electric potential	Geometry	Domain 2
V	Lagrange (Quadratic)	V	Electric potential	Mesh	Domain 2

Weak expressions

Weak expression	Integration order	Integration frame	Selection
- 2*(es.DR*test(VR)+es.DZ*test(VZ))*es.d *pi*R	4	Material	Domain 2

2.3.8 Charge Conservation (membrane)



Charge Conservation (membrane)

SELECTION

Geometric entity level	Domain
Name	Membrane
Selection	Domain 3

EQUATIONS

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

Electric field

SETTINGS

Description	Value
Constitutive relation	Relative permittivity
Relative permittivity	User defined
Relative permittivity	{{epsr_membrane, 0, 0}, {0, epsr_membrane, 0}, {0, 0, epsr_membrane}}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	0	C/m²	Surface charge density	Boundaries 29–31, 33–36, 66, 70–72, 79, 92, 100–103, 108, 112–113, 122–133, 135, 140–142, 153, 197–198	+ operation
es.epsilonr_iso	epsr_membrane	1	Relative permittivity, isotropic value	Domain 3	
es.Dr	(spatial.F11*es.DR+spatial.F31*es.DZ)*spatial.detInvF	C/m²	Electric displacement field, r component	Domain 3	
es.Dphi	if(Rg>0.001*h,r/R,rR)*es.DPHI*spatial.detInvF	C/m²	Electric displacement field, phi component	Domain 3	

Name	Expression	Unit	Description	Selection	Details
es.Dz	(spatial.F13*es.DR+spatial.F33*es.DZ)*spatial.detInvF	C/m²	Electric displacement field, z component	Domain 3	
es.Pr	(spatial.F11*es.PR+spatial.F31*es.PZ)*spatial.detInvF	C/m²	Polarization, r component	Domain 3	
es.Pphi	if(Rg>0.001*h,r/R,rR)*es.PPHI*spatial.detInvF	C/m²	Polarization, phi component	Domain 3	
es.Pz	(spatial.F13*es.PR+spatial.F33*es.PZ)*spatial.detInvF	C/m²	Polarization, z component	Domain 3	
es.normD	sqrt(realdot(es.Dr,es.Dr)+realdot(es.Dphi,es.Dphi)+realdot(es.Dz,es.Dz))	C/m²	Electric displacement field norm	Domain 3	
es.normP	sqrt(realdot(es.Pr,es.Pr)+realdot(es.Pphi,es.Pphi)+realdot(es.Pz,es.Pz))	C/m²	Polarization norm	Domain 3	
es.Er	spatial.invF11*es.ER+spatial.invF13*es.EZ	V/m	Electric field, r component	Domain 3	
es.Ephi	if(Rg>0.001*h,R/r,Rr)*es.EPHI	V/m	Electric field, phi component	Domain 3	
es.Ez	spatial.invF31*es.ER+spatial.invF33*es.EZ	V/m	Electric field, z component	Domain 3	
es.tEr	spatial.invF11*es.tER+spatial.invF13*es.tEZ	V/m	Tangential electric field, r component	Boundaries 29–31, 33–36, 66, 70–72, 79, 92, 100–103, 108, 112–113, 122–133, 135, 140–142, 153, 197–198	
es.tEphi	if(Rg>0.001*h,R/r,Rr)*es.tEPHI	V/m	Tangential electric field, phi component	Boundaries 29–31, 33–36, 66, 70–72, 79, 92, 100–103, 108, 112–113, 122–133, 135, 140–142, 153, 197–198	

Name	Expression	Unit	Description	Selection	Details
es.tEz	spatial.invF31*es.tER+spatial.invF33*es.tEZ	V/m	Tangential electric field, z component	Boundaries 29–31, 33–36, 66, 70–72, 79, 92, 100–103, 108, 112–113, 122–133, 135, 140–142, 153, 197–198	
es.normE	sqrt(realdot(es.Er,es.Er)+realdot(es.Ephi,es.Ephi)+realdot(es.Ez,es.Ez))	V/m	Electric field norm	Domain 3	
es.normJ	sqrt(realdot(es.JR,es.JR)+realdot(es.JPHI,es.JPHI)+realdot(es.JZ,es.JZ))*spatial.detInvF^2	A/m²	Current density norm	Domain 3	
es.W	es.We	J/m³	Energy density	Domain 3	+ operation
es.dWe	2*es.We*pi*R	J/m²	Integrand for total electric energy	Domain 3	
es.We	0.5*epsilon0_const*(((es.I_sRR+es.chiRR)*es.ER+(es.I_sRPHI+es.chiRPHI)*es.EPHI+(es.I_sRZ+es.chiRZ)*es.EZ)*es.ER+((es.I_sPHIR+es.chiPHIR)*es.ER+(es.I_sPHIPHI+es.chiPHIPHI)*es.EPHI+(es.I_sPHIZ+es.chiPHIZ)*es.EZ)*es.EPHI+((es.I_sZR+es.chiZR)*es.ER+(es.I_sZPHI+es.chiZPHI)*es.EPHI+(es.I_sZZ+es.chiZZ)*es.EZ)*es.EZ)*spatial.detInvF	J/m³	Electric energy density	Domain 3	
es.epsilonrRR	epsr_membrane	1	Relative permittivity, RR component	Domain 3	
es.epsilonrPHIR	0	1	Relative permittivity, PHIR component	Domain 3	
es.epsilonrZR	0	1	Relative permittivity, ZR	Domain 3	

Name	Expression	Unit	Description	Selection	Details
			component		
es.epsilonrRPHI	0	1	Relative permittivity, RPHI component	Domain 3	
es.epsilonrPHIPHI	epsr_membrane	1	Relative permittivity, PHIPHI component	Domain 3	
es.epsilonrZPHI	0	1	Relative permittivity, ZPHI component	Domain 3	
es.epsilonrRZ	0	1	Relative permittivity, RZ component	Domain 3	
es.epsilonrPHIZ	0	1	Relative permittivity, PHIZ component	Domain 3	
es.epsilonrZZ	epsr_membrane	1	Relative permittivity, ZZ component	Domain 3	
es.DR	epsilon0_const*es.I_sRR*es.ER+epsilon0_const*es.I_sRPHI*es.EPHI+epsilon0_const*es.I_sRZ*es.EZ+es.PR	C/m²	Electric displacement field, R component	Domain 3	
es.DPHI	epsilon0_const*es.I_sPHIR*es.ER+epsilon0_const*es.I_sPHIPHI*es.EPHI+epsilon0_const*es.I_sPHIZ*es.EZ+es.PPHI	C/m²	Electric displacement field, PHI component	Domain 3	
es.DZ	epsilon0_const*es.I_sZR*es.ER+epsilon0_const*es.I_sZPHI*es.EPHI+epsilon0_const*es.I_sZZ*es.EZ+es.PZ	C/m²	Electric displacement field, Z component	Domain 3	
es.PR	epsilon0_const*(es.chiRR*es.ER+es.chiRPHI*es.EPHI+es.chiRZ*es.EZ)	C/m²	Polarization, R component	Domain 3	+ operation
es.PPHI	epsilon0_const*(es.chiPHIR*es.ER+es.chiPHIPHI*es.EPHI+es.chiPHIZ*es.EZ)	C/m²	Polarization, PHI component	Domain 3	+ operation

Name	Expression	Unit	Description	Selection	Details
es.PZ	epsilon0_const*(es.chiZR*es.ER+es.chiZPHI*es.EPHI+es.chiZZ*es.EZ)	C/m²	Polarization, Z component	Domain 3	+ operation
es.chiRR	-1+es.epsilonrRR	1	Electric susceptibility, RR component	Domain 3	
es.chiPHIR	es.epsilonrPHIR	1	Electric susceptibility, PHIR component	Domain 3	
es.chiZR	es.epsilonrZR	1	Electric susceptibility, ZR component	Domain 3	
es.chiRPHI	es.epsilonrRPHI	1	Electric susceptibility, RPHI component	Domain 3	
es.chiPHIPHI	-1+es.epsilonrPHIPHI	1	Electric susceptibility, PHIPHI component	Domain 3	
es.chiZPHI	es.epsilonrZPHI	1	Electric susceptibility, ZPHI component	Domain 3	
es.chiRZ	es.epsilonrRZ	1	Electric susceptibility, RZ component	Domain 3	
es.chiPHIZ	es.epsilonrPHIZ	1	Electric susceptibility, PHIZ component	Domain 3	
es.chiZZ	-1+es.epsilonrZZ	1	Electric susceptibility, ZZ component	Domain 3	
es.ER	-VR	V/m	Electric field, R component	Domain 3	+ operation
es.EPHI	0	V/m	Electric field, PHI component	Domain 3	+ operation
es.EZ	-VZ	V/m	Electric field, Z component	Domain 3	+ operation
es.tER	-VTR	V/m	Tangential electric field, R component	Boundaries 29–31, 33–36, 66, 70–72, 79, 92, 100–103, 108, 112–113,	

Name	Expression	Unit	Description	Selection	Details
				122–133, 135, 140–142, 153, 197–198	
es.tEPHI	0	V/m	Tangential electric field, PHI component	Boundaries 29–31, 33–36, 66, 70–72, 79, 92, 100–103, 108, 112–113, 122–133, 135, 140–142, 153, 197–198	
es.tEZ	-VTZ	V/m	Tangential electric field, Z component	Boundaries 29–31, 33–36, 66, 70–72, 79, 92, 100–103, 108, 112–113, 122–133, 135, 140–142, 153, 197–198	
es.JR	es.JdR	A/m²	Current density, R component	Domain 3	+ operation
es.JPHI	es.JdPHI	A/m²	Current density, PHI component	Domain 3	+ operation
es.JZ	es.JdZ	A/m²	Current density, Z component	Domain 3	+ operation
es.JdR	0	A/m²	Displacement current density, R component	Domain 3	
es.JdPHI	0	A/m²	Displacement current density, PHI component	Domain 3	
es.JdZ	0	A/m²	Displacement current density, Z component	Domain 3	
es.ccn3.nJ	es.dnr*(spatial.invF11*up(es.JR)+spatial.invF13*up(es.JZ))+es.dnphi*if(Rg>0.001*h,R/r,Rr)*up(es.JPHI)+es.dnz*(spatial.invF31*up(es.JR)+spatial.invF33*up(es.JZ))	A/m²	Inward current density	Boundaries 30, 153	
es.ccn3.nJ	es.unr*(spatial.invF11*down(es.JR)+spatial.	A/m²	Inward current density	Boundaries 29, 31, 33–36,	

Name	Expression	Unit	Description	Selection	Details
	invF13*down(es.JZ))+es.unphi*if(Rg>0.001*h,R/r,Rr)*down(es.JPHI)+es.unz*(spatial.invF31*down(es.JR)+spatial.invF33*down(es.JZ))			66, 70–72, 79, 92, 100–103, 108, 112–113, 122–133, 135, 140–142, 197–198	

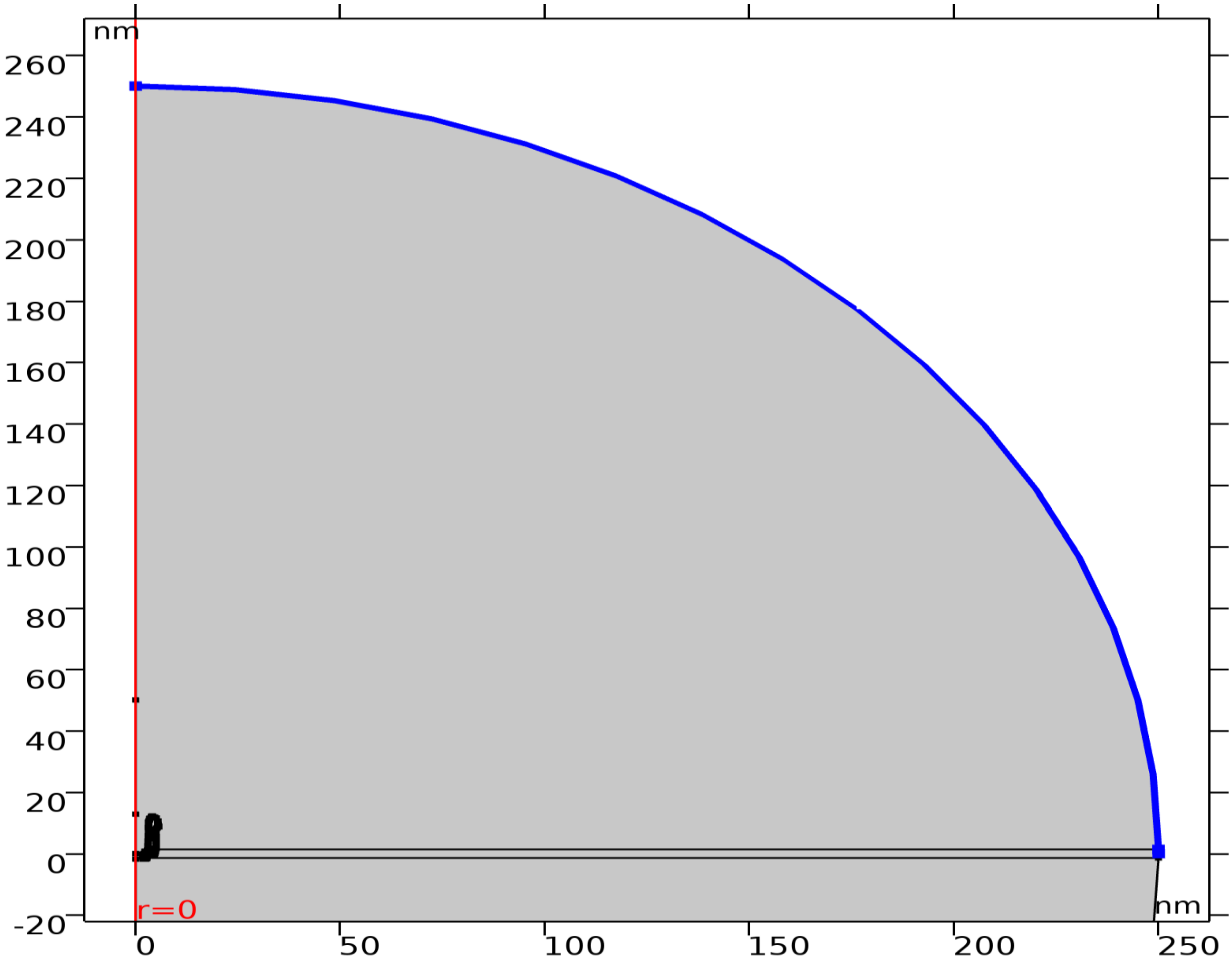
Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
V	Lagrange (Quadratic)	V	Electric potential	Material	Domain 3
V	Lagrange (Quadratic)	V	Electric potential	Spatial	Domain 3
V	Lagrange (Quadratic)	V	Electric potential	Geometry	Domain 3
V	Lagrange (Quadratic)	V	Electric potential	Mesh	Domain 3

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-2*(es.DR*test(VR)+es.DZ*test(VZ))*es.d*pi*R	4	Material	Domain 3

2.3.9 Ground



Ground

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 196, 198

EQUATIONS

$$V = 0$$

Constraint settings

SETTINGS

Description	Value
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off

Description	Value
Constraint method	Elemental

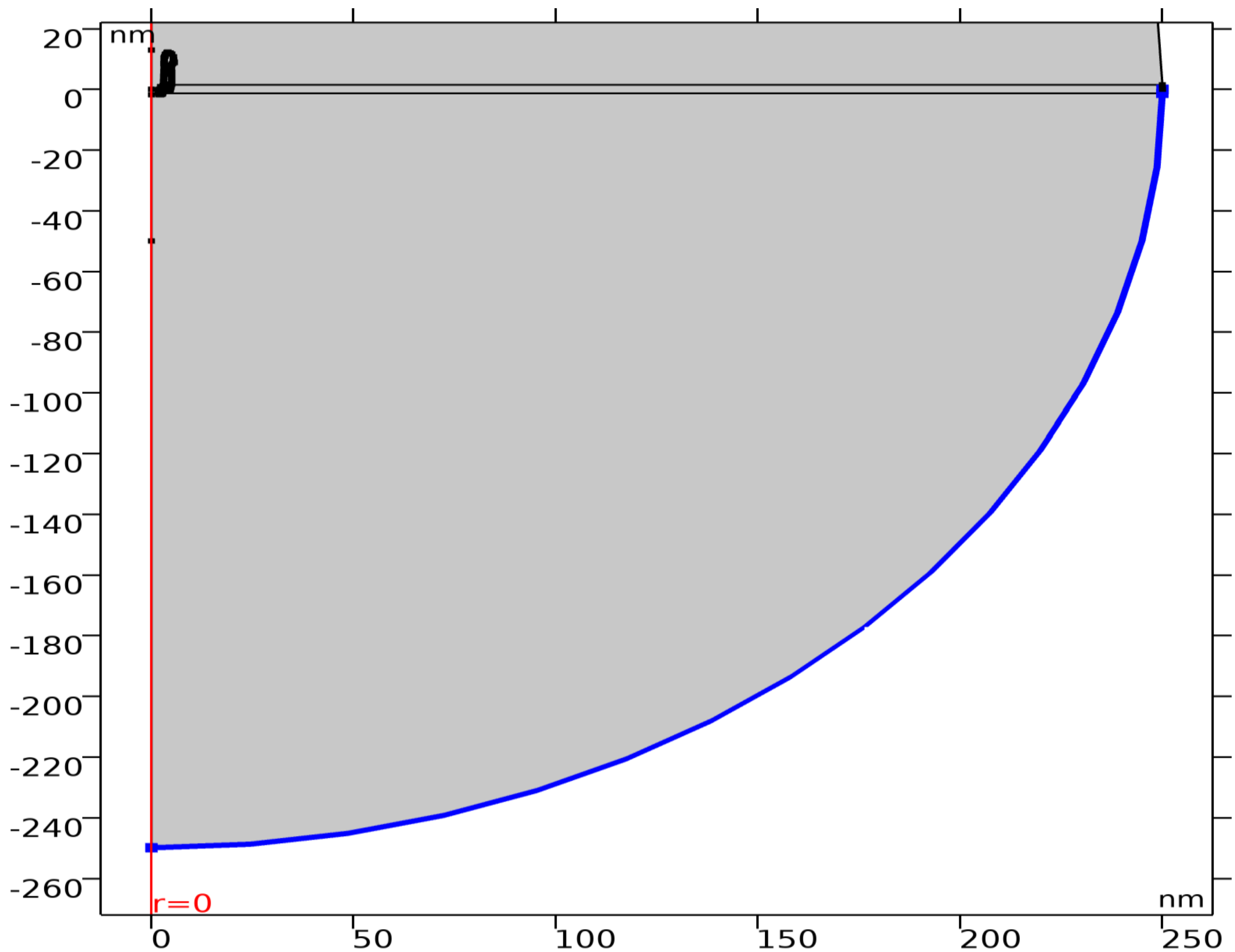
Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	es.unr*down(es.Dr)+es.unphi*down(es.Dphi)+es.unz*down(es.Dz)	C/m^2	Surface charge density	Boundaries 196, 198	+ operation

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-V	test(-V)	Lagrange (Quadratic)	Boundaries 196, 198	Elemental

2.3.10 Electric Potential



Electric Potential

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 195, 197

EQUATIONS

$$V = V_0$$

Electric potential

SETTINGS

Description	Value
Electric potential	V_bias

Constraint settings

SETTINGS

Description	Value
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off
Constraint method	Elemental

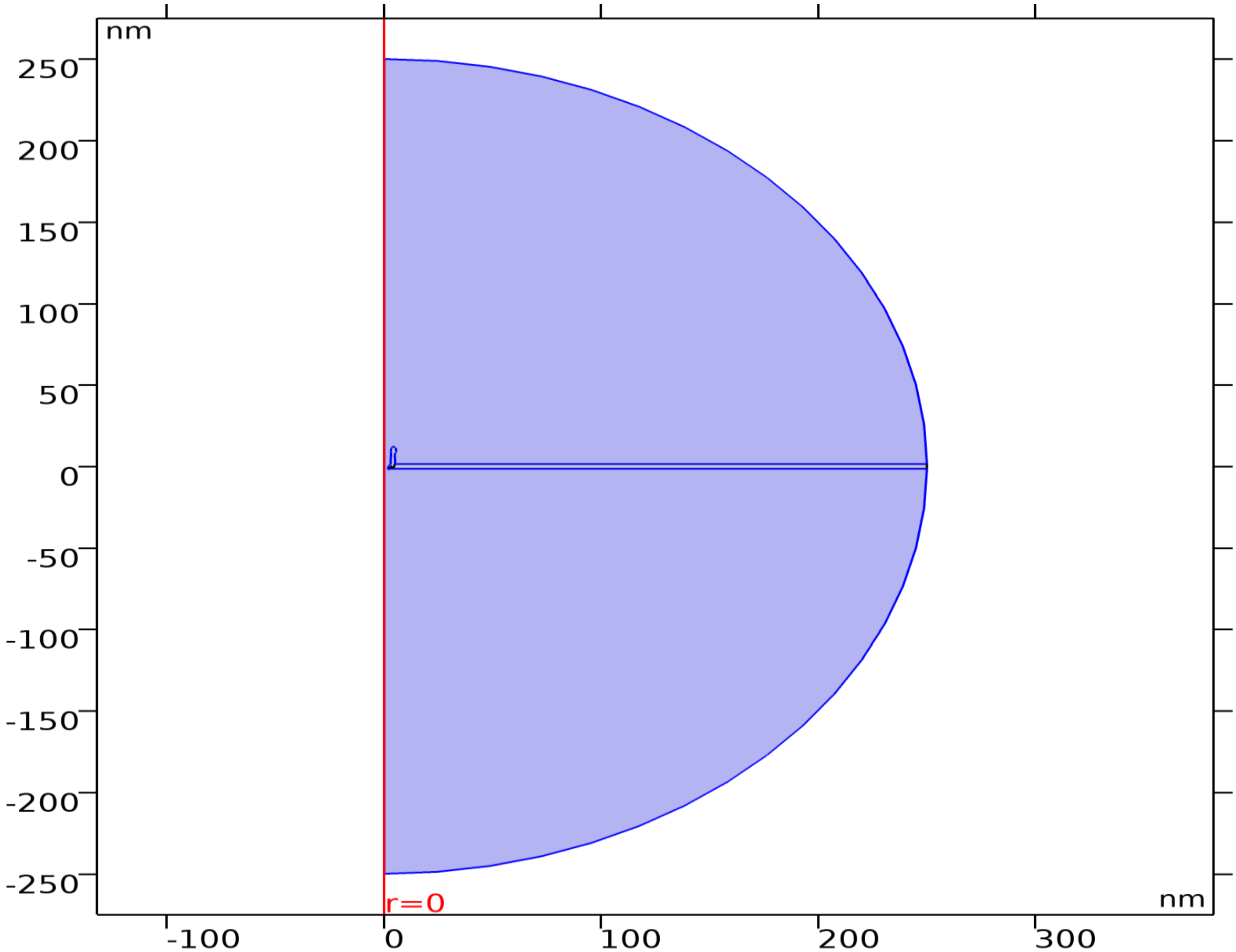
Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	es.unr*down(es.Dr)+es.unphi*down(es.Dphi)+es.unz*down(es.Dz)	C/m^2	Surface charge density	Boundaries 195, 197	+ operation
es.V0	V_bias	V	Electric potential	Boundaries 195, 197	

Constraints

Constraint	Constraint force	Shape function	Selection	Details
es.V0-V	test(es.V0-V)	Lagrange (Quadratic)	Boundaries 195, 197	Elemental

2.3.11 Space Charge Density (ions)



Space Charge Density (ions)

SELECTION

Geometric entity level	Domain
Name	Reservoir
Selection	Domain 1

EQUATIONS

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

Coordinate system selection

SETTINGS

Description	**Value**
Coordinate system	Global coordinate system

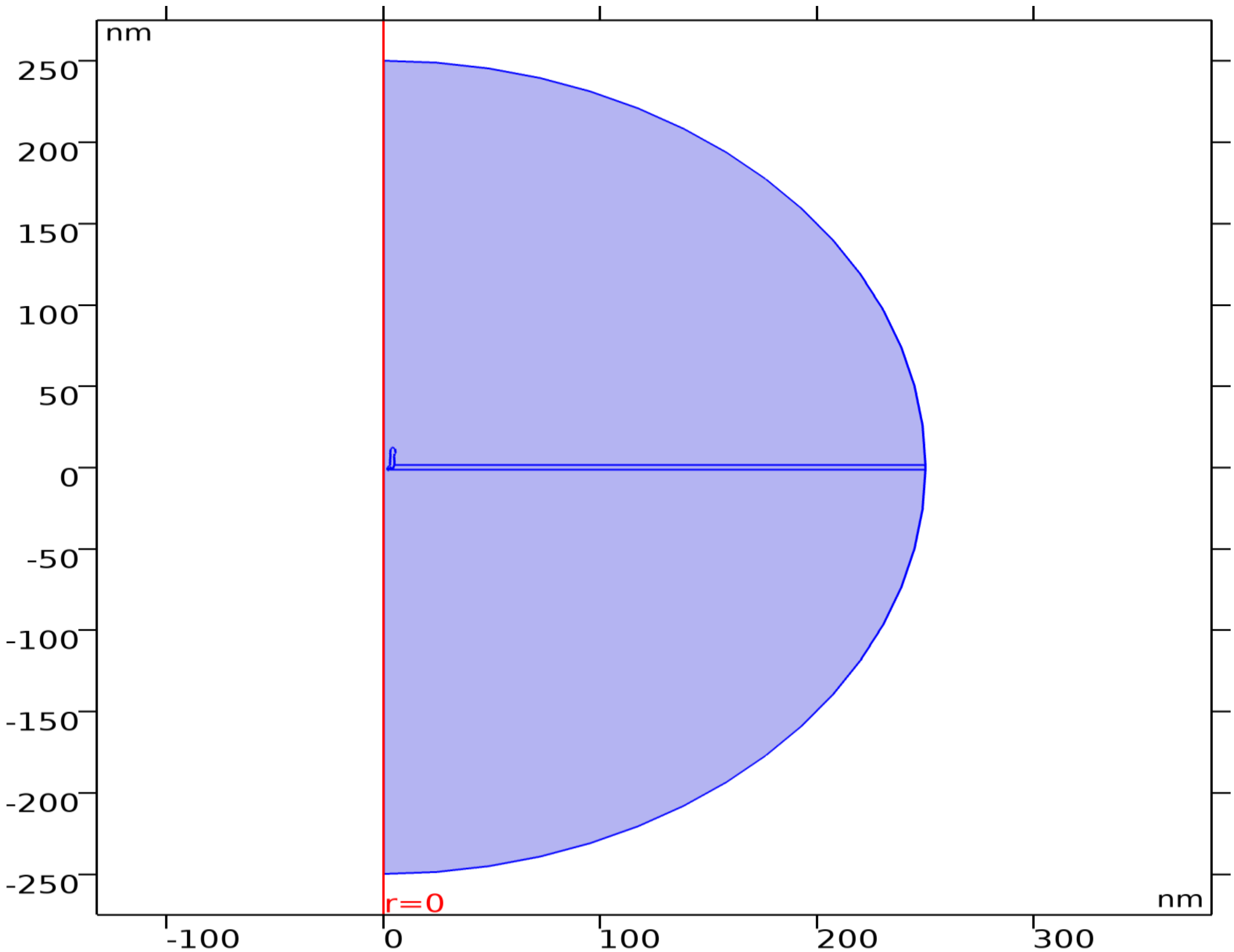
Variables

Name	Expression	Unit	Description	Selection	Details
es.rhoq	es.scd1.rhoq	C/m^3	Space charge density	Domain 1	+ operation
es.scd1.rhoq	scd_ions	C/m^3	Space charge density	Domain 1	

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-2*es.scd1.rhoq*test(V)*es.d*pi*r	4	Spatial	Domain 1

2.3.12 Space Charge Density (nanopore)



Space Charge Density (nanopore)

SELECTION

Geometric entity level	Domain
Selection	Domains 1–3

EQUATIONS

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

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection	Details
es.rhoq	es.scd2.rhoq	C/m^3	Space charge density	Domains 1–3	+ operation
es.scd2.rhoq	scd_pore	C/m^3	Space charge density	Domains 1–3	

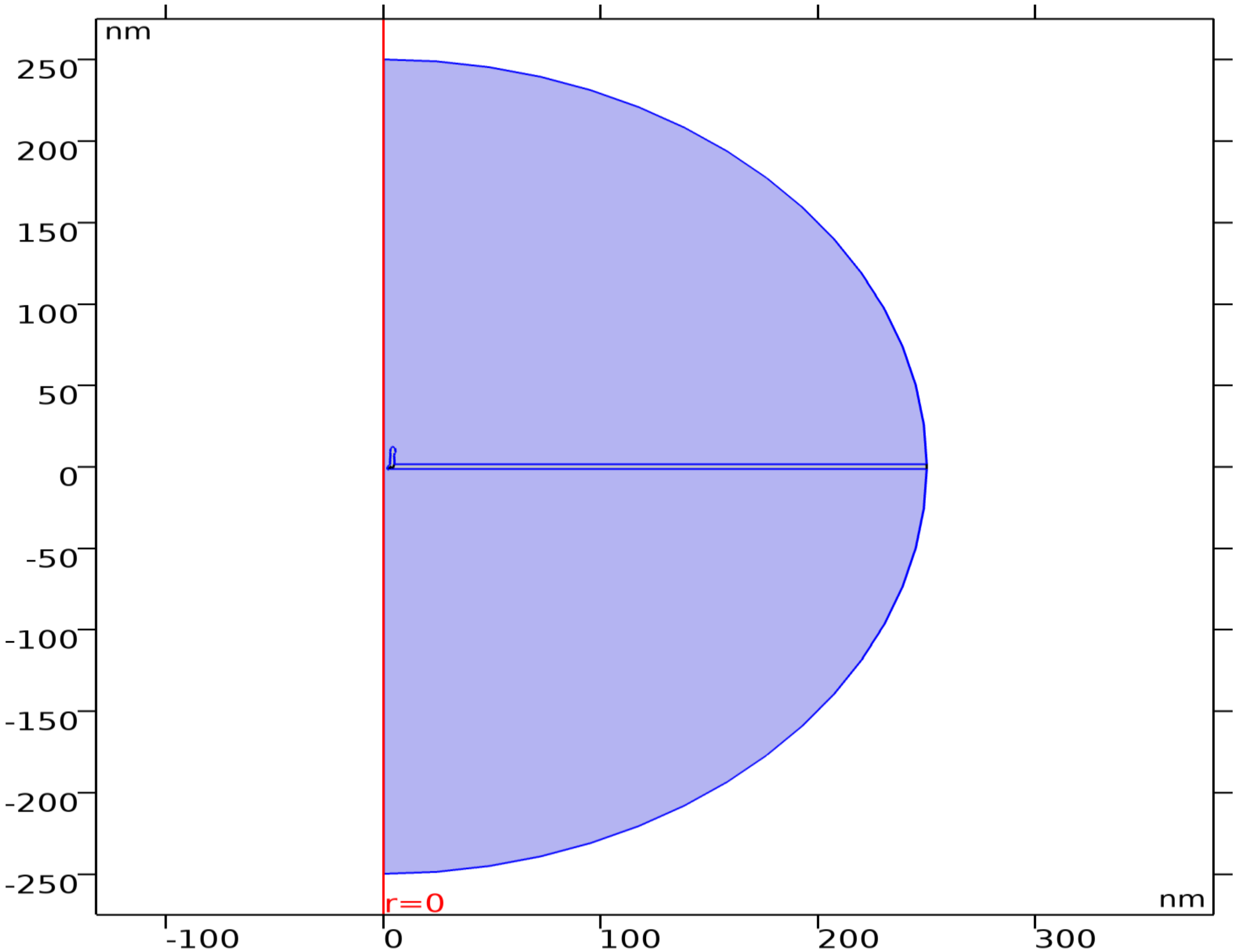
Weak expressions

Weak expression	Integration order	Integration frame	Selection
-2*es.scd2.rhoq*test(V)*es.d*pi*r	4	Spatial	Domains 1–3

2.4 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module



Transport of Diluted Species

SELECTION

Geometric entity level	Domain
Name	Reservoir
Selection	Domain 1

EQUATIONS

$$\nabla \cdot (\mathbf{J}_i + \mathbf{u}c_i) = R_i$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$

2.4.1 Interface settings

Discretization

SETTINGS

Description	**Value**

Description	Value
Concentration	Quadratic

Transport mechanisms

SETTINGS

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

Consistent stabilization

SETTINGS

Description	Value
Streamline diffusion	On
Crosswind diffusion	On
Equation residual	Approximate residual
Crosswind diffusion type	Do Carmo and Galeão

Inconsistent stabilization

SETTINGS

Description	Value
Isotropic diffusion	Off

Advanced settings

SETTINGS

Description	Value
Convective term	Conservative form

2.4.2 Variables

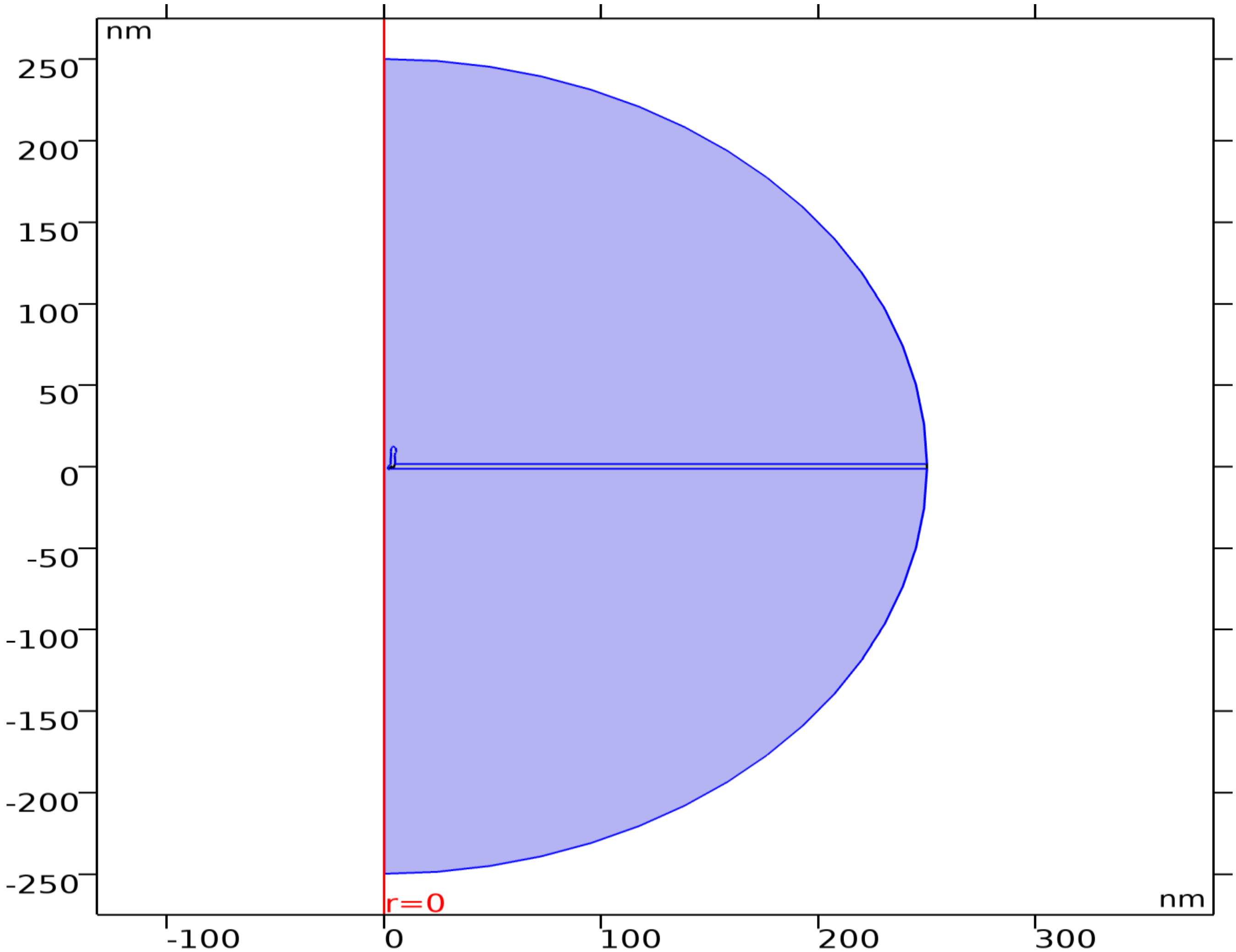
Name	Expression	Unit	Description	Selection	Details
tds.R_cpos	0	mol/(m^3·s)	Total rate expression	Domain 1	+ operation
tds.R_cneg	0	mol/(m^3·s)	Total rate expression	Domain 1	+ operation
tds.epsilon_p	1	1	Porosity	Domain 1	
tds.theta	tds.epsilon_p	1	Liquid volume fraction	Domain 1	
tds.av	0	1	Gas volume fraction	Domain 1	

Name	Expression	Unit	Description	Selection	Details
tds.nr	dnr	1	Normal vector, r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nphi	0	1	Normal vector, phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nz	dnz	1	Normal vector, z component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nrmesh	dnrmesh	1	Normal vector (mesh), r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nphimesh	0	1	Normal vector (mesh), phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nzmesh	dnzmesh	1	Normal vector	Boundaries 1–	

Name	Expression	Unit	Description	Selection	Details
			(mesh), z component	28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nrc	root.nrc/tds.ncLen	1	Normal vector, r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nphic	0	1	Normal vector, phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nzc	root.nzc/tds.ncLen	1	Normal vector, z component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.ncLen	sqrt(root.nrc^2+root.nzc^2+eps)	1	Help variable	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.cbf_cpos	0	mol/(m²·s)	Convective boundary flux	Boundaries 1–28, 30, 32, 37–	

Name	Expression	Unit	Description	Selection	Details
				65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.u	0	m/s	Velocity field, r component	Domain 1	
tds.v	0	m/s	Velocity field, phi component	Domain 1	
tds.w	0	m/s	Velocity field, z component	Domain 1	
tds.cbf_cneg	0	$mol/(m^2\cdot s)$	Convective boundary flux	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	

2.4.3 Transport Properties



Transport Properties

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

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

$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$

Diffusion

SETTINGS

Description	**Value**
Material	None

Description	Value
Diffusion coefficient	User defined
Diffusion coefficient	{{D_cpos, 0, 0}, {0, D_cpos, 0}, {0, 0, D_cpos}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_cneg, 0, 0}, {0, D_cneg, 0}, {0, 0, D_cneg}}

Migration in electric field

SETTINGS

Description	Value
Mobility	User defined
Mobility	{{{mu_cpos, 0, 0}, {0, mu_cpos, 0}, {0, 0, mu_cpos}}, {{mu_cneg, 0, 0}, {0, mu_cneg, 0}, {0, 0, mu_cneg}}}
Charge number	{z_cpos, z_cneg}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T_system

Variables

Name	Expression	Unit	Description	Selection	Details
domflux.cposr	2*(tds.dflux_cposr+tds.cflux_cposr+tds.mflux_cposr+smp.sflux_cposr)*pi*r	mol/(m·s)	Domain flux, r component	Domain 1	
domflux.cposz	2*(tds.dflux_cposz+tds.cflux_cposz+tds.mflux_cposz+smp.sflux_cposz)*pi*r	mol/(m·s)	Domain flux, z component	Domain 1	
domflux.cnegr	2*(tds.dflux_cnegr+tds.cflux_cnegr+tds.mflux_cnegr+smp.sflux_cnegr)*pi*r	mol/(m·s)	Domain flux, r component	Domain 1	
domflux.cnegz	2*(tds.dflux_cnegz+tds.cflux_cnegz+tds.	mol/(m·s)	Domain flux, z	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	mflux_cnegz+smp.sflux_cnegz)*pi*r		component		
tds.ndflux_cpos	tds.dflux_cposr*tds.nrc+tds.dflux_cposphi*tds.nphic+tds.dflux_cposz*tds.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.ncflux_cpos	tds.cflux_cposr*tds.nrc+tds.cflux_cposphi*tds.nphic+tds.cflux_cposz*tds.nzc	mol/(m²·s)	Normal convective flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nmflux_cpos	tds.mflux_cposr*tds.nrc+tds.mflux_cposphi*tds.nphic+tds.mflux_cposz*tds.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.ntflux_cpos	tds.bndFlux_cpos	mol/(m²·s)	Normal total flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.ndflux_cneg	tds.dflux_cnegr*tds.nrc+tds.dflux_cnegphi*tds.nphic+tds.dflux_cnegz*tds.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139,	

Name	Expression	Unit	Description	Selection	Details
				143–196	
tds.ncflux_cneg	tds.cflux_cnegr*tds.nrc+tds.cflux_cnegphi*tds.nphic+tds.cflux_cnegz*tds.nzc	mol/(m²·s)	Normal convective flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.nmflux_cneg	tds.mflux_cnegr*tds.nrc+tds.mflux_cnegphi*tds.nphic+tds.mflux_cnegz*tds.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.ntflux_cneg	tds.bndFlux_cneg	mol/(m²·s)	Normal total flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.u	model.input.u1	m/s	Velocity field, r component	Domain 1	Meta
tds.v	model.input.u2	m/s	Velocity field, phi component	Domain 1	Meta
tds.w	model.input.u3	m/s	Velocity field, z component	Domain 1	Meta
tds.bndFlux_cpos	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cpos)/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.bndFlux_cneg	if(r>0.001/sqrt(sqrt(mean(emetric2))),-	mol/(m²·s)	Boundary flux	Boundaries 1–28, 30, 32, 37–	

Name	Expression	Unit	Description	Selection	Details
	0.5*dflux_spatial(cneg)/(pi*r),NaN)			65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
tds.D_cposrr	D_cpos	m^2/s	Diffusion coefficient, rr component	Domain 1	+ operation
tds.D_cposphir	0	m^2/s	Diffusion coefficient, phir component	Domain 1	+ operation
tds.D_cposzr	0	m^2/s	Diffusion coefficient, zr component	Domain 1	+ operation
tds.D_cposrphi	0	m^2/s	Diffusion coefficient, rphi component	Domain 1	+ operation
tds.D_cposphiphi	D_cpos	m^2/s	Diffusion coefficient, phiphi component	Domain 1	+ operation
tds.D_cposzphi	0	m^2/s	Diffusion coefficient, zphi component	Domain 1	+ operation
tds.D_cposrz	0	m^2/s	Diffusion coefficient, rz component	Domain 1	+ operation
tds.D_cposphiz	0	m^2/s	Diffusion coefficient, phiz component	Domain 1	+ operation
tds.D_cposzz	D_cpos	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.D_cnegrr	D_cneg	m^2/s	Diffusion coefficient, rr component	Domain 1	+ operation
tds.D_cnegphir	0	m^2/s	Diffusion coefficient, phir component	Domain 1	+ operation
tds.D_cnegzr	0	m^2/s	Diffusion coefficient, zr component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
tds.D_cnegrphi	0	m²/s	Diffusion coefficient, rphi component	Domain 1	+ operation
tds.D_cnegphiphi	D_cneg	m²/s	Diffusion coefficient, phiphi component	Domain 1	+ operation
tds.D_cnegzphi	0	m²/s	Diffusion coefficient, zphi component	Domain 1	+ operation
tds.D_cnegrz	0	m²/s	Diffusion coefficient, rz component	Domain 1	+ operation
tds.D_cnegphiz	0	m²/s	Diffusion coefficient, phiz component	Domain 1	+ operation
tds.D_cnegzz	D_cneg	m²/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.Dav_cpos	0.5*(tds.D_cposrr+tds.D_cposzz)	m²/s	Average diffusion coefficient	Domain 1	
tds.Dav_cneg	0.5*(tds.D_cnegrr+tds.D_cnegzz)	m²/s	Average diffusion coefficient	Domain 1	
tds.tflux_cposr	tds.dflux_cposr+tds.mflux_cposr+tds.cflux_cposr+smp.sflux_cposr	mol/(m²·s)	Total flux, r component	Domain 1	+ operation
tds.tflux_cposphi	tds.dflux_cposphi+tds.mflux_cposphi+tds.cflux_cposphi+smp.sflux_cposphi	mol/(m²·s)	Total flux, phi component	Domain 1	+ operation
tds.tflux_cposz	tds.dflux_cposz+tds.mflux_cposz+tds.cflux_cposz+smp.sflux_cposz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cpos	sqrt(tds.dflux_cposr^2+tds.dflux_cposphi^2+tds.dflux_cposz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cpos	sqrt(tds.tflux_cposr^2+tds.tflux_cposphi^2+tds.tflux_cposz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
tds.mflux_cposr	tds.z_cpos*F_const*	mol/(m²·s)	Electrophoretic	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	cpos*(-tds.um_cposrr*d(tds.V,r)-tds.um_cposrz*d(tds.V,z))		flux, r component		
tds.mflux_cposphi	tds.z_cpos*F_const*cpos*(-tds.um_cposphir*d(tds.V,r)-tds.um_cposphiz*d(tds.V,z))	mol/(m²·s)	Electrophoretic flux, phi component	Domain 1	
tds.mflux_cposz	tds.z_cpos*F_const*cpos*(-tds.um_cposzr*d(tds.V,r)-tds.um_cposzz*d(tds.V,z))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
tds.tflux_cnegr	tds.dflux_cnegr+tds.mflux_cnegr+tds.cflux_cnegr+smp.sflux_cnegr	mol/(m²·s)	Total flux, r component	Domain 1	+ operation
tds.tflux_cnegphi	tds.dflux_cnegphi+tds.mflux_cnegphi+tds.cflux_cnegphi+smp.sflux_cnegphi	mol/(m²·s)	Total flux, phi component	Domain 1	+ operation
tds.tflux_cnegz	tds.dflux_cnegz+tds.mflux_cnegz+tds.cflux_cnegz+smp.sflux_cnegz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cneg	sqrt(tds.dflux_cnegr^2+tds.dflux_cnegphi^2+tds.dflux_cnegz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cneg	sqrt(tds.tflux_cnegr^2+tds.tflux_cnegphi^2+tds.tflux_cnegz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
tds.mflux_cnegr	tds.z_cneg*F_const*cneg*(-tds.um_cnegrr*d(tds.V,r)-tds.um_cnegrz*d(tds.V,z))	mol/(m²·s)	Electrophoretic flux, r component	Domain 1	
tds.mflux_cnegph	tds.z_cneg*F_const*	mol/(m²·s)	Electrophoretic	Domain 1	

Name	Expression	Unit	Description	Selection	Details
i	cneg*(-tds.um_cnegphir*d(tds.V,r)-tds.um_cnegphiz*d(tds.V,z))		flux, phi component		
tds.mflux_cnegz	tds.z_cneg*F_const*cneg*(-tds.um_cnegzr*d(tds.V,r)-tds.um_cnegzz*d(tds.V,z))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
tds.dflux_cposr	-tds.D_cposrr*cposr-tds.D_cposrz*cposz	mol/(m²·s)	Diffusive flux, r component	Domain 1	
tds.dflux_cposphi	-tds.D_cposphir*cposr-tds.D_cposphiz*cposz	mol/(m²·s)	Diffusive flux, phi component	Domain 1	
tds.dflux_cposz	-tds.D_cposzr*cposr-tds.D_cposzz*cposz	mol/(m²·s)	Diffusive flux, z component	Domain 1	
tds.grad_cposr	cposr	mol/m⁴	Concentration gradient, r component	Domain 1	
tds.grad_cposphi	0	mol/m⁴	Concentration gradient, phi component	Domain 1	
tds.grad_cposz	cposz	mol/m⁴	Concentration gradient, z component	Domain 1	
tds.dflux_cnegr	-tds.D_cnegrr*cnegr-tds.D_cnegrz*cnegz	mol/(m²·s)	Diffusive flux, r component	Domain 1	
tds.dflux_cnegphi	-tds.D_cnegphir*cnegr-tds.D_cnegphiz*cnegz	mol/(m²·s)	Diffusive flux, phi component	Domain 1	
tds.dflux_cnegz	-tds.D_cnegzr*cnegr-tds.D_cnegzz*cnegz	mol/(m²·s)	Diffusive flux, z component	Domain 1	
tds.grad_cnegr	cnegr	mol/m⁴	Concentration gradient, r	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			component		
tds.grad_cnegphi	0	mol/m⁴	Concentration gradient, phi component	Domain 1	
tds.grad_cnegz	cnegz	mol/m⁴	Concentration gradient, z component	Domain 1	
tds.um_cposrr	mu_cpos	s·mol/kg	Mobility, rr component	Domain 1	
tds.um_cposphir	0	s·mol/kg	Mobility, phir component	Domain 1	
tds.um_cposzr	0	s·mol/kg	Mobility, zr component	Domain 1	
tds.um_cposrphi	0	s·mol/kg	Mobility, rphi component	Domain 1	
tds.um_cposphiphi	mu_cpos	s·mol/kg	Mobility, phiphi component	Domain 1	
tds.um_cposzphi	0	s·mol/kg	Mobility, zphi component	Domain 1	
tds.um_cposrz	0	s·mol/kg	Mobility, rz component	Domain 1	
tds.um_cposphiz	0	s·mol/kg	Mobility, phiz component	Domain 1	
tds.um_cposzz	mu_cpos	s·mol/kg	Mobility, zz component	Domain 1	
tds.z_cpos	z_cpos	1	Charge number	Domain 1	
tds.um_cnegrr	mu_cneg	s·mol/kg	Mobility, rr component	Domain 1	
tds.um_cnegphir	0	s·mol/kg	Mobility, phir component	Domain 1	
tds.um_cnegzr	0	s·mol/kg	Mobility, zr component	Domain 1	
tds.um_cnegrphi	0	s·mol/kg	Mobility, rphi component	Domain 1	
tds.um_cnegphiphi	mu_cneg	s·mol/kg	Mobility, phiphi component	Domain 1	
tds.um_cnegzphi	0	s·mol/kg	Mobility, zphi component	Domain 1	
tds.um_cnegrz	0	s·mol/kg	Mobility, rz component	Domain 1	
tds.um_cnegphiz	0	s·mol/kg	Mobility, phiz	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			component		
tds.um_cnegzz	mu_cneg	s·mol/kg	Mobility, zz component	Domain 1	
tds.z_cneg	z_cneg	1	Charge number	Domain 1	
tds.V	model.input.V	V	Electric potential	Domain 1	Meta
tds.T	tds.cdm1.minput_temperature	K	Temperature	Domain 1	
tds.cflux_cposr	cpos*tds.u	mol/(m²·s)	Convective flux, r component	Domain 1	
tds.cflux_cposphi	cpos*tds.v	mol/(m²·s)	Convective flux, phi component	Domain 1	
tds.cflux_cposz	cpos*tds.w	mol/(m²·s)	Convective flux, z component	Domain 1	
tds.cfluxMag_cpos	sqrt(tds.cflux_cposr^2+tds.cflux_cposphi^2+tds.cflux_cposz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
tds.cflux_cnegr	cneg*tds.u	mol/(m²·s)	Convective flux, r component	Domain 1	
tds.cflux_cnegphi	cneg*tds.v	mol/(m²·s)	Convective flux, phi component	Domain 1	
tds.cflux_cnegz	cneg*tds.w	mol/(m²·s)	Convective flux, z component	Domain 1	
tds.cfluxMag_cneg	sqrt(tds.cflux_cnegr^2+tds.cflux_cnegphi^2+tds.cflux_cnegz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
tds.Res_cpos	-tds.D_cposrr*cposrr-tds.D_cposrz*cposrz-tds.D_cposzr*cposzr-tds.D_cposzz*cposzz+d(cpos*(tds.u-tds.z_cpos*tds.um_cposrr*F_const*d(tds.V,r)-tds.z_cpos*tds.um_cposrz*F_const*d(tds.V,z)),r)+if(abs(r)<0.001*h_spatial,d(cpos*	mol/(m³·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	(tds.u-tds.z_cpos*tds.um_cposrr*F_const*d(tds.V,r)-tds.z_cpos*tds.um_cposrz*F_const*d(tds.V,z)),r),cpos*(tds.u-tds.z_cpos*tds.um_cposrr*F_const*d(tds.V,r)-tds.z_cpos*tds.um_cposrz*F_const*d(tds.V,z))/r)+d(cpos*(tds.w-tds.z_cpos*tds.um_cposzr*F_const*d(tds.V,r)-tds.z_cpos*tds.um_cposzz*F_const*d(tds.V,z)),z)-tds.R_cpos				
tds.Res_cneg	-tds.D_cnegrr*cnegrr-tds.D_cnegrz*cnegrz-tds.D_cnegzr*cnegzr-tds.D_cnegzz*cnegzz+d(cneg*(tds.u-tds.z_cneg*tds.um_cnegrr*F_const*d(tds.V,r)-tds.z_cneg*tds.um_cnegrz*F_const*d(tds.V,z)),r)+if(abs(r)<0.001*h_spatial,d(cneg*(tds.u-tds.z_cneg*tds.um_cnegrr*F_const*d(tds.V,r)-tds.z_cneg*tds.um_cnegrz*F_const*d(tds.V,z)),r),cneg*(tds.u-tds.z_cneg*tds.um_cnegrr*F_const*d(tds.V,r)-tds.z_cneg*tds.um_c	mol/(m^3·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	negrz*F_const*d(tds.V,z))/r)+d(cneg*(tds.w-tds.z_cneg*tds.um_cnegzr*F_const*d(tds.V,r)-tds.z_cneg*tds.um_cnegzz*F_const*d(tds.V,z)),z)-tds.R_cneg				

Shape functions

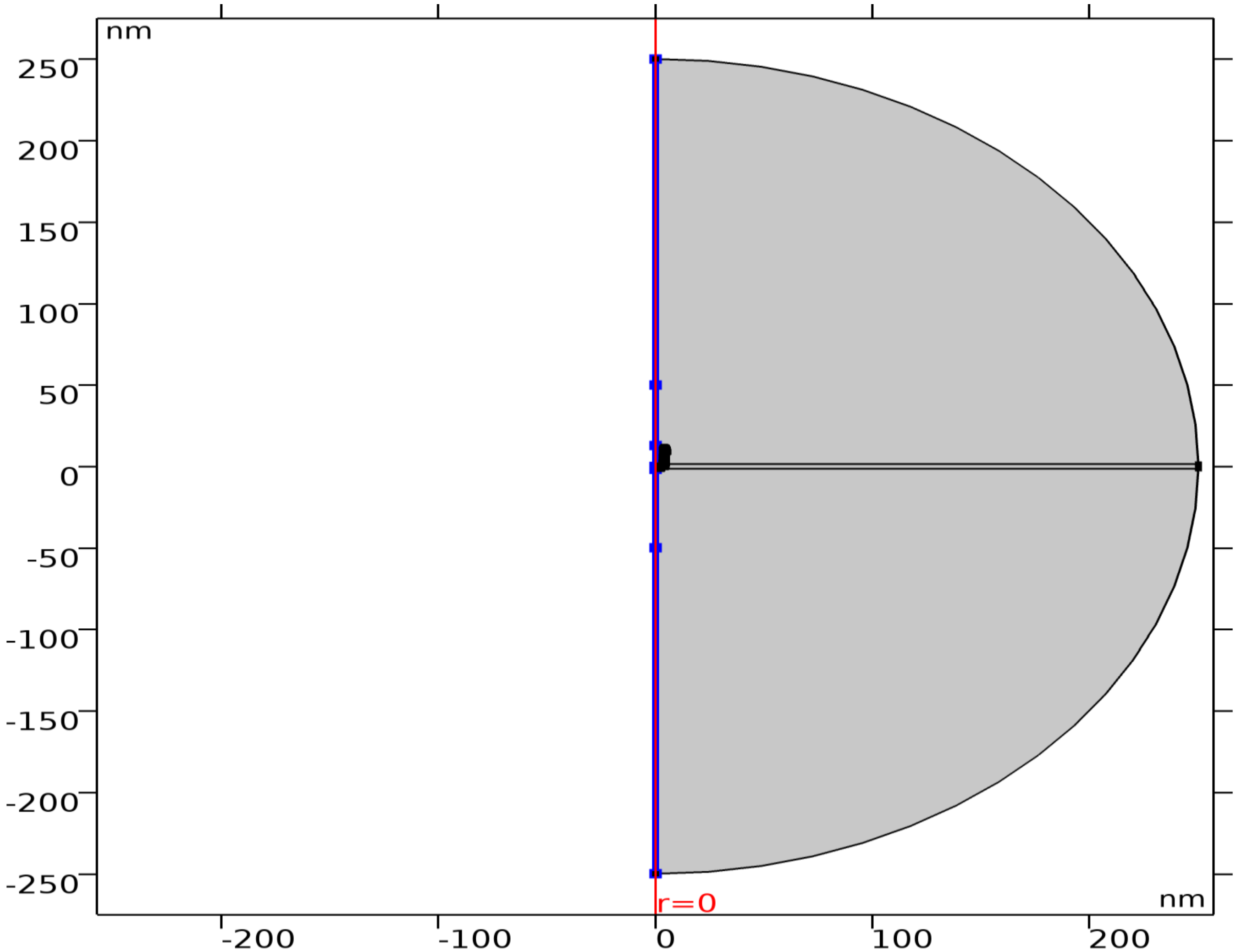
Name	Shape function	Unit	Description	Shape frame	Selection
cpos	Lagrange (Quadratic)	mol/m^3	Concentration	Spatial	Domain 1
cneg	Lagrange (Quadratic)	mol/m^3	Concentration	Spatial	Domain 1

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(tds.dflux_cposr*test(cposr)+tds.dflux_cposz*test(cposz))*pi*r	4	Spatial	Domain 1
2*(tds.dflux_cnegr*test(cnegr)+tds.dflux_cnegz*test(cnegz))*pi*r	4	Spatial	Domain 1
2*tds.z_cpos*F_const*cpos*((-tds.um_cposrr*d(tds.V,r)-tds.um_cposrz*d(tds.V,z))*test(cposr)+(-tds.um_cposzr*d(tds.V,r)-tds.um_cposzz*d(tds.V,z))*test(cposz))*pi*r	4	Spatial	Domain 1
2*tds.z_cneg*F_const*cneg*((-tds.um_cnegrr*d(tds.V,r)-tds.um_cnegrz*d(tds.V,z))*test(cnegr)+(-tds.um_cnegzr*d(tds.V,r)-tds.um_cnegzz*d(tds.V,z))*test(cnegz))*pi*r	4	Spatial	Domain 1
2*cpos*(tds.u*test(cposr)+tds.w*test(cposz))*(isScalingSystemDomain==0)*pi*r	4	Spatial	Domain 1
2*tds.cbf_cpos*test(cpos)*pi*r	4	Spatial	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139,

Weak expression	Integration order	Integration frame	Selection
			143–196
2*cneg*(tds.u*test(cnegr)+tds.w*test(cnegz))*(isScalingSystemDomain==0)*pi*r	4	Spatial	Domain 1
2*tds.cbf_cneg*test(cneg)*pi*r	4	Spatial	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196
2*tds.streamline*(isScalingSystemDomain==0)*pi*r	4	Spatial	Domain 1
2*tds.crosswind*(isScalingSystemDomain==0)*pi*r	6	Spatial	Domain 1

2.4.4 Axial Symmetry

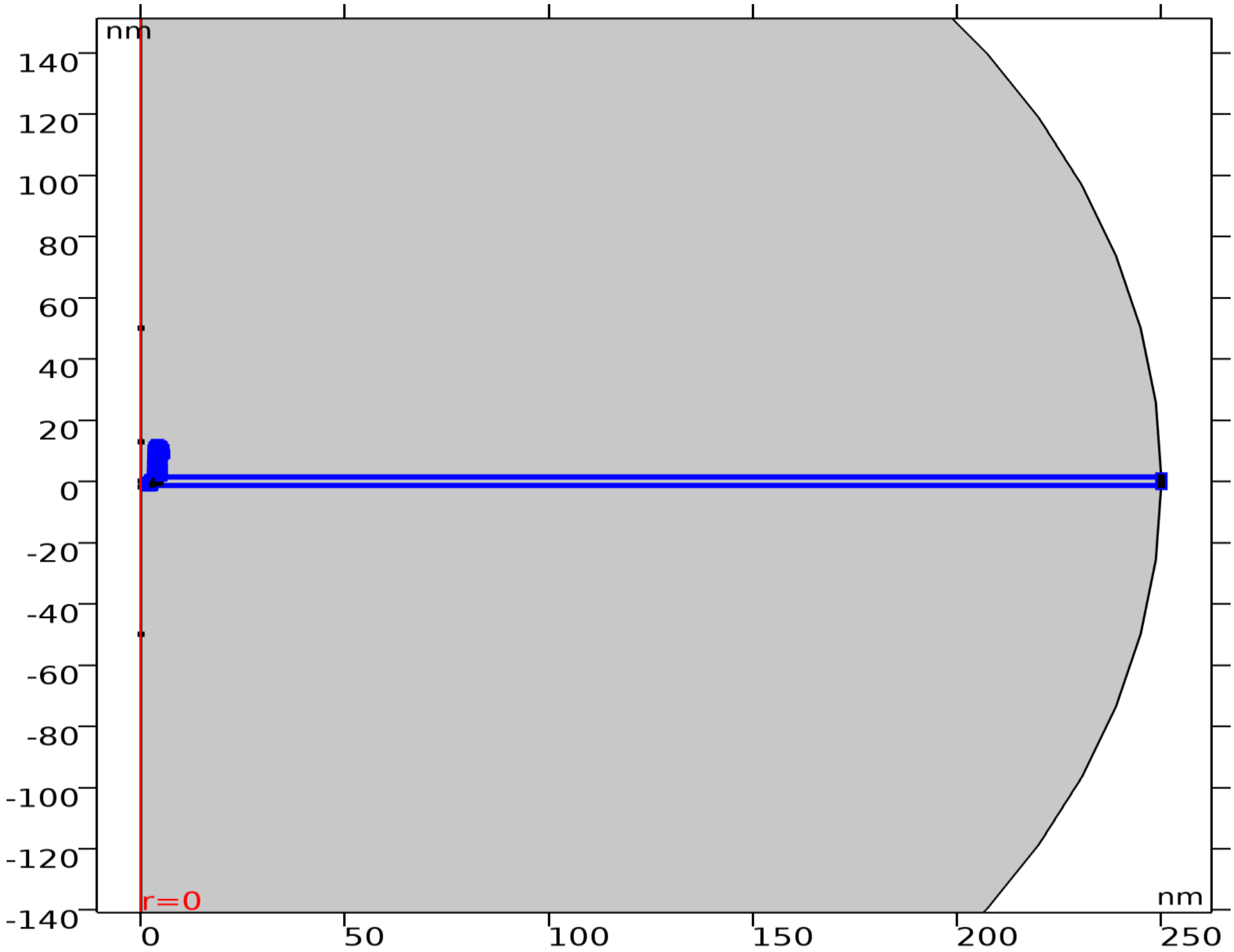


Axial Symmetry

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1–6

2.4.5 No Flux



No Flux

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194

EQUATIONS

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

Convection

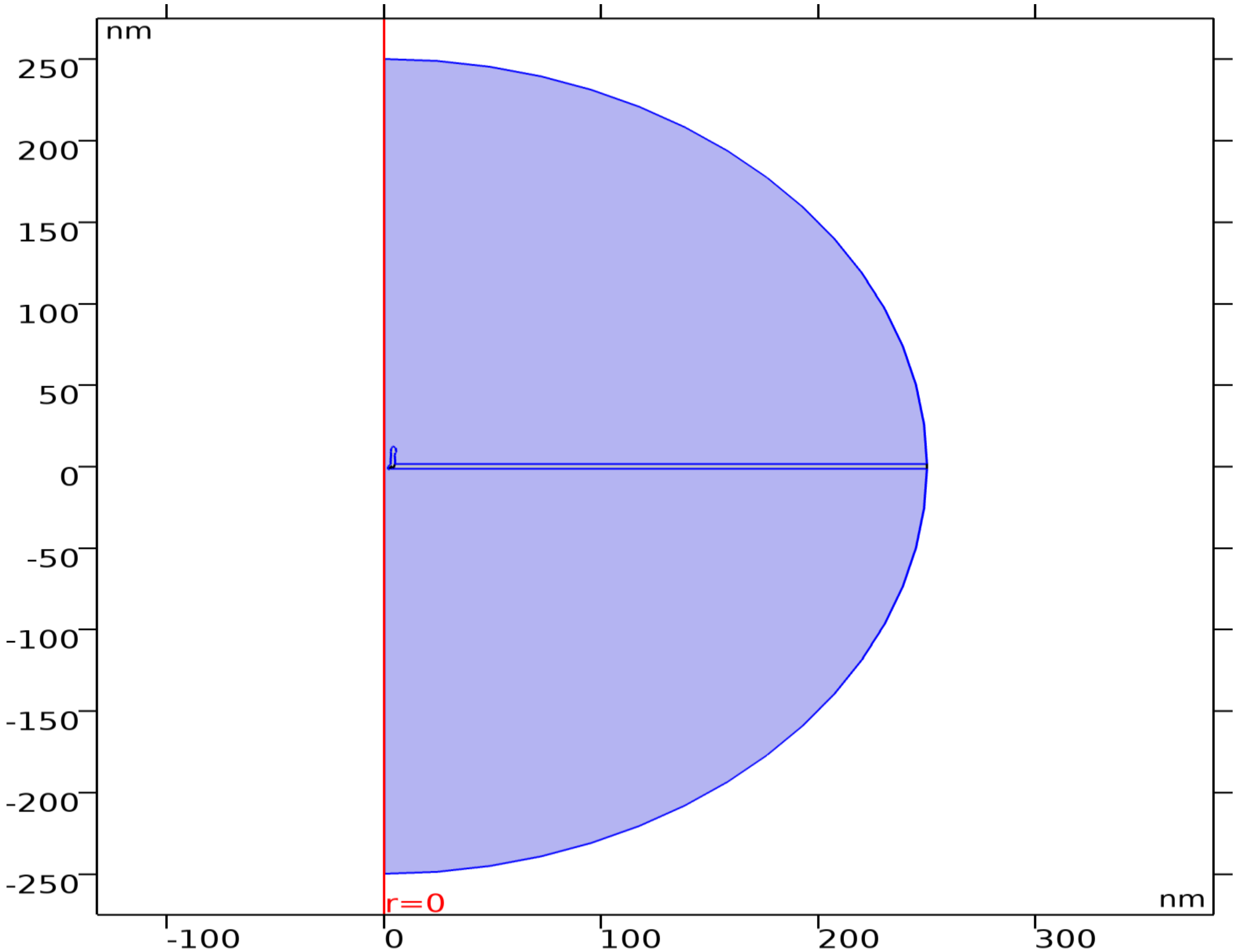
SETTINGS

Description	Value
Include	Off

Variables

Name	Expression	Unit	Description	Selection
tds.cbf_cpos	cpos*(-tds.u*tds.nrmesh-tds.v*tds.nphimesh-tds.w*tds.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194
tds.cbf_cneg	cneg*(-tds.u*tds.nrmesh-tds.v*tds.nphimesh-tds.w*tds.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194

2.4.6 Initial Values



Initial Values

SELECTION

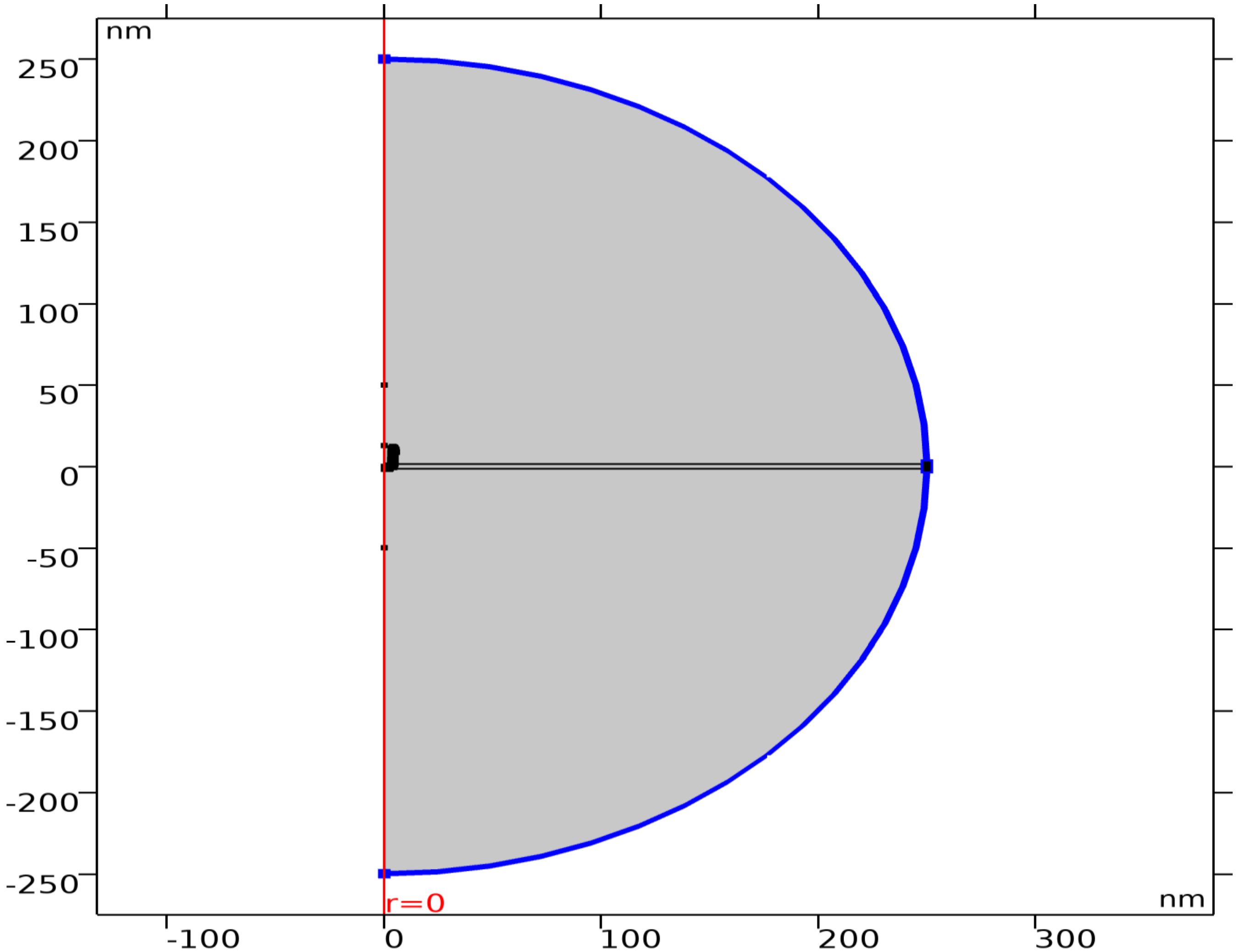
Geometric entity level	Domain
Selection	Domain 1

Initial values

SETTINGS

Description	**Value**
Concentration	{cpos_init, cneg_init}

2.4.7 Concentration



Concentration

SELECTION

Geometric entity level	Boundary
Name	Reservoir exterior boundary
Selection	Boundaries 195–196

EQUATIONS

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

Concentration

SETTINGS

Description	**Value**
Species cpos	On

Description	Value
Species cneg	On
Concentration	{if(z<0, c_trans, c_cis), if(z<0, c_trans, c_cis)}

Constraint settings

SETTINGS

Description	Value
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off
Constraint method	Elemental

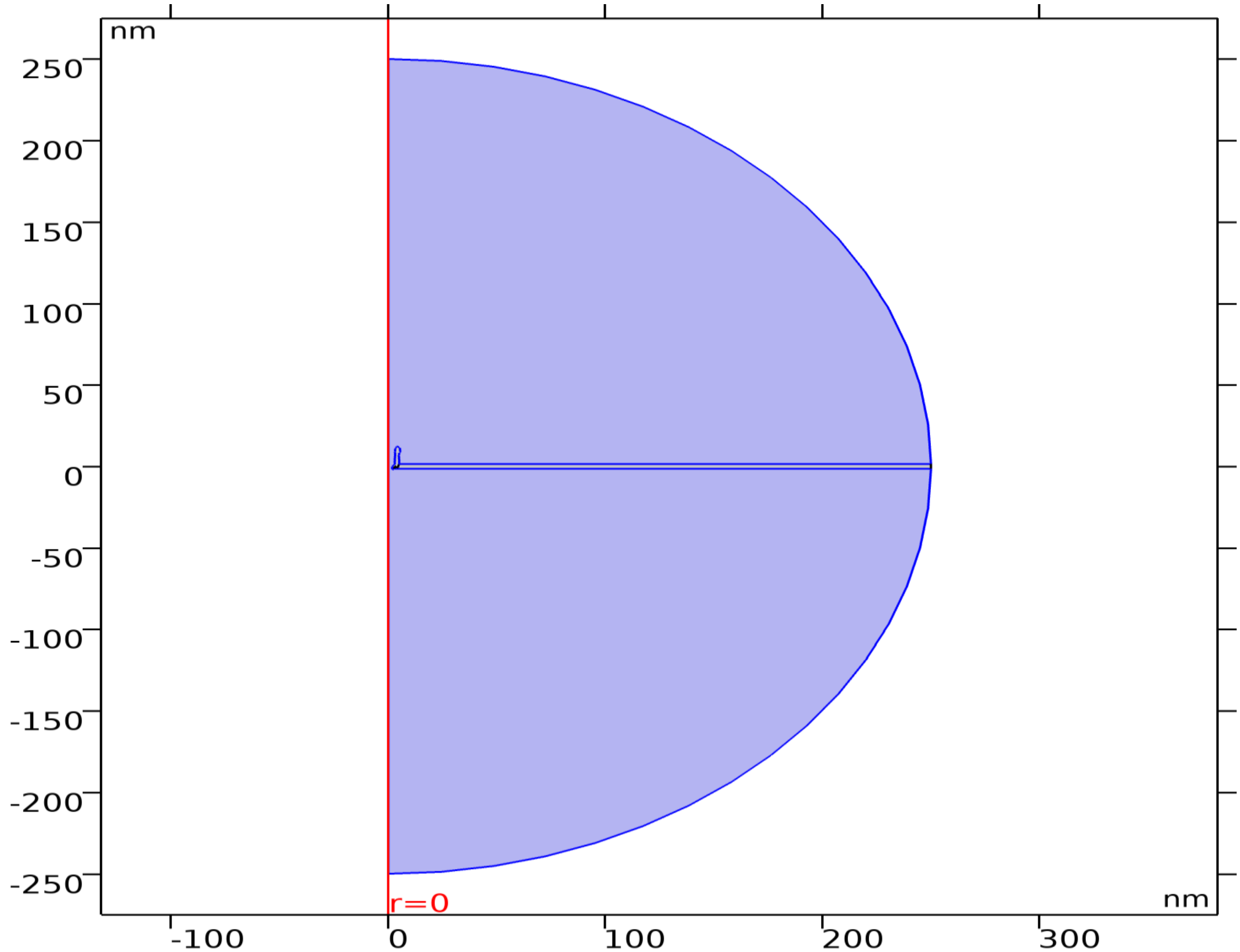
Variables

Name	Expression	Unit	Description	Selection
tds.c0_cpos	if(z<0,c_trans,c_cis)	mol/m³	Concentration	Boundaries 195–196
tds.c0_cneg	if(z<0,c_trans,c_cis)	mol/m³	Concentration	Boundaries 195–196

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-cpos+tds.c0_cpos	test(-cpos+tds.c0_cpos)	Lagrange (Quadratic)	Boundaries 195–196	Elemental
-cneg+tds.c0_cneg	test(-cneg+tds.c0_cneg)	Lagrange (Quadratic)	Boundaries 195–196	Elemental

2.4.8 Steric Flux Vector (cpos)



Steric Flux Vector (cpos)

SELECTION

Geometric entity level	Domain
Selection	Domain 1

Weak contribution

SETTINGS

Description	Value
Weak expression	smp.enable*smp.alpha_cpos*cpos*(smp.rad3_cpos*((-tds.D_cposrr*cposr - tds.D_cposrz*cposz)*test(cposr) + (-tds.D_cposzr*cposr - tds.D_cposzz*cposz)*test(cposz)) + smp.rad3_cneg*((-tds.D_cposrr*cnegr - tds.D_cposrz*cnegz)*test(cposr) + (-tds.D_cposzr*cnegr - tds.D_cposzz*cnegz)*test(cposz)))

Quadrature settings

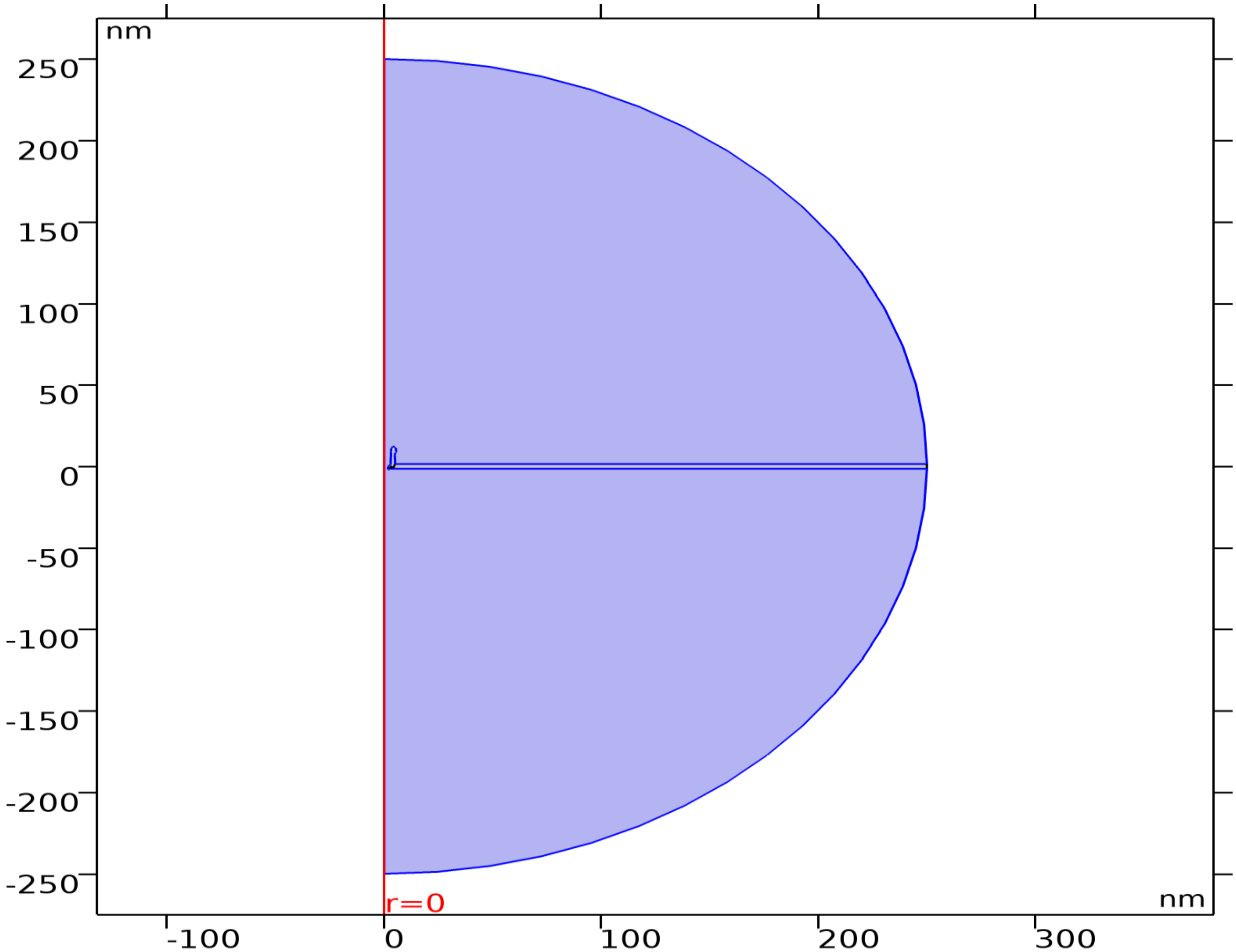
SETTINGS

Description	Value
Use automatic quadrature settings	On

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*smp.enable*smp.alpha_cpos*cpos*(smp.rad3_cpos*((-tds.D_cposrr*cposr-tds.D_cposrz*cposz)*test(cposr)+(-tds.D_cposzr*cposr-tds.D_cposzz*cposz)*test(cposz))+smp.rad3_cneg*((-tds.D_cposrr*cnegr-tds.D_cposrz*cnegz)*test(cposr)+(-tds.D_cposzr*cnegr-tds.D_cposzz*cnegz)*test(cposz)))*pi*r	4	Spatial	Domain 1

2.4.9 Steric Flux Vector (cneg)



Steric Flux Vector (cneg)

SELECTION

Geometric entity level	Domain
Selection	Domain 1

Weak contribution

SETTINGS

Description	**Value**
Weak expression	smp.enable*smp.alpha_cneg*cneg*(smp.rad3_cpos*((-tds.D_cnegrr*cposr - tds.D_cnegrz*cposz)*test(cnegr) + (-tds.D_cnegzr*cposr - tds.D_cnegzz*cposz)*test(cnegz)) + smp.rad3_cneg*((-tds.D_cnegrr*cnegr - tds.D_cnegrz*cnegz)*test(cnegr) + (-tds.D_cnegzr*cnegr - tds.D_cnegzz*cnegz)*test(cnegz)))

Quadrature settings

SETTINGS

Description	Value
Use automatic quadrature settings	On

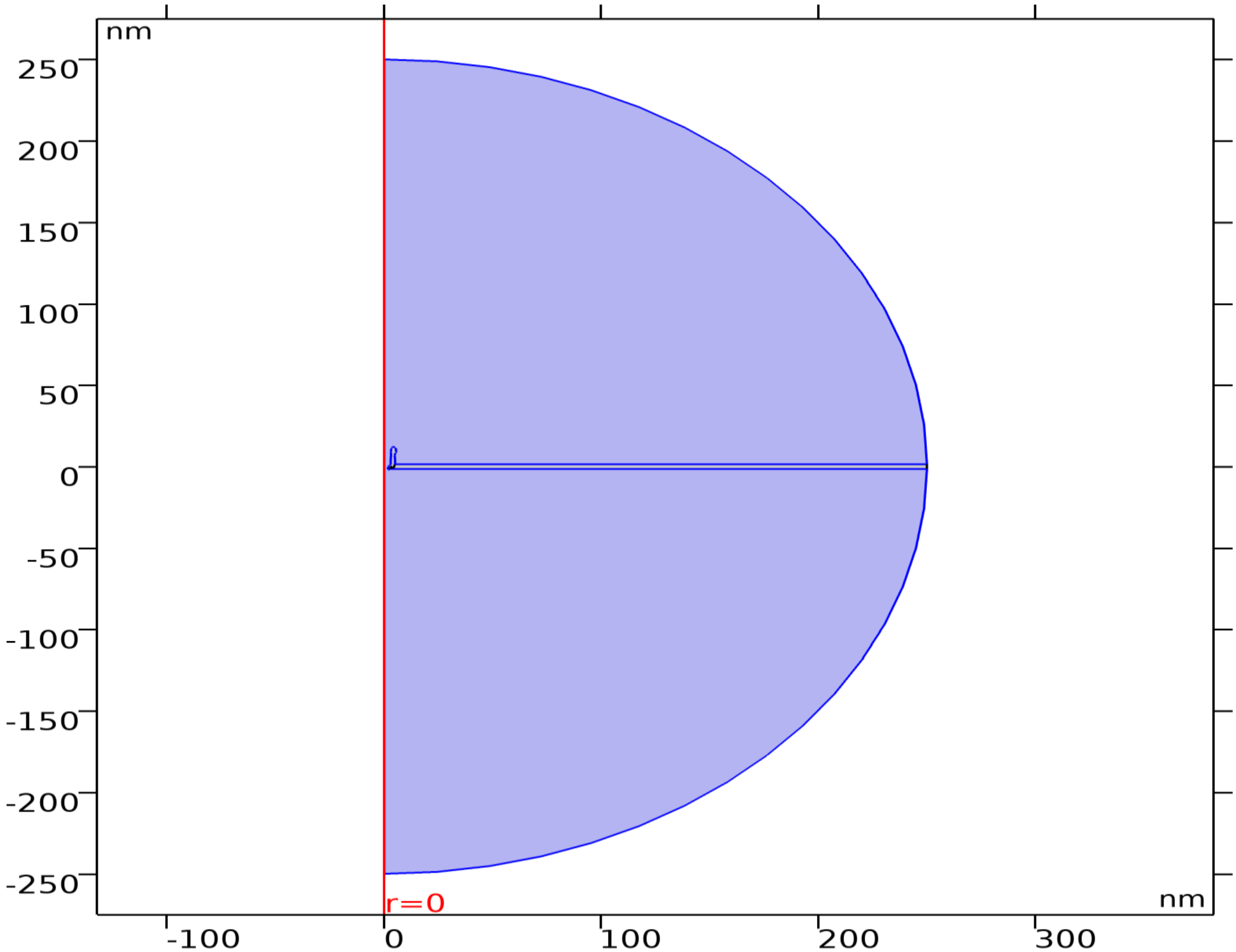
Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*smp.enable*smp.alpha_cneg*cneg*(smp.rad3_cpos*((-tds.D_cnegrr*cposr-tds.D_cnegrz*cposz)*test(cnegr)+(-tds.D_cnegzr*cposr-tds.D_cnegzz*cposz)*test(cnegz))+smp.rad3_cneg*((-tds.D_cnegrr*cnegr-tds.D_cnegrz*cnegz)*test(cnegr)+(-tds.D_cnegzr*cnegr-tds.D_cnegzz*cnegz)*test(cnegz)))*pi*r	4	Spatial	Domain 1

2.5 LAMINAR FLOW

USED PRODUCTS

COMSOL Multiphysics



Laminar Flow

SELECTION

Geometric entity level	Domain
Name	Reservoir
Selection	Domain 1

EQUATIONS

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mathbf{K}]+\mathbf{F}$$
$$\rho\nabla\cdot(\mathbf{u}) = 0$$
$$\mathbf{K} = \mu\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T}\right)$$

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
Enable porous media domains	Off
Reference temperature	User defined
Reference temperature	T_system
Reference pressure level	1[atm]

Turbulence

SETTINGS

Description	Value
Turbulence model type	None

Consistent stabilization

SETTINGS

Description	Value
Streamline diffusion	On
Crosswind diffusion	On

Inconsistent stabilization

SETTINGS

Description	Value
Isotropic diffusion	Off

Advanced settings

SETTINGS

Description	Value
Use pseudo time stepping for stationary equation form	Automatic from physics
CFL number expression	Automatic

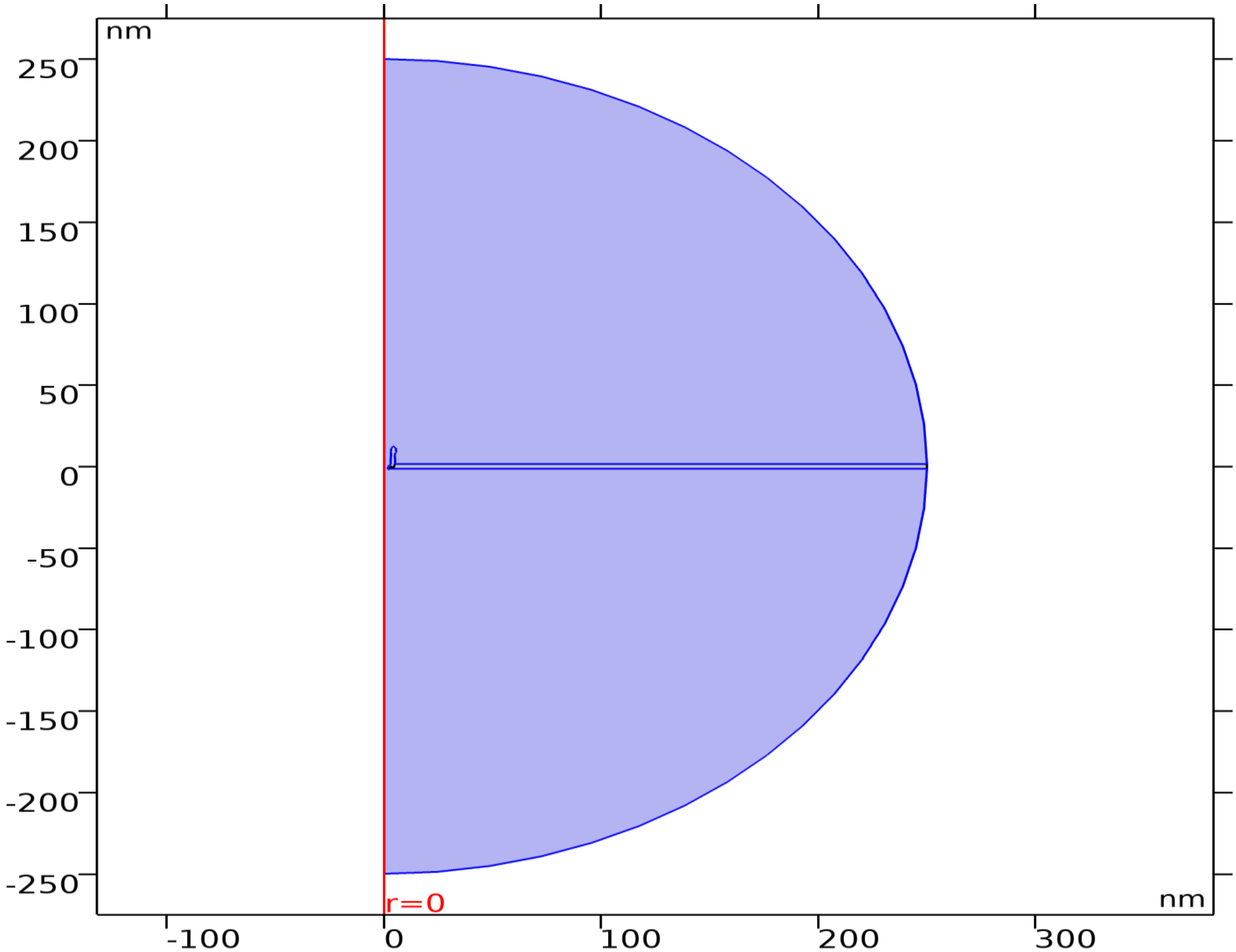
2.5.2 Variables

Name	Expression	Unit	Description	Selection	Details
spf.Tref	model.input.Tref	K	Reference	Global	Meta

Name	Expression	Unit	Description	Selection	Details
			temperature		
spf.dz	1	m	Thickness	Domain 1	
spf.pref	1[atm]	Pa	Reference pressure level	Domain 1	
spf.pA	p+spf.pref	Pa	Absolute pressure	Domain 1	
spf.hasWF	0		Help variable	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
spf.usePseudoTimeStepping	0	1	Help variable	Global	+ operation
spf.localCFLvalue	1.3^min(niterCMP,9)+if(niterCMP>=25,9*1.3^min(-25+niterCMP,9),0)+if(niterCMP>=45,90*1.3^min(-45+niterCMP,9),0)		Local CFL number	Domain 1	
spf.locCFL	CFLCMP	1	Local CFL number	Domain 1	
spf.geometryLengthScale	6.250000000000002E-8	m	Geometry length scale	Domain 1	
spf.time_step_inv	max(sqrt(emetric_spatial(u,w)*2^gmg_level^2),spf.nu/spf.geometryLengthScale^2)	Hz	Inverse time step	Domain 1	
spf.tsti	nojac(spf.time_step_inv/spf.locCFL)	1/s	Help variable	Domain 1	
spf.nr	dnr	1	Normal vector, r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	

Name	Expression	Unit	Description	Selection	Details
spf.nphi	0	1	Normal vector, phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
spf.nz	dnz	1	Normal vector, z component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
spf.nrmesh	dnrmesh	1	Normal vector, r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
spf.nphimesh	0	1	Normal vector, phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
spf.nzmesh	dnzmesh	1	Normal vector, z component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	

2.5.3 Fluid Properties



Fluid Properties

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I}+\mathbf{K}]+\mathbf{F}$$
$$\rho\nabla\cdot(\mathbf{u}) = 0$$
$$\mathbf{K} = \mu\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}\right)$$

Fluid properties

SETTINGS

Description	Value

Description	Value
Density	User defined
Density	rho
Dynamic viscosity	User defined
Dynamic viscosity	eta

Variables

Name	Expression	Unit	Description	Selection	Details
spf.Fr	0	N/m³	Volume force, r component	Domain 1	+ operation
spf.Fphi	0	N/m³	Volume force, phi component	Domain 1	+ operation
spf.Fz	0	N/m³	Volume force, z component	Domain 1	+ operation
spf.rho	material.rho	kg/m³	Density	Domain 1	Meta
spf.mu	material.mu	Pa·s	Dynamic viscosity	Domain 1	Meta
spf.Trho	spf.fp1.minput_temperature	K	Temperature for density evaluation	Domain 1	
spf.prho	spf.fp1.minput_pressure	Pa	Pressure for the evaluation of density	Domain 1	
spf.rhoref	subst(material.rho,spf.fp1.minput_temperature,spf.Tref,spf.fp1.minput_pressure,spf.pref)	kg/m³	Reference density	Domain 1	Meta
spf.mumat	material.mu	Pa·s	Dynamic viscosity	Domain 1	Meta
spf.srijrr	ur	1/s	Strain rate tensor, rr component	Domain 1	
spf.srijphir	0	1/s	Strain rate tensor, phir component	Domain 1	
spf.srijzr	0.5*(wr+uz)	1/s	Strain rate tensor, zr component	Domain 1	
spf.srijrphi	0	1/s	Strain rate tensor, rphi component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
spf.srijphiphi	if(abs(r)<0.001*h_spatial,ur,u/r)	1/s	Strain rate tensor, phiphi component	Domain 1	
spf.srijzphi	0	1/s	Strain rate tensor, zphi component	Domain 1	
spf.srijrz	0.5*(uz+wr)	1/s	Strain rate tensor, rz component	Domain 1	
spf.srijphiz	0	1/s	Strain rate tensor, phiz component	Domain 1	
spf.srijzz	wz	1/s	Strain rate tensor, zz component	Domain 1	
spf.srijmeanrr	0.5*root.comp1.spf.elemint(2*ur)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, rr component	Domain 1	
spf.srijmeanphir	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, phir component	Domain 1	
spf.srijmeanzr	0.5*root.comp1.spf.elemint(wr+uz)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zr component	Domain 1	
spf.srijmeanrphi	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, rphi component	Domain 1	
spf.srijmeanphiphi	0.5*root.comp1.spf.elemint(2*if(abs(r)<0.001*h_spatial,ur,u/r))/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, phiphi component	Domain 1	
spf.srijmeanzphi	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zphi component	Domain 1	
spf.srijmeanrz	0.5*root.comp1.spf.elemint(uz+wr)/root.comp1.spf.ele	1/s	Strain rate tensor, rz component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	mint(1)				
spf.srijmeanphiz	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, phiz component	Domain 1	
spf.srijmeanzz	0.5*root.comp1.spf.elemint(2*wz)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zz component	Domain 1	
spf.rrijrr	0	1/s	Rotation rate tensor, rr component	Domain 1	
spf.rrijphir	0	1/s	Rotation rate tensor, phir component	Domain 1	
spf.rrijzr	0.5*(wr-uz)	1/s	Rotation rate tensor, zr component	Domain 1	
spf.rrijrphi	0	1/s	Rotation rate tensor, rphi component	Domain 1	
spf.rrijphiphi	0	1/s	Rotation rate tensor, phiphi component	Domain 1	
spf.rrijzphi	0	1/s	Rotation rate tensor, zphi component	Domain 1	
spf.rrijrz	0.5*(uz-wr)	1/s	Rotation rate tensor, rz component	Domain 1	
spf.rrijphiz	0	1/s	Rotation rate tensor, phiz component	Domain 1	
spf.rrijzz	0	1/s	Rotation rate tensor, zz component	Domain 1	
spf.sr	sqrt(2*spf.srijrr^2+2*spf.srijrphi^2+2*spf.srijrz^2+2*spf.srijphir^2+2*spf.srijphiphi^2+2*spf.srijphiz^2+2*spf.srijzr^2+2*spf.	1/s	Shear rate	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	srijzphi^2+2*spf.srijzz^2+eps)				
spf.divu	d(spf.rho*u,r)+spf.rho*if(abs(r)<0.001*h,d(u,r),u/r)+d(spf.rho*w,z)-u*d(spf.rho,r)-w*d(spf.rho,z)	1/s	Divergence of velocity field	Domain 1	
spf.U	sqrt(u^2+w^2)	m/s	Velocity magnitude	Domain 1	
spf.vorticityr	0	1/s	Vorticity field, r component	Domain 1	
spf.vorticityphi	-wr+uz	1/s	Vorticity field, phi component	Domain 1	
spf.vorticityz	0	1/s	Vorticity field, z component	Domain 1	
spf.vort_magn	sqrt(spf.vorticityr^2+spf.vorticityphi^2+spf.vorticityz^2)	1/s	Vorticity magnitude	Domain 1	
spf.cellRe	0.25*spf.rho*sqrt(emetric_spatial(u-d(r,TIME),w-d(z,TIME))/emetric2_spatial)/spf.mu	1	Cell Reynolds number	Domain 1	
spf.nu	spf.mu/spf.rho	m^2/s	Kinematic viscosity	Domain 1	
spf.betaT	0	1/Pa	Isothermal compressibility coefficient	Domain 1	
spf.Qm	0	$kg/(m^3 \cdot s)$	Source term	Domain 1	+ operation
spf.Fgtotr	0	N/m^3	Gravity force, r component	Domain 1	+ operation
spf.Fgtotphi	0	N/m^3	Gravity force, phi component	Domain 1	+ operation
spf.Fgtotz	0	N/m^3	Gravity force, z component	Domain 1	+ operation
spf.mu_eff	spf.mu+spf.muT	Pa·s	Dynamic viscosity	Domain 1	
spf.muT	0	Pa·s	Turbulent dynamic viscosity	Domain 1	

Name	Expression	Unit	Description	Selection	Details
spf.T_stressr	spf.K_stressr-p*spf.nrmesh	N/m²	Total stress, r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	+ operation
spf.T_stressphi	spf.K_stressphi-p*spf.nphimesh	N/m²	Total stress, phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	+ operation
spf.T_stressz	spf.K_stressz-p*spf.nzmesh	N/m²	Total stress, z component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	+ operation
spf.K_stressr	spf.mu_eff*(2*ur*spf.nrmesh+(uz+wr)*spf.nzmesh)	N/m²	Viscous stress, r component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	+ operation
spf.K_stressphi	2*spf.mu_eff*if(abs(r)<0.001*h_spatial,ur,u/r)*spf.nphimesh	N/m²	Viscous stress, phi component	Boundaries 1–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	+ operation
spf.K_stressz	spf.mu_eff*((wr+u	N/m²	Viscous stress, z	Boundaries 1–	+ operation

Name	Expression	Unit	Description	Selection	Details
	z)*spf.nrmesh+2*wz*spf.nzmesh)		component	28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–196	
spf.K_stress_tensorrr	2*spf.mu_eff*ur	N/m²	Viscous stress tensor, rr component	Domain 1	+ operation
spf.K_stress_tensorphir	0	N/m²	Viscous stress tensor, phir component	Domain 1	+ operation
spf.K_stress_tensorzr	spf.mu_eff*(wr+uz)	N/m²	Viscous stress tensor, zr component	Domain 1	+ operation
spf.K_stress_tensorrphi	0	N/m²	Viscous stress tensor, rphi component	Domain 1	+ operation
spf.K_stress_tensorphiphi	2*spf.mu_eff*if(abs(r)<0.001*h_spatial,ur,u/r)	N/m²	Viscous stress tensor, phiphi component	Domain 1	+ operation
spf.K_stress_tensorzphi	0	N/m²	Viscous stress tensor, zphi component	Domain 1	+ operation
spf.K_stress_tensorrz	spf.mu_eff*(uz+wr)	N/m²	Viscous stress tensor, rz component	Domain 1	+ operation
spf.K_stress_tensorphiz	0	N/m²	Viscous stress tensor, phiz component	Domain 1	+ operation
spf.K_stress_tensorzz	2*spf.mu_eff*wz	N/m²	Viscous stress tensor, zz component	Domain 1	+ operation
spf.K_stress_tensor_testrr	2*spf.mu_eff*test(ur)	N/m²	Viscous stress tensor test, rr component	Domain 1	+ operation
spf.K_stress_tensor_testphir	0	N/m²	Viscous stress tensor test, phir component	Domain 1	+ operation
spf.K_stress_tensor_testzr	spf.mu_eff*(test(wr)+test(uz))	N/m²	Viscous stress tensor test, zr	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			component		
spf.K_stress_tensor_testrphi	0	N/m²	Viscous stress tensor test, rphi component	Domain 1	+ operation
spf.K_stress_tensor_testphiphi	2*spf.mu_eff*if(abs(r)<0.001*h_spatial,test(ur),test(u)/r)	N/m²	Viscous stress tensor test, phiphi component	Domain 1	+ operation
spf.K_stress_tensor_testzphi	0	N/m²	Viscous stress tensor test, zphi component	Domain 1	+ operation
spf.K_stress_tensor_testrz	spf.mu_eff*(test(uz)+test(wr))	N/m²	Viscous stress tensor test, rz component	Domain 1	+ operation
spf.K_stress_tensor_testphiz	0	N/m²	Viscous stress tensor test, phiz component	Domain 1	+ operation
spf.K_stress_tensor_testzz	2*spf.mu_eff*test(wz)	N/m²	Viscous stress tensor test, zz component	Domain 1	+ operation
spf.upwind_helpr	u-d(r,TIME)	m/s	Upwind term, r component	Domain 1	+ operation
spf.upwind_helpphi	0	m/s	Upwind term, phi component	Domain 1	+ operation
spf.upwind_helpz	w-d(z,TIME)	m/s	Upwind term, z component	Domain 1	+ operation
spf.tau_vdrr	2*spf.mu*spf.srijrr	Pa	Viscous stress tensor, rr component	Domain 1	+ operation
spf.tau_vdphir	2*spf.mu*spf.srijphir	Pa	Viscous stress tensor, phir component	Domain 1	+ operation
spf.tau_vdzr	2*spf.mu*spf.srijzr	Pa	Viscous stress tensor, zr component	Domain 1	+ operation
spf.tau_vdrphi	2*spf.mu*spf.srijrphi	Pa	Viscous stress tensor, rphi component	Domain 1	+ operation
spf.tau_vdphiphi	2*spf.mu*spf.srijphiphi	Pa	Viscous stress tensor, phiphi component	Domain 1	+ operation
spf.tau_vdzphi	2*spf.mu*spf.srijz	Pa	Viscous stress	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	phi		tensor, zphi component		
spf.tau_vdrz	2*spf.mu*spf.srijrz	Pa	Viscous stress tensor, rz component	Domain 1	+ operation
spf.tau_vdphiz	2*spf.mu*spf.srijphiz	Pa	Viscous stress tensor, phiz component	Domain 1	+ operation
spf.tau_vdzz	2*spf.mu*spf.srijzz	Pa	Viscous stress tensor, zz component	Domain 1	+ operation
spf.Qvd	spf.tau_vdrr*ur+spf.tau_vdrz*uz+spf.tau_vdphiphi*if(abs(r)<0.001*h_spatial,ur,u/r)+spf.tau_vdzr*wr+spf.tau_vdzz*wz	W/m³	Viscous dissipation	Domain 1	+ operation
spf.epsilon_p	1	1	Porosity	Domain 1	
spf.Fst_tensorrr	0	N/m²	Surface tension force, rr component	Domain 1	+ operation
spf.Fst_tensorphir	0	N/m²	Surface tension force, phir component	Domain 1	+ operation
spf.Fst_tensorzr	0	N/m²	Surface tension force, zr component	Domain 1	+ operation
spf.Fst_tensorrphi	0	N/m²	Surface tension force, rphi component	Domain 1	+ operation
spf.Fst_tensorphiphi	0	N/m²	Surface tension force, phiphi component	Domain 1	+ operation
spf.Fst_tensorzphi	0	N/m²	Surface tension force, zphi component	Domain 1	+ operation
spf.Fst_tensorrz	0	N/m²	Surface tension force, rz component	Domain 1	+ operation
spf.Fst_tensorphiz	0	N/m²	Surface tension force, phiz component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
spf.Fst_tensorzz	0	N/m²	Surface tension force, zz component	Domain 1	+ operation
spf.continuityEquation	spf.divu	kg/(m³·s)	Continuity equation	Domain 1	
spf.contCoeff	spf.rho	kg/m³	Help variable	Domain 1	
spf.res_u	pr+spf.rho*u*ur+spf.rho*w*uz-(d(2*ur,r)+if(abs(r)<0.001*h_spatial,d(2*ur,r),2*ur/r)+d(uz+wr,z)-2*if(abs(r)<0.001*h_spatial,ur,u/r)/r)*spf.mu-spf.Fr	N/m³	Equation residual	Domain 1	
spf.res_v	-spf.Fphi	N/m³	Equation residual	Domain 1	
spf.res_w	spf.rho*u*wr+pz+spf.rho*w*wz-(d(wr+uz,r)+if(abs(r)<0.001*h_spatial,d(wr+uz,r),(wr+uz)/r)+d(2*wz,z))*spf.mu-spf.Fz	N/m³	Equation residual	Domain 1	
spf.res_p	spf.rho*spf.divu	kg/(m³·s)	Pressure equation residual	Domain 1	

Shape functions

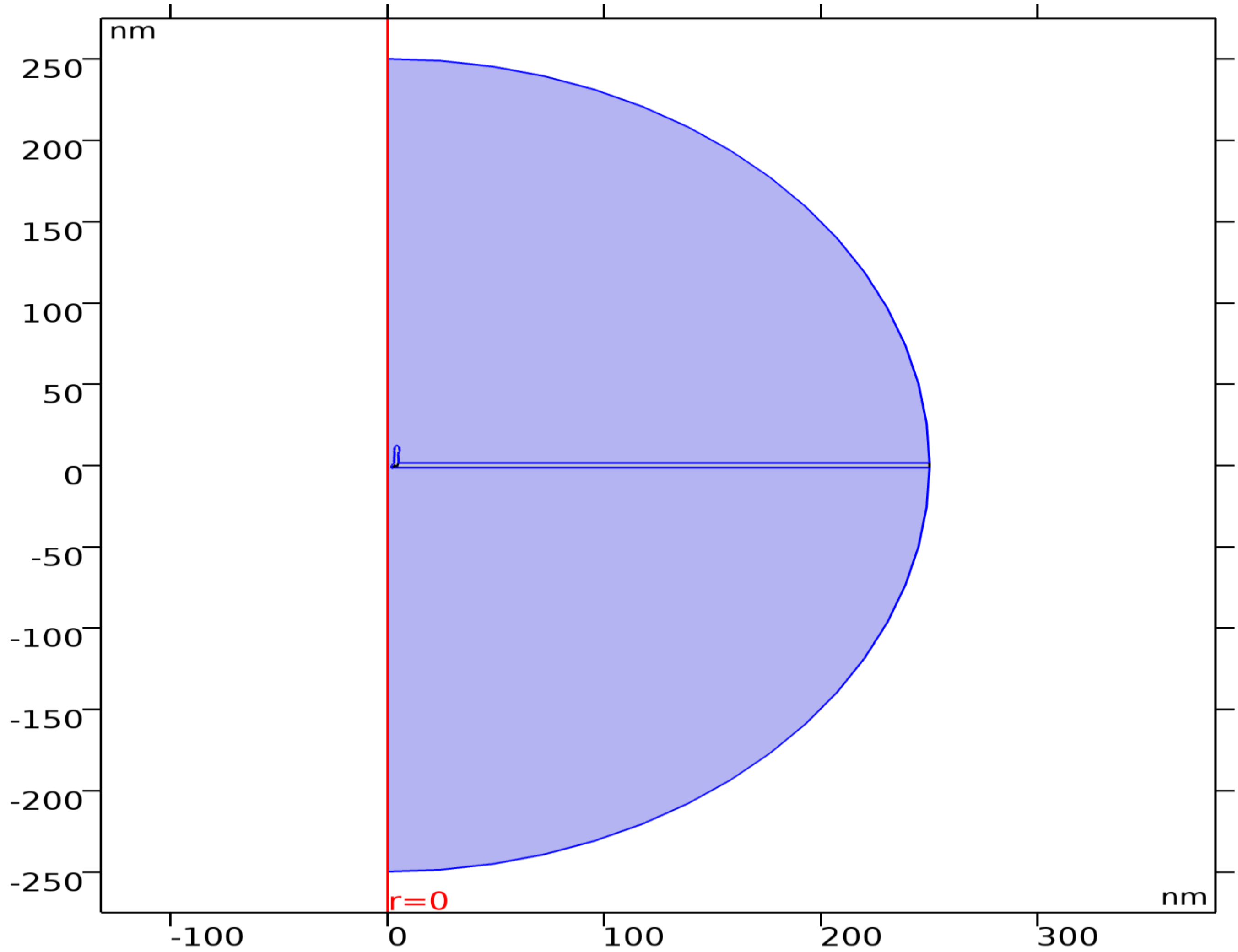
Name	Shape function	Unit	Description	Shape frame	Selection
u	Lagrange (Linear)	m/s	Velocity field, r component	Spatial	Domain 1
w	Lagrange (Linear)	m/s	Velocity field, z component	Spatial	Domain 1
p	Lagrange (Linear)	Pa	Pressure	Spatial	Domain 1

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*((p-spf.K_stress_tensorrr)*test(ur)-spf.K_stress_tensorrz*test(uz)+(p-spf.K_stress_tensorphiphi)*if(abs(r)<0.001*h_spatial,test(ur),test(u)/r)-spf.K_stress_tensorzr*test(wr)+(p-	2	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
spf.K_stress_tensorzz)*test(wz))*pi*r			
2*(spf.Fr*test(u)+spf.Fz*test(w))*pi*r	2	Spatial	Domain 1
2*(-(d(spf.rho*u,r)*u+d(spf.rho*u,z)*w)*test(u)-(d(spf.rho*w,r)*u+d(spf.rho*w,z)*w)*test(w))*pi*r	2	Spatial	Domain 1
-2*spf.continuityEquation*test(p)*pi*r	2	Spatial	Domain 1
2*spf.streamlinens*pi*r	2	Spatial	Domain 1
2*spf.crosswindns*pi*r	2	Spatial	Domain 1
2*(spf.usePseudoTimeStepping>0)*spf.rho*spf.tsti*(-(u-nojac(u))*test(u)-(w-nojac(w))*test(w))*pi*r	2	Spatial	Domain 1

2.5.4 Initial Values



Initial Values

SELECTION

Geometric entity level	Domain
Selection	Domain 1

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

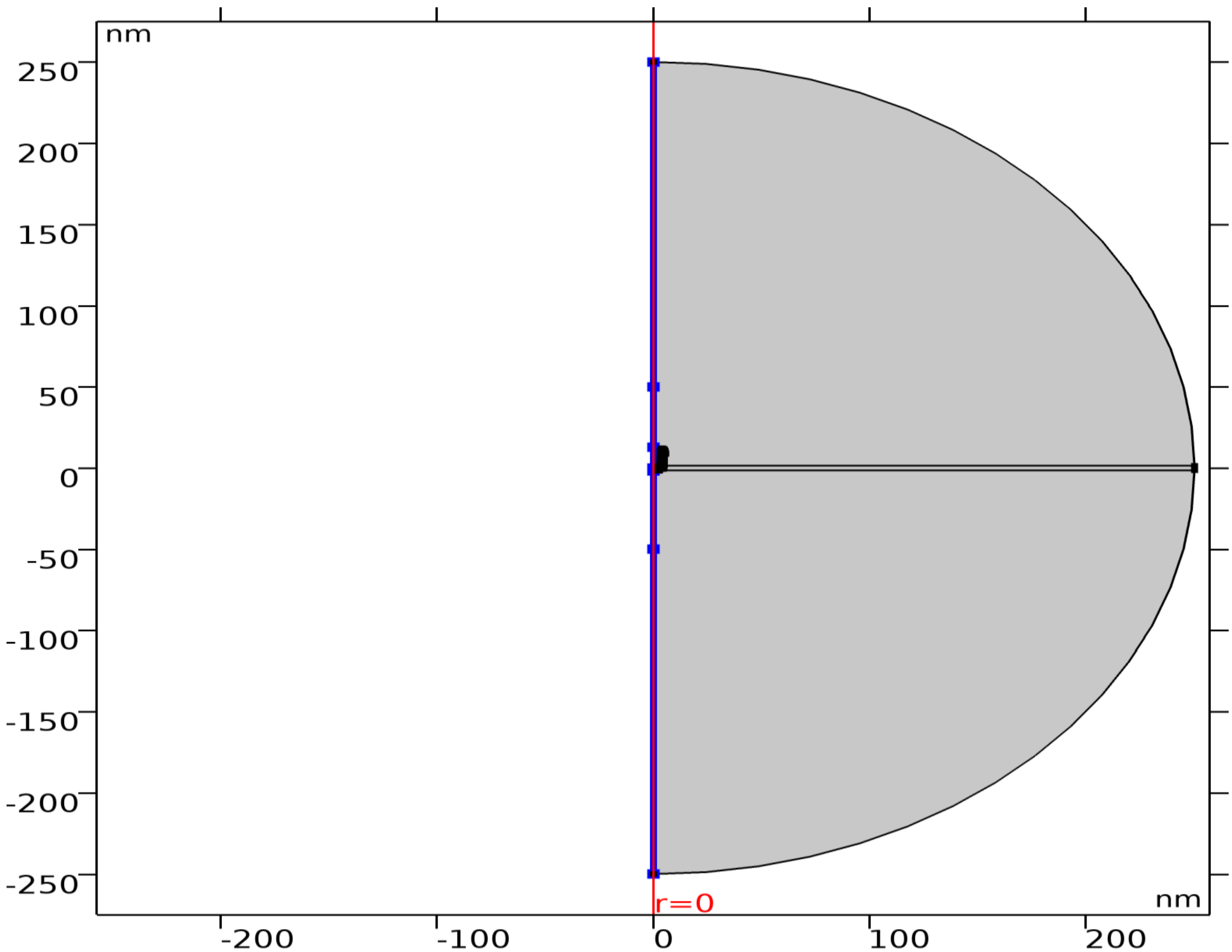
SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection
spf.u_initr	0	m/s	Velocity field, r component	Domain 1
spf.u_initphi	0	m/s	Velocity field, phi component	Domain 1
spf.u_initz	0	m/s	Velocity field, z component	Domain 1
spf.p_init	0	Pa	Pressure	Domain 1

2.5.5 Axial Symmetry



Axial Symmetry

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1–6

Constraint settings

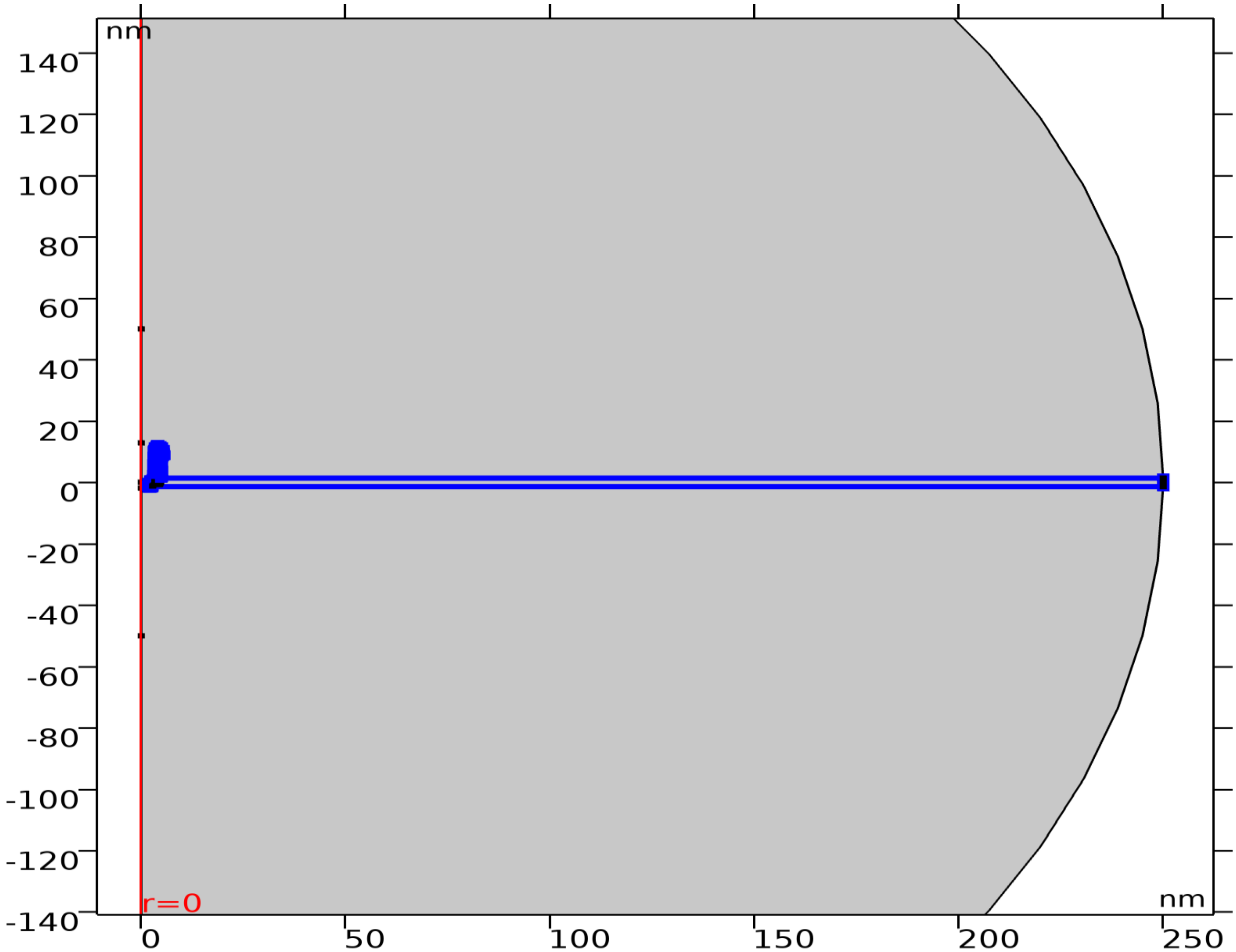
SETTINGS

Description	Value
Apply reaction terms on	All physics (symmetric)
Constraint method	Elemental

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-u	test(-u)	Lagrange (Linear)	Boundaries 1–6	Elemental

2.5.6 Wall



Wall

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194

EQUATIONS

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

Boundary condition

SETTINGS

Description	Value
Wall condition	No slip

Wall movement

SETTINGS

Description	Value
Translational velocity	Automatic from frame
Sliding wall	Off

Constraint settings

SETTINGS

Description	Value
Apply reaction terms on	Individual dependent variables
Use weak constraints	Off
Constraint method	Elemental

Variables

Name	Expression	Unit	Description	Selection	Details
spf.ubndr	0	m/s	Velocity at boundary, r component	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	+ operation
spf.ubndphi	0	m/s	Velocity at boundary, phi component	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	+ operation
spf.ubndz	0	m/s	Velocity at boundary, z component	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	+ operation
spf.uLeakager	0	m/s	Leakage	Boundaries 7–	+ operation

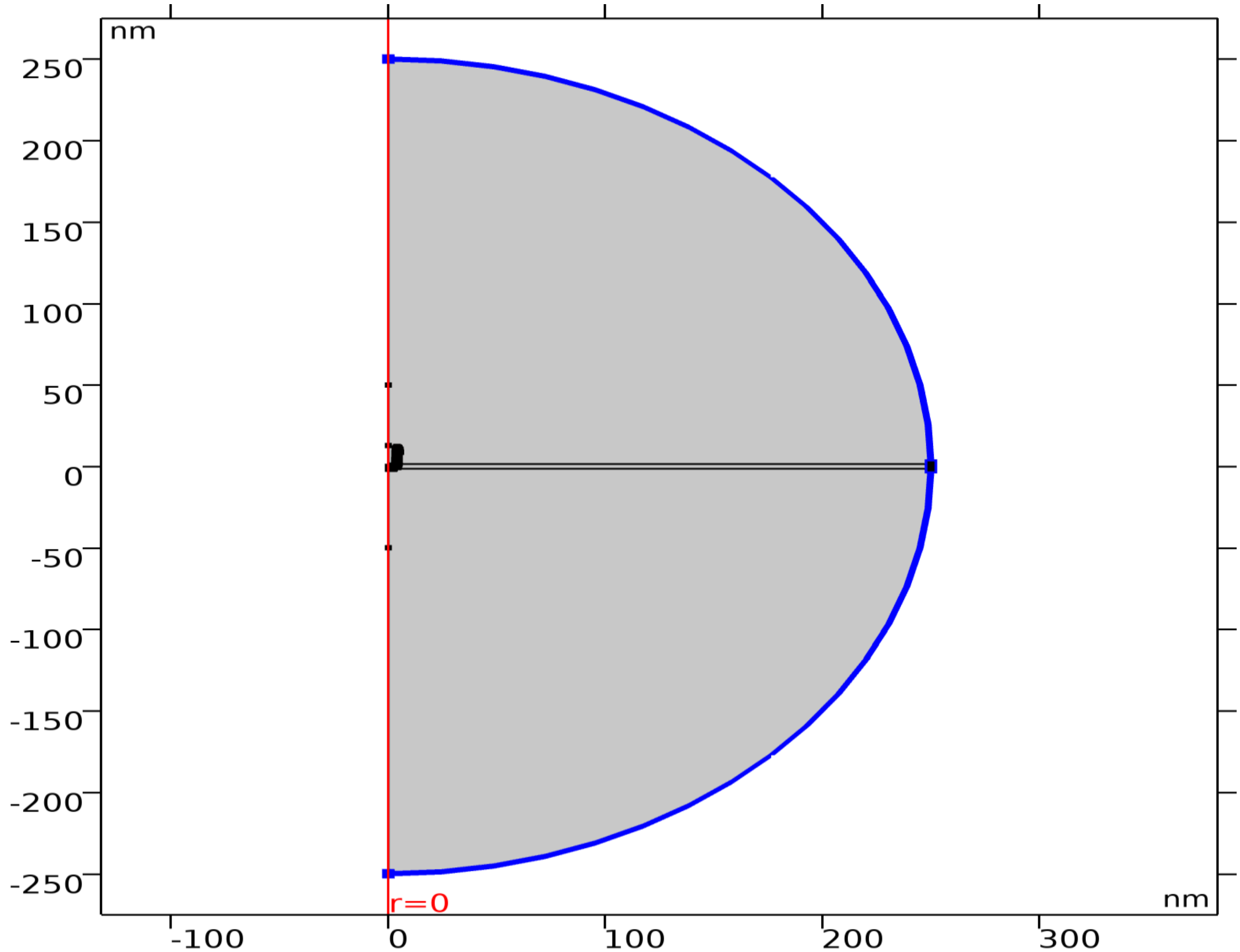
Name	Expression	Unit	Description	Selection	Details
			velocity, r component	28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	
spf.uLeakagephi	0	m/s	Leakage velocity, phi component	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	+ operation
spf.uLeakagez	0	m/s	Leakage velocity, z component	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	+ operation
spf.noSlipWall	1	1	Help variable	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-u+spf.ubndr+spf.uLeakager	test(-u)	Lagrange (Linear)	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134,	Elemental

Constraint	Constraint force	Shape function	Selection	Details
			136–139, 143–194	
spf.ubndphi+spf.uLeakagephi	0		Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	Elemental
-w+spf.ubndz+spf.uLeakagez	test(-w)	Lagrange (Linear)	Boundaries 7–28, 30, 32, 37–65, 67–69, 73–78, 80–91, 93–99, 104–107, 109–111, 114–121, 134, 136–139, 143–194	Elemental

2.5.7 Open Boundary



Open Boundary

SELECTION

Geometric entity level	Boundary
Name	Reservoir exterior boundary
Selection	Boundaries 195–196

EQUATIONS

$$[-p\mathbf{I} + \mathbf{K}]\mathbf{n} = -f_0\mathbf{n}$$

Boundary condition

SETTINGS

Description	**Value**
Boundary condition	Normal stress

Description	Value
Normal stress	0

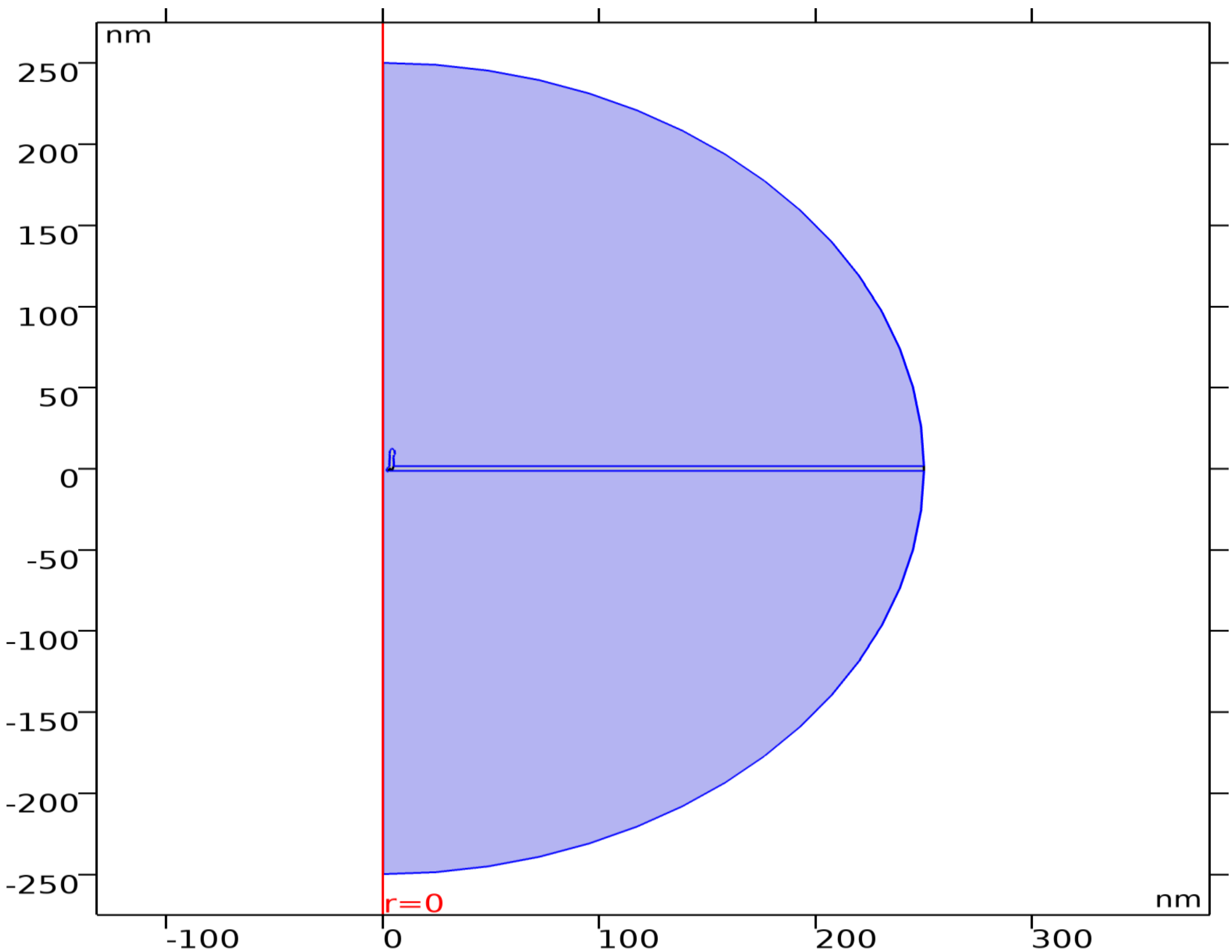
Variables

Name	Expression	Unit	Description	Selection
spf.f0	0	N/m²	Normal stress	Boundaries 195–196

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-2*spf.f0*(test(u)*spf.nrmesh+test(w)*spf.nzmesh)*pi*r	2	Spatial	Boundaries 195–196

2.5.8 Body Force (scd_ions)



Body Force (scd_ions)

SELECTION

Geometric entity level	Domain
Selection	Domain 1

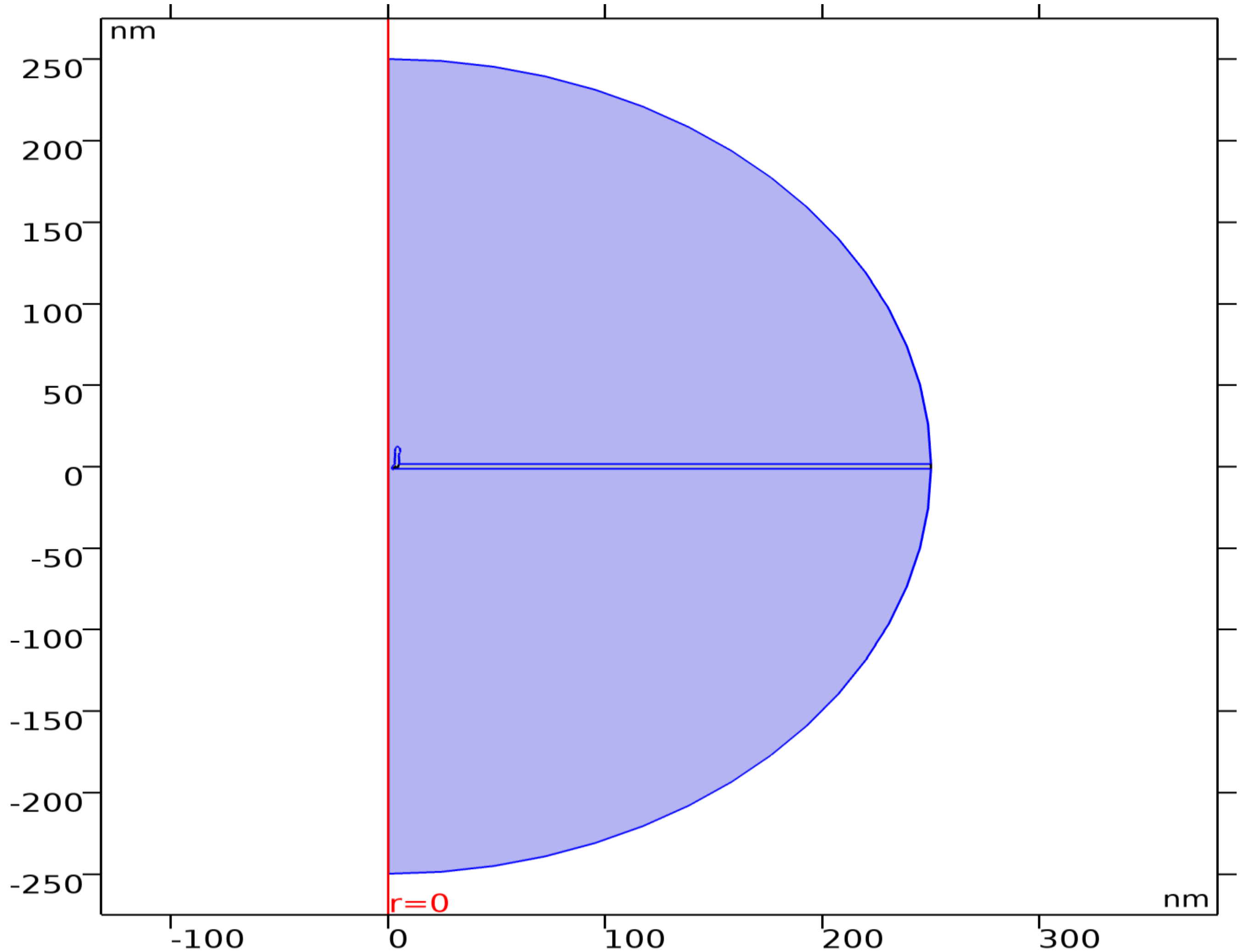
EQUATIONS

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

Variables

Name	Expression	Unit	Description	Selection	Details
spf.Fr	es.Er*scd_ions	N/m^3	Volume force, r component	Domain 1	+ operation
spf.Fphi	0	N/m^3	Volume force, phi component	Domain 1	+ operation
spf.Fz	es.Ez*scd_ions	N/m^3	Volume force, z component	Domain 1	+ operation

2.5.9 Density Continuity



Density Continuity

SELECTION

Geometric entity level	Domain
Selection	Domain 1

Weak contribution

SETTINGS

Description	Value
Weak expression	(u*d(spf.rho, r) + w*d(spf.rho, z))*test(p)

Quadrature settings

SETTINGS

Description	Value

Description	Value
Use automatic quadrature settings	On

Weak expressions

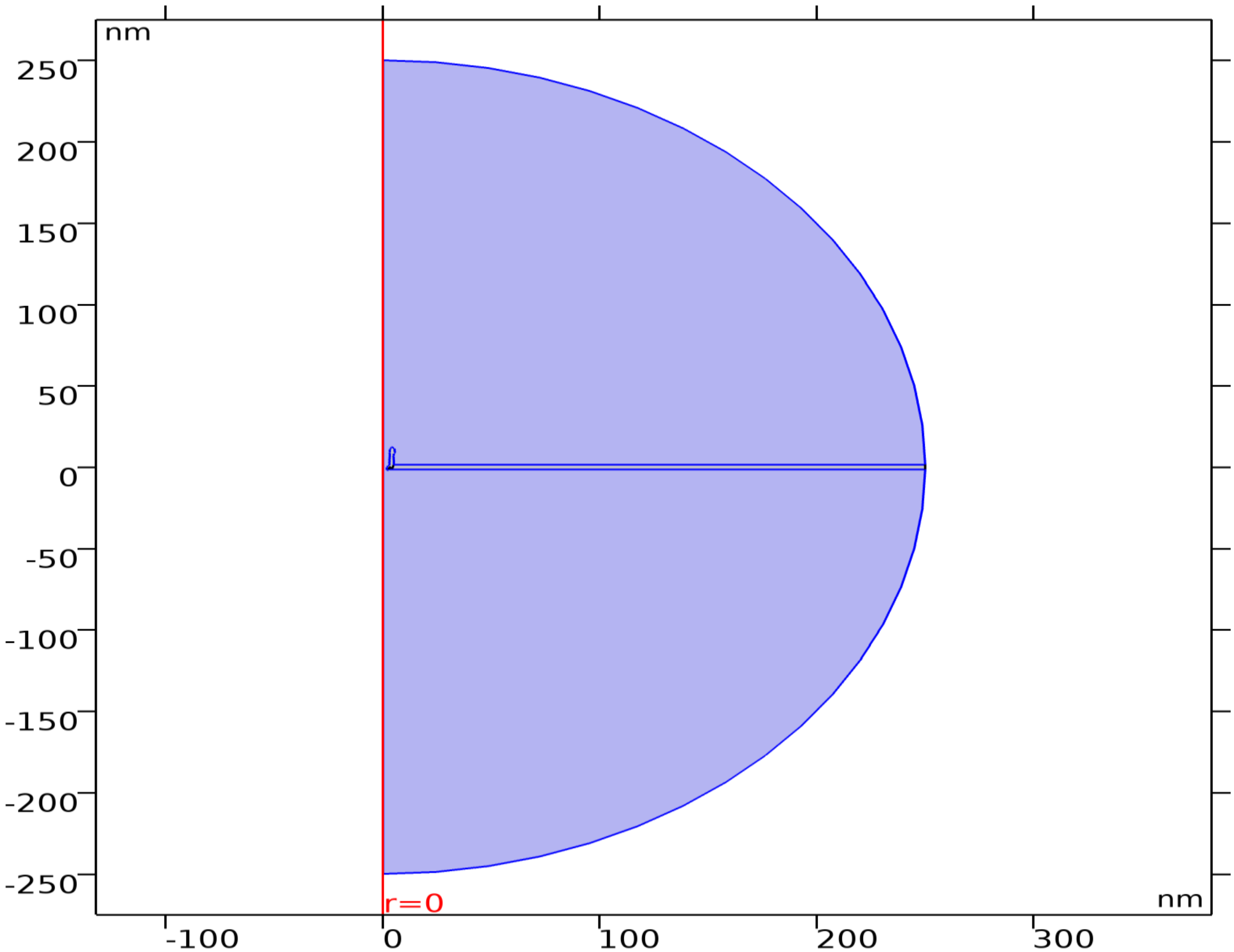
Weak expression	Integration order	Integration frame	Selection
2*(u*d(spf.rho,r)+w*d(spf.rho,z))*test(p)*pi*r	2	Spatial	Domain 1

2.6 MULTIPHYSICS

2.6.1 Potential Coupling 1

USED PRODUCTS

COMSOL Multiphysics



Potential Coupling 1

SELECTION

Geometric entity level	Domain
Selection	Domain 1

Coupled interfaces

SETTINGS

Description	Value
Source	Electrostatics (es)
Destination	Transport of Diluted Species (tds)

Variables

Name	Expression	Unit	Description	Selection
pc1.V	V	V	Electric potential	Domain 1

2.6.2 Flow Coupling 1

USED PRODUCTS

COMSOL Multiphysics

Coupled interfaces

SETTINGS

Description	Value
Source	Laminar Flow (spf)
Destination	Transport of Diluted Species (tds)

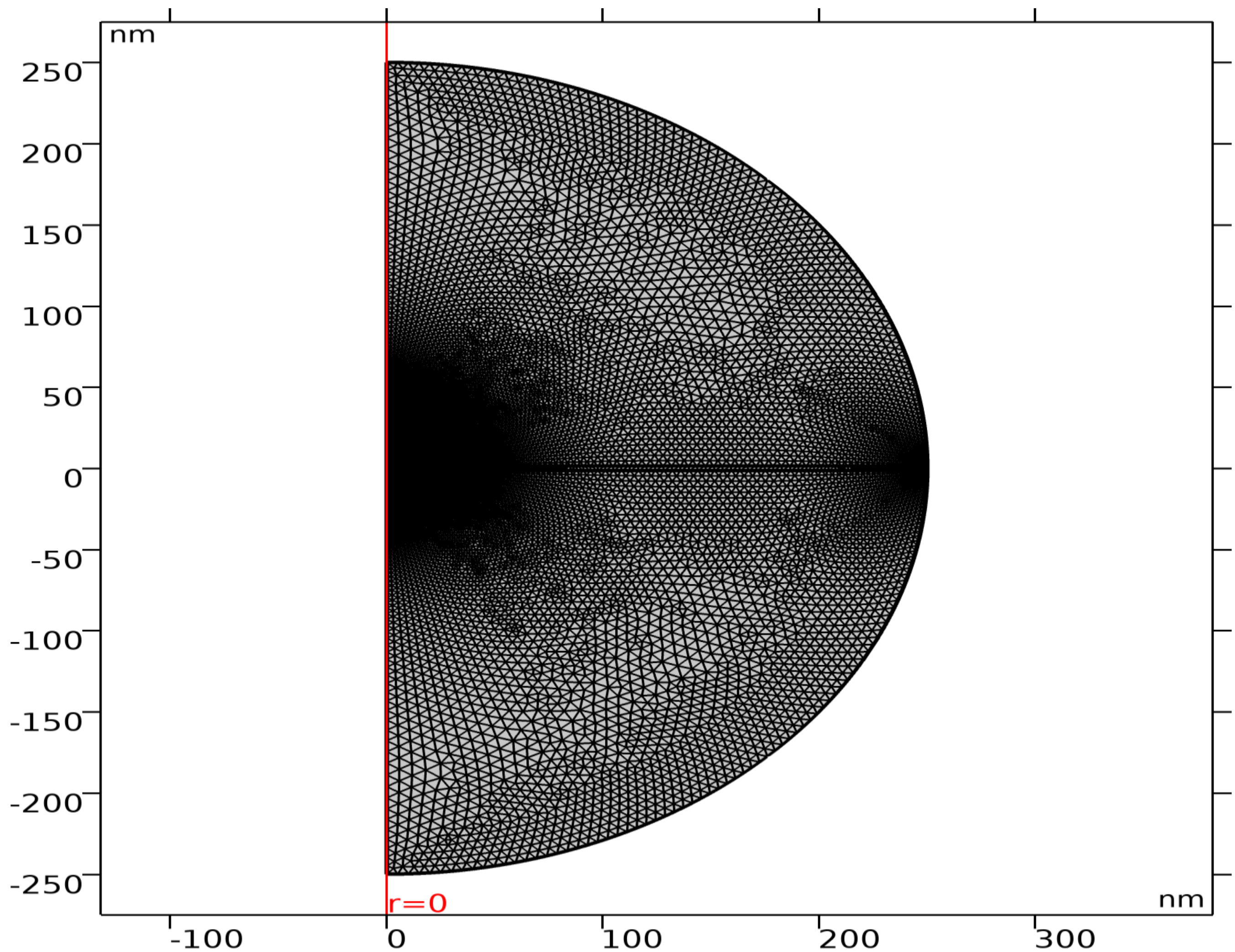
Variables

Name	Expression	Unit	Description	Selection
fc1.uR	spatial.invF11*u+spatial.invF31*w	m/s	Velocity field, R component	Global
fc1.uPHI	0	m/s	Velocity field, PHI component	Global
fc1.uZ	spatial.invF13*u+spatial.invF33*w	m/s	Velocity field, Z component	Global
fc1.p	p	Pa	Pressure	Global
fc1.pA	spf.pA	Pa	Absolute pressure	Global

2.7 MESH

MESH STATISTICS

Description	Value
Minimum element quality	0.6378
Average element quality	0.9765
Triangle	120917
Edge element	1879
Vertex element	196



Mesh

2.7.1 Size (global) (size)

SETTINGS

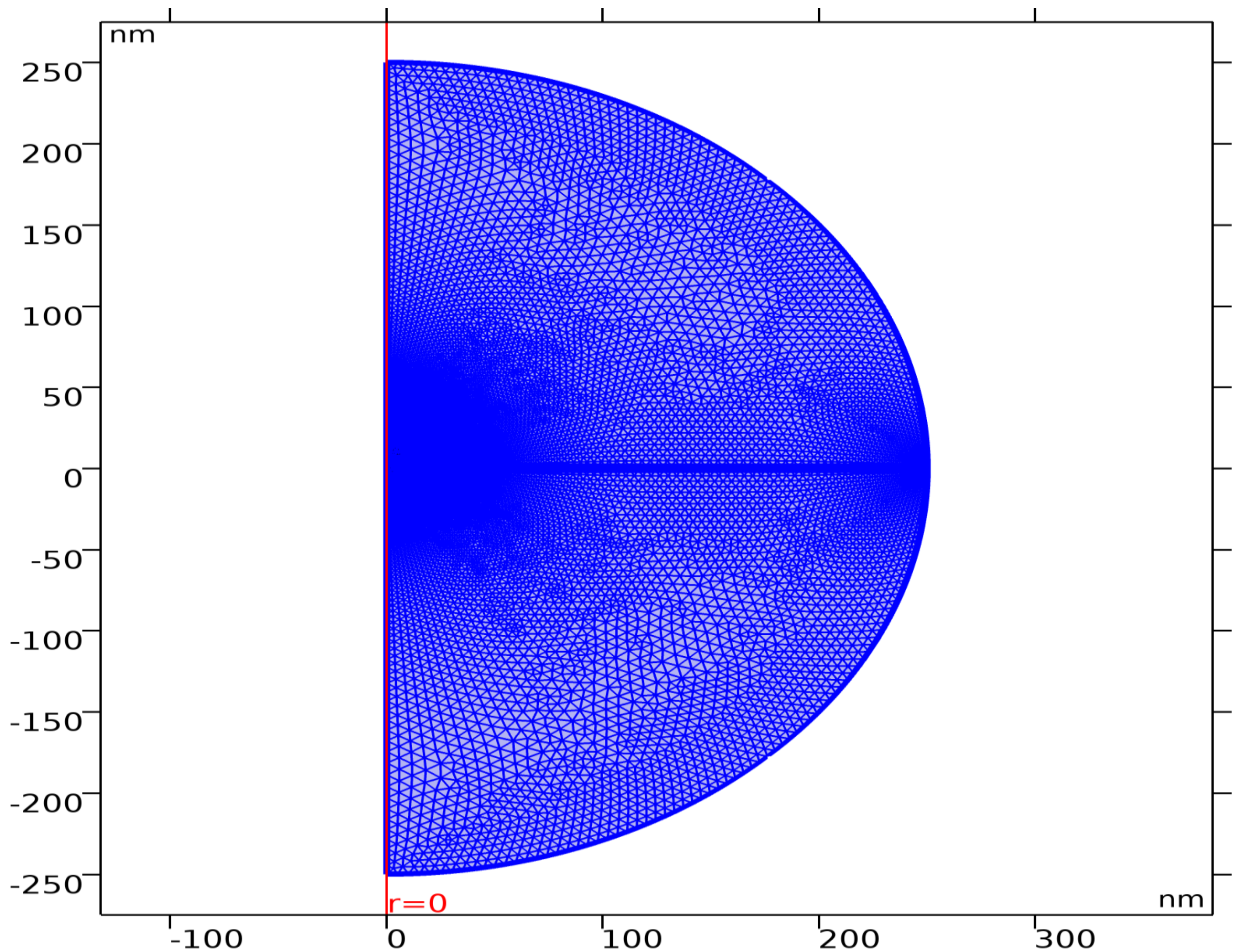
Description	Value
Maximum element size	10
Minimum element size	0.001

Description	Value
Curvature factor	0.25
Maximum element growth rate	1.05
Predefined size	Finer
Custom element size	Custom

2.7.2 Free Triangular (not pore) (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Domains 1, 3

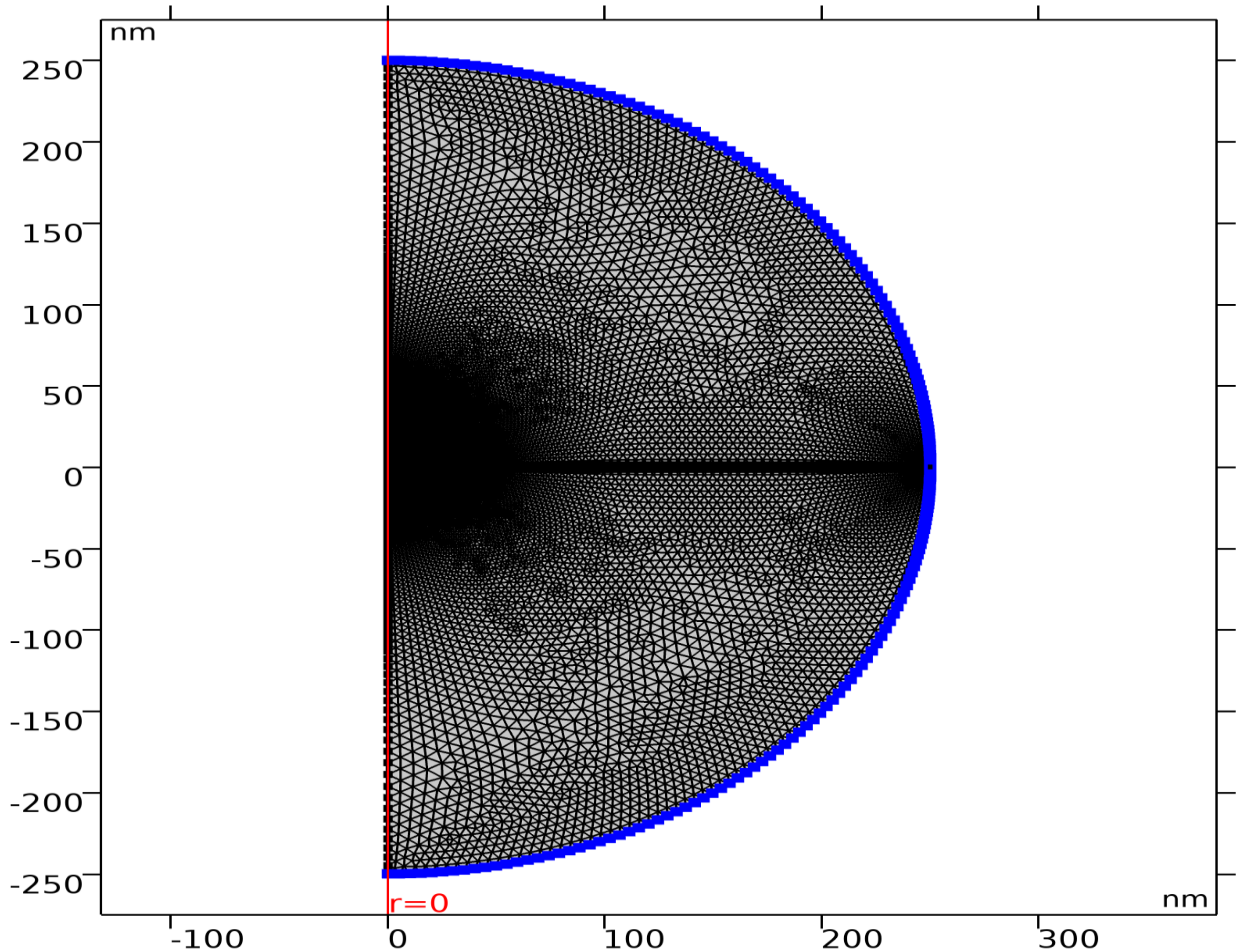


Free Triangular (not pore)

Size (reservoir boundary) (size1)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 195–196



Size (reservoir boundary)

SETTINGS

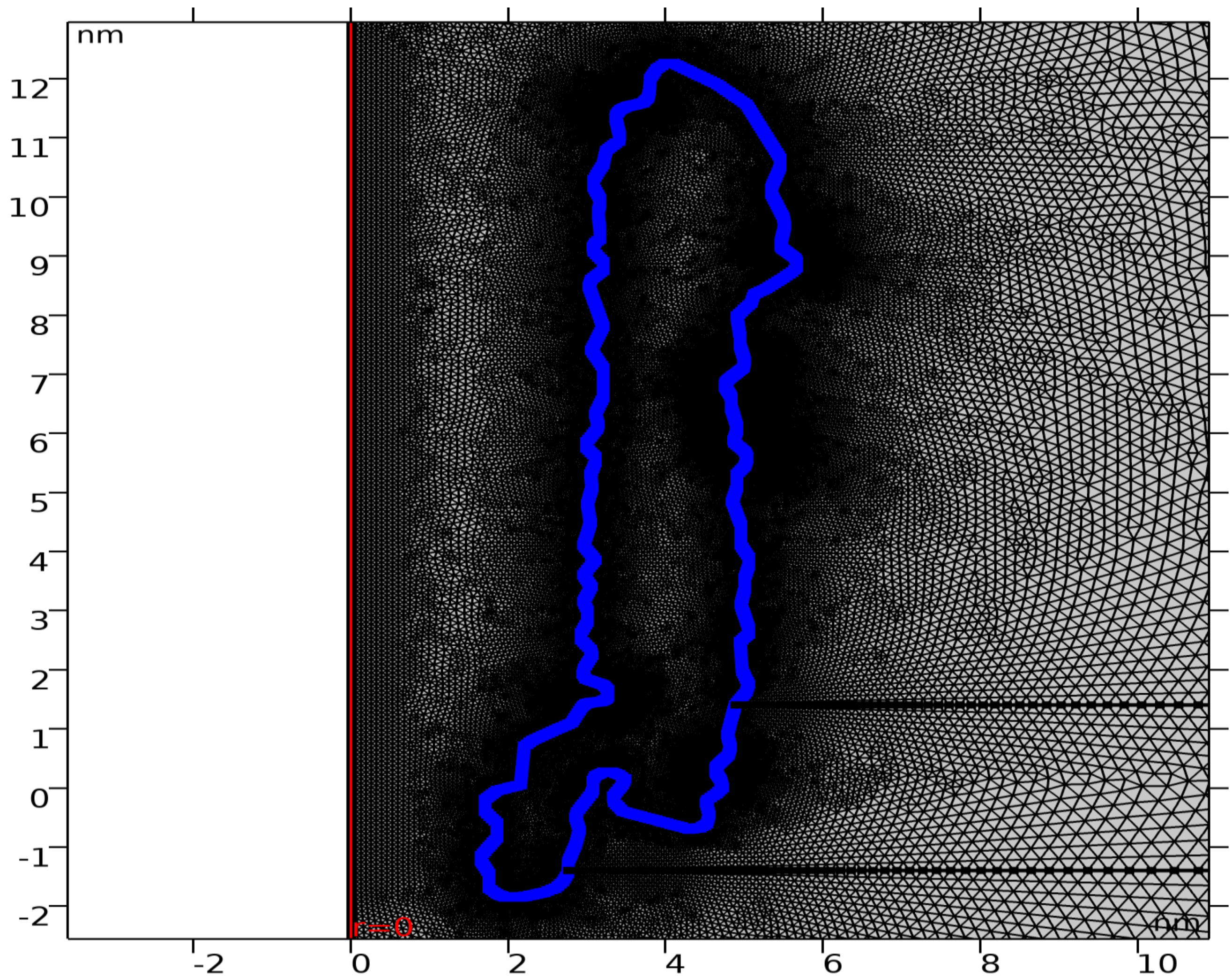
Description	Value
Maximum element size	5
Minimum element size	0.025
Minimum element size	Off
Curvature factor	0.25
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.25
Maximum element growth rate	Off

Description	Value
Predefined size	Finer
Custom element size	Custom

Size (pore boundary) (size5)

SELECTION

Geometric entity level	Boundary
Name	Nanopore
Selection	Boundaries 7–29, 31–152, 154–194



Size (pore boundary)

SETTINGS

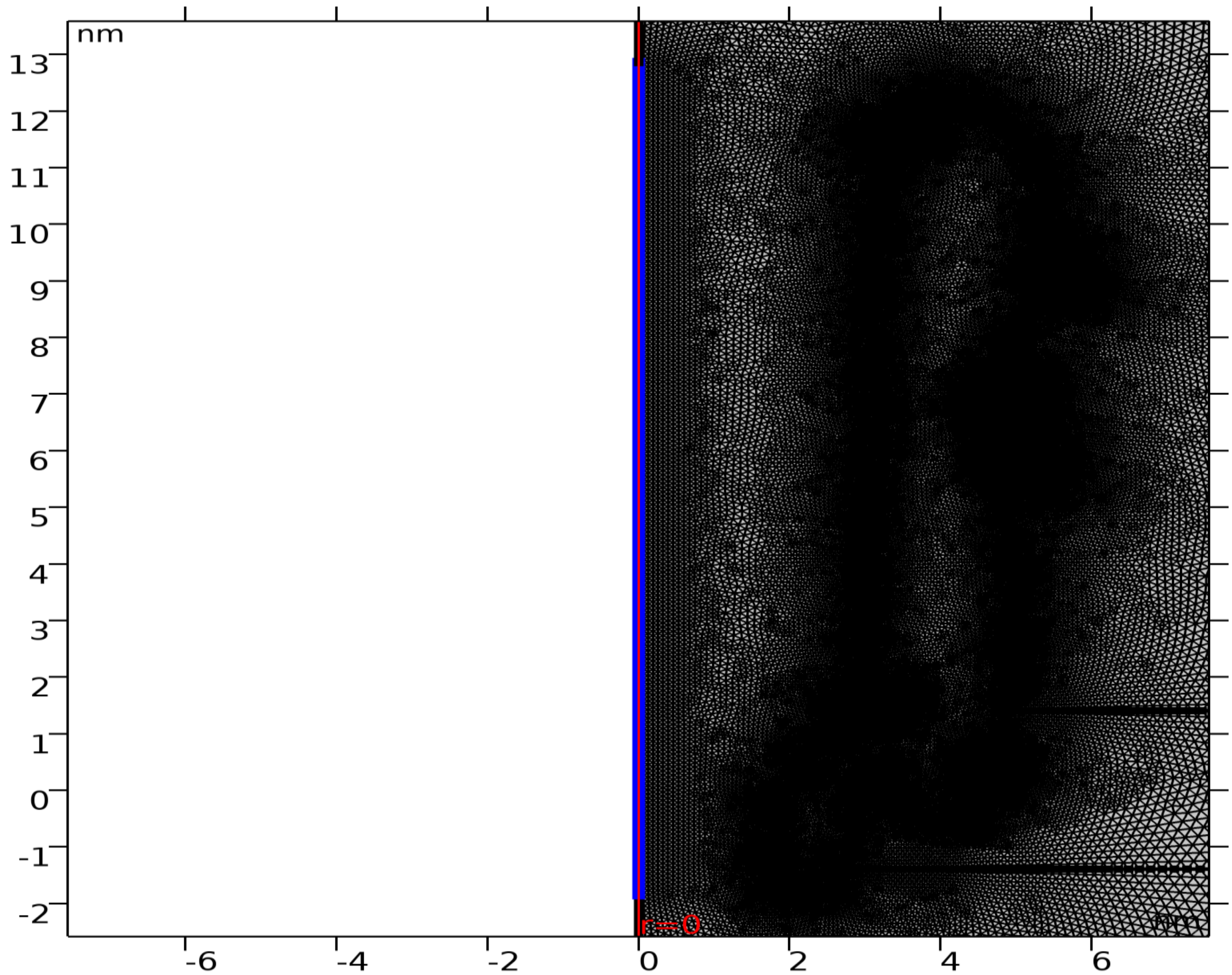
Description	Value
Maximum element size	0.05

Description	Value
Minimum element size	0.001
Curvature factor	0.25
Maximum element growth rate	1.05
Predefined size	Finer
Custom element size	Custom

Size (symmetry axis inside pore) (size6)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 3–4



Size (symmetry axis inside pore)

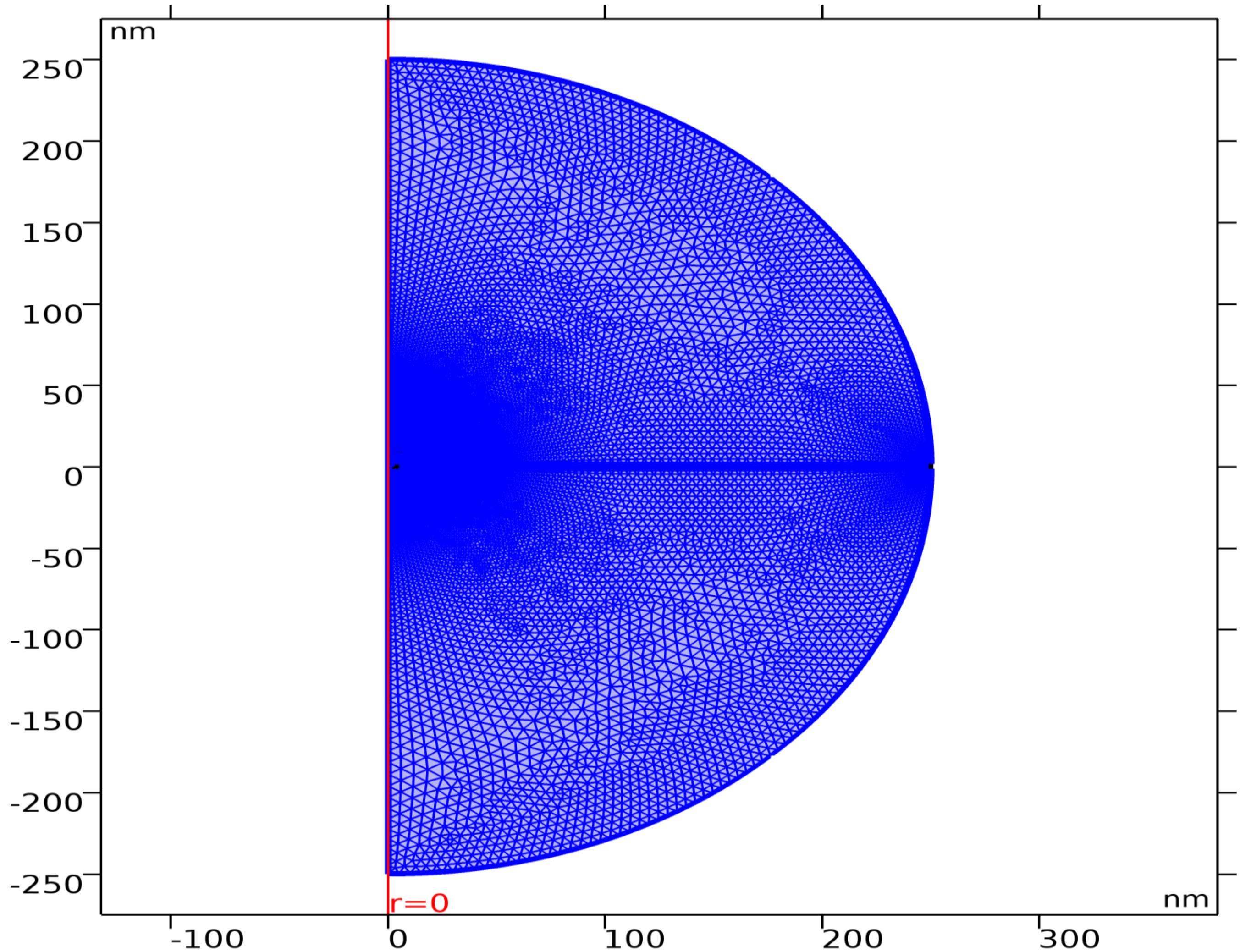
SETTINGS

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	0.075
Minimum element size	0.04
Minimum element size	Off
Curvature factor	0.25
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	Off
Predefined size	Finer
Custom element size	Custom

Size (reservoir domain) (size3)

SELECTION

Geometric entity level	Domain
Name	Reservoir
Selection	Domain 1



Size (reservoir domain)

SETTINGS

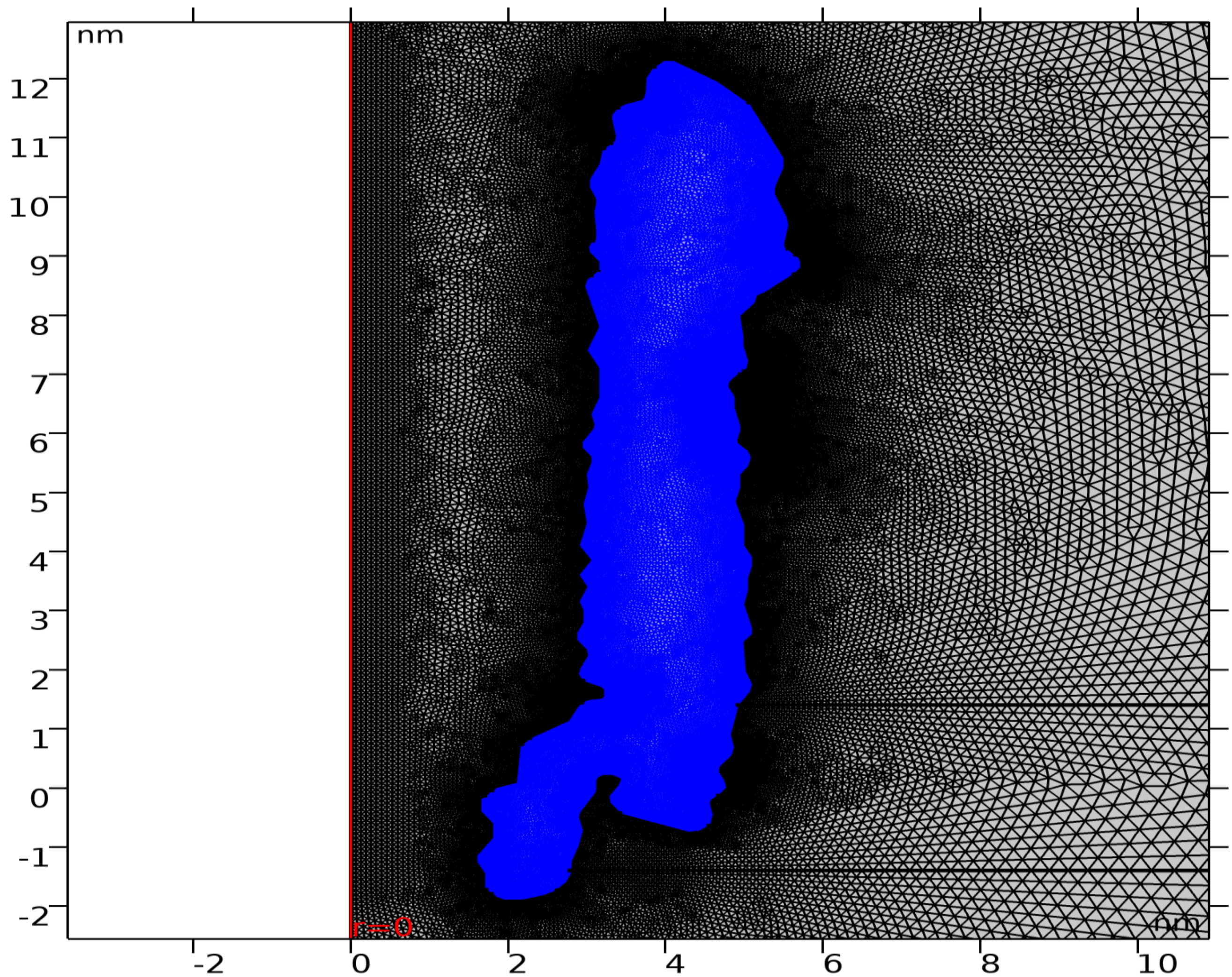
Description	Value
Calibrate for	Fluid dynamics
Maximum element size	2.8
Maximum element size	Off
Minimum element size	0.04
Minimum element size	Off
Curvature factor	0.25
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.04
Predefined size	Finer

Description	Value
Custom element size	Custom

2.7.3 Free Triangular (pore) (ftri2)

SELECTION

Geometric entity level	Domain
Selection	Remaining

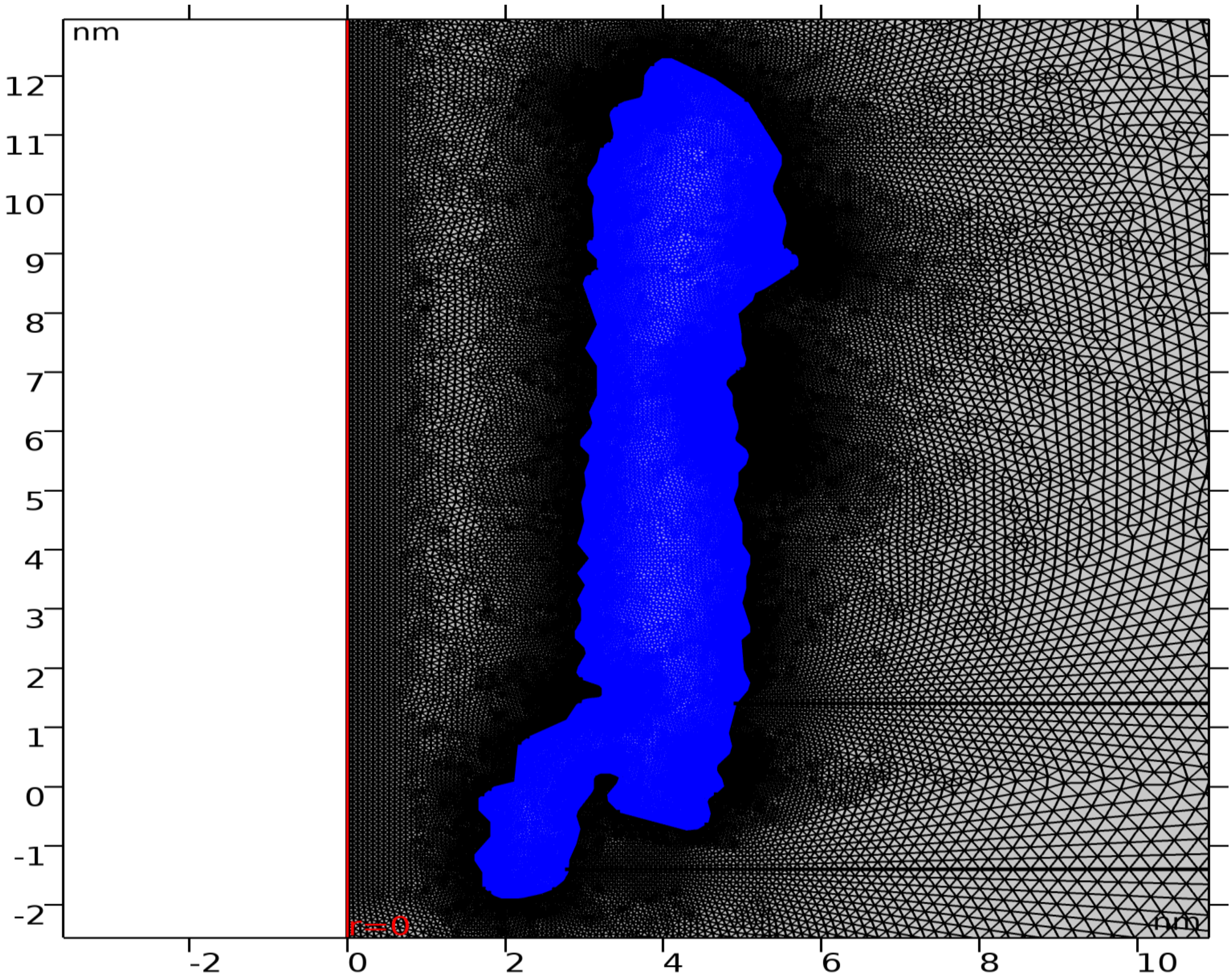


Free Triangular (pore)

Size (pore domain) (size2)

SELECTION

Geometric entity level	Domain
Name	Nanopore
Selection	Domain 2



Size (pore domain)

SETTINGS

Description	Value
Maximum element size	0.1
Minimum element size	0.004
Minimum element size	Off
Curvature factor	0.2
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	Off
Predefined size	Extremely fine
Custom element size	Custom

3 Study 1: Demo

COMPUTATION INFORMATION

Computation time	3 min 10 s
CPU	AMD64 Family 23 Model 113 Stepping 0, 12 cores
Operating system	Windows 10

3.1 STATIONARY

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

MESH SELECTION

Geometry	Mesh
mesh2	mesh2

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Electrostatics (es)	physics
Transport of Diluted Species (tds)	physics
Laminar Flow (spf)	physics

MESH SELECTION

Geometry	Mesh
Geometry (geom1)	mesh2

3.2 SOLVER CONFIGURATIONS

3.2.1 Solution 1

Compile Equations: Stationary (st1)

STUDY AND STEP

Description	Value
Use study	Study 1: Demo
Use study step	Stationary

Dependent Variables 1 (v1)

GENERAL

Description	Value
Defined by study step	Stationary

Concentration (comp1.cneg) (comp1_cneg)

GENERAL

Description	Value
Field components	comp1.cneg

Concentration (comp1.cpos) (comp1_cpos)

GENERAL

Description	Value
Field components	comp1.cpos

Pressure (comp1.p) (comp1_p)

GENERAL

Description	Value
Field components	comp1.p

Velocity field (comp1.u) (comp1_u)

GENERAL

Description	Value
Field components	{comp1.u, comp1.w}

Electric potential (comp1.V) (comp1_V)

GENERAL

Description	Value
Field components	comp1.V

Stationary Solver 1 (s1)

GENERAL

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

Advanced (aDef)

ASSEMBLY SETTINGS

Description	Value
Reuse sparsity pattern	On

Fully Coupled 1 (fc1)

GENERAL

Description	Value

Description	Value
Linear solver	Direct 1

METHOD AND TERMINATION

Description	Value
Initial damping factor	0.2
Minimum damping factor	1.0E-2
Recovery damping factor	0.2
Maximum number of iterations	100

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO
Pivoting perturbation	1.0E-13

4 Study 2: Full sweep

COMPUTATION INFORMATION

Computation time	41 h 3 min 51 s
CPU	AMD64 Family 23 Model 113 Stepping 0, 12 cores
Operating system	Windows 10

4.1 PARAMETRIC SWEEP

STUDY SETTINGS

Description	Value
Sweep type	Parameter switch

STUDY SETTINGS

Switch	Cases	Case numbers
Enabled Physics	All	range(1,1,5)
Electrolyte	User defined	1

4.2 STATIONARY

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

MESH SELECTION

Geometry	Mesh
mesh2	mesh2

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Electrostatics (es)	physics
Transport of Diluted Species (tds)	physics
Laminar Flow (spf)	physics

MESH SELECTION

Geometry	Mesh
Geometry (geom1)	mesh2

4.2.1 Study extensions

STUDY EXTENSIONS

Description	Value

Description	Value
Sweep type	All combinations
Run continuation for	Manual
Continuation parameter	V_bias

PARAMETERS

Parameter name	Parameter value list	Parameter unit
V_bias (Applied bias voltage)	range(-500,100,-300),range(-200,25,-125),range(-100,10,100),range(125,25,200),range(300,100,500)	mV
c_salt (Bulk salt concentration)	5,10,25,50,75,100,125,150,200,250,300,400,500,750,1000,1500,2000,2500,3000,4000,5000	mM

4.3 SOLVER CONFIGURATIONS

4.3.1 Solution 2

Compile Equations: Stationary (st1)

STUDY AND STEP

Description	Value
Use study	Study 2: Full sweep
Use study step	Stationary

LOG

```
<---- Compile Equations: Stationary in Study 2: Full sweep/Solution 2 (sol2) ---
Started at May 22, 2020 4:42:41 PM.
Geometry shape order: Linear
Running on AMD64 Family 23 Model 113 Stepping 0, AuthenticAMD.
Using 1 socket with 12 cores in total on beasty.
Available memory: 32.22 GB.
Parameter enable_wdf = 1.0 .
Parameter enable_cdf = 1.0 .
Parameter enable_smp = 1.0 .
Parameter enable_cdf_rho = 1.0 .
Parameter enable_cdf_epsr = 1.0 .
Parameter enable_cdf_eta = 1.0 .
Parameter enable_cdf_mob = 1.0 .
Parameter a_cpos = 5.0E-10 .
Parameter a_cneg = 5.0E-10 .
Parameter a_sol = 3.11E-10 .
Parameter z_cpos = 1.0 .
Parameter z_cneg = -1.0 .
Parameter epsr0 = 78.15 .
Parameter epsr_alpha = 11.5 .
Parameter epsr_ms = 30.08 .
Parameter rho0 = 996.9999999999999 .
Parameter rho1 = 0.04047 .
Parameter rho2 = -6.149E-4 .
Parameter eta0 = 8.904E-4 .
Parameter eta1 = 0.007558 .
Parameter eta2 = 0.07769 .
Parameter eta3 = 0.01192 .
Parameter eta4 = 5.951E-4 .
Parameter d0_cpos = 1.334E-9 .
Parameter d0_cneg = 2.032E-9 .
Parameter l0_cpos = 0.0050096752508337495 .
Parameter l0_cneg = 0.0076309296174619035 .
Parameter d1_cpos = 0.202 .
Parameter d2_cpos = -0.3048 .
Parameter d3_cpos = 0.219 .
Parameter d4_cpos = -0.03124 .
Parameter d1_cneg = 0.149 .
Parameter d2_cneg = -0.04933 .
Parameter d3_cneg = 0.03392 .
Parameter d4_cneg = 0.01431 .
Parameter l1_cpos = 0.7907 .
Parameter l2_cpos = -0.3529 .
Parameter l3_cpos = 0.1459 .
Parameter l4_cpos = 0.009241 .
Parameter l1_cneg = 0.6289 .
Parameter l2_cneg = -0.4286 .
Parameter l3_cneg = 0.2123 .
Parameter l4_cneg = -0.01068 .
Parameter cmax = 5300.0 .
Time: 8 s.
Physical memory: 2.85 GB
Virtual memory: 3.96 GB
Ended at May 22, 2020 4:42:49 PM.
----- Compile Equations: Stationary in Study 2: Full sweep/Solution 2 (sol2) -->
```

Dependent Variables 1 (v1)

GENERAL

Description	Value
Defined by study step	Stationary

INITIAL VALUE CALCULATION CONSTANTS

Constant name	Initial value source
V_bias	range(-500,100,-300)[mV] range(-200,25,-125)[mV] range(-100,10,100)[mV] range(125,25,200)[mV] range(300,100,500)[mV]
c_salt	5[mM] 10[mM] 25[mM] 50[mM] 75[mM] 100[mM] 125[mM] 150[mM] 200[mM] 250[mM] 300[mM] 400[mM] 500[mM] 750[mM] 1000[mM] 1500[mM] 2000[mM] 2500[mM] 3000[mM] 4000[mM] 5000[mM]

LOG

```
<---- Dependent Variables 1 in Study 2: Full sweep/Solution 2 (sol2) -----------
Started at May 22, 2020 4:42:49 PM.
Solution time: 1 s.
Physical memory: 2.99 GB
Virtual memory: 4.1 GB
Ended at May 22, 2020 4:42:50 PM.
----- Dependent Variables 1 in Study 2: Full sweep/Solution 2 (sol2) ---------->
```

Concentration (comp1.cneg) (comp1_cneg)

GENERAL

Description	Value
Field components	comp1.cneg

Concentration (comp1.cpos) (comp1_cpos)

GENERAL

Description	Value
Field components	comp1.cpos

Pressure (comp1.p) (comp1_p)

GENERAL

Description	Value
Field components	comp1.p

Velocity field (comp1.u) (comp1_u)

GENERAL

Description	Value
Field components	{comp1.u, comp1.w}

Electric potential (comp1.V) (comp1_V)

GENERAL

Description	Value
Field components	comp1.V

Stationary Solver 1 (s1)

GENERAL

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

RESULTS WHILE SOLVING

Description	Value
Probes	None

Advanced (aDef)

ASSEMBLY SETTINGS

Description	Value
Reuse sparsity pattern	On

Parametric 1 (p1)

GENERAL

Description	Value
Defined by study step	Stationary
Sweep type	All combinations
Run continuation for	Manual
Continuation parameter	V_bias
On error	Store empty solution

PARAMETERS

Parameter name	Parameter value list	Parameter unit
V_bias	range(-500,100,-300),range(-200,25,-125),range(-100,10,100),range(125,25,200),range(300,100,500)	mV
c_salt	5,10,25,50,75,100,125,150,200,250,300,400,500,750,1000,1500,2000,2500,3000,4000,5000	mM

CLUSTER SETTINGS

Description	Value
Distribute parameters	On

Fully Coupled 1 (fc1)

GENERAL

Description	Value
Linear solver	Direct 1

METHOD AND TERMINATION

Description	Value
Initial damping factor	0.2
Minimum damping factor	1.0E-2
Recovery damping factor	0.2
Maximum number of iterations	100

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO
Pivoting perturbation	1.0E-13

4.3.2 Parametric Solutions 1

enable_wdf=1, enable_cdf=1, enable_smp=1, enable_cdf_rho=1, enable_cdf_epsr=1, enable_cdf_eta=1, enable_cdf_mob=1, a_cpos=5E-10, a_cneg=5E-10, a_sol=3.11E-10, z_cpos=1, z_cneg=-1, epsr0=78.15, epsr_alpha=11.5, epsr_ms=30.08, rho0=997, rho1=0.04047, rho2=-6.149E-4, eta0=8.904E-4, eta1=0.007558, eta2=0.07769, eta3=0.01192, eta4=5.951E-4, d0_cpos=1.334E-9, d0_cneg=2.032E-9, l0_cpos=0.0050097, l0_cneg=0.0076309, d1_cpos=0.202, d2_cpos=-0.3048, d3_cpos=0.219, d4_cpos=-0.03124, d1_cneg=0.149, d2_cneg=-0.04933, d3_cneg=0.03392, d4_cneg=0.01431, l1_cpos=0.7907, l2_cpos=-0.3529, l3_cpos=0.1459, l4_cpos=0.009241, l1_cneg=0.6289, l2_cneg=-0.4286, l3_cneg=0.2123, l4_cneg=-0.01068, cmax=5300 (su1)

GENERAL

Description	Value
Solution	enable_wdf=1, enable_cdf=1, enable_smp=1, enable_cdf_rho=1, enable_cdf_epsr=1, enable_cdf_eta=1, enable_cdf_mob=1, a_cpos=5E-10, a_cneg=5E-10, a_sol=3.11E-10, z_cpos=1, z_cneg= - 1, epsr0=78.15, epsr_alpha=11.5, epsr_ms=30.08, rho0=997, rho1=0.04047, rho2= - 6.149E-4, eta0=8.904E-4, eta1=0.007558, eta2=0.07769, eta3=0.01192, eta4=5.951E-4, d0_cpos=1.334E-9, d0_cneg=2.032E-9, l0_cpos=0.0050097, l0_cneg=0.0076309, d1_cpos=0.202, d2_cpos= - 0.3048, d3_cpos=0.219, d4_cpos= - 0.03124, d1_cneg=0.149, d2_cneg= - 0.04933, d3_cneg=0.03392, d4_cneg=0.01431, l1_cpos=0.7907, l2_cpos= - 0.3529, l3_cpos=0.1459, l4_cpos=0.009241, l1_cneg=0.6289, l2_cneg= - 0.4286, l3_cneg=0.2123, l4_cneg= - 0.01068, cmax=5300

LOG

```
<---- Compile Equations: Stationary in Study 2: Full sweep/Solution 2 (sol2) ---
Started at May 22, 2020 4:42:41 PM.
Geometry shape order: Linear
Running on AMD64 Family 23 Model 113 Stepping 0, AuthenticAMD.
Using 1 socket with 12 cores in total on beasty.
Available memory: 32.22 GB.
Parameter enable_wdf = 1.0 .
Parameter enable_cdf = 1.0 .
Parameter enable_smp = 1.0 .
Parameter enable_cdf_rho = 1.0 .
Parameter enable_cdf_epsr = 1.0 .
Parameter enable_cdf_eta = 1.0 .
Parameter enable_cdf_mob = 1.0 .
Parameter a_cpos = 5.0E-10 .
Parameter a_cneg = 5.0E-10 .
Parameter a_sol = 3.11E-10 .
Parameter z_cpos = 1.0 .
Parameter z_cneg = -1.0 .
Parameter epsr0 = 78.15 .
Parameter epsr_alpha = 11.5 .
Parameter epsr_ms = 30.08 .
Parameter rho0 = 996.9999999999999 .
Parameter rho1 = 0.04047 .
Parameter rho2 = -6.149E-4 .
Parameter eta0 = 8.904E-4 .
Parameter eta1 = 0.007558 .
Parameter eta2 = 0.07769 .
Parameter eta3 = 0.01192 .
Parameter eta4 = 5.951E-4 .
Parameter d0_cpos = 1.334E-9 .
Parameter d0_cneg = 2.032E-9 .
Parameter l0_cpos = 0.0050096752508337495 .
Parameter l0_cneg = 0.0076309296174619035 .
Parameter d1_cpos = 0.202 .
Parameter d2_cpos = -0.3048 .
Parameter d3_cpos = 0.219 .
Parameter d4_cpos = -0.03124 .
Parameter d1_cneg = 0.149 .
Parameter d2_cneg = -0.04933 .
Parameter d3_cneg = 0.03392 .
Parameter d4_cneg = 0.01431 .
Parameter l1_cpos = 0.7907 .
Parameter l2_cpos = -0.3529 .
Parameter l3_cpos = 0.1459 .
Parameter l4_cpos = 0.009241 .
Parameter l1_cneg = 0.6289 .
Parameter l2_cneg = -0.4286 .
Parameter l3_cneg = 0.2123 .
Parameter l4_cneg = -0.01068 .
Parameter cmax = 5300.0 .
Time: 8 s.
Physical memory: 2.85 GB
Virtual memory: 3.96 GB
Ended at May 22, 2020 4:42:49 PM.
----- Compile Equations: Stationary in Study 2: Full sweep/Solution 2 (sol2) -->
```

```
<---- Dependent Variables 1 in Study 2: Full sweep/Solution 2 (sol2) -----------
Started at May 22, 2020 4:42:49 PM.
Solution time: 1 s.
Physical memory: 2.99 GB
Virtual memory: 4.1 GB
Ended at May 22, 2020 4:42:50 PM.
----- Dependent Variables 1 in Study 2: Full sweep/Solution 2 (sol2) ---------->
```

5 Results

5.1 DERIVED VALUES

5.1.1 conductance

OUTPUT

Evaluated in	conductance (NaCl, ePNP-NS)

EXPRESSIONS

Expression	Unit	Description
F_const*(tds.z_cpos*tds.ntflux_cpos+tds.z_cneg*tds.ntflux_cneg)		current
F_const*tds.z_cpos*tds.ntflux_cpos		current_cation
F_const*tds.z_cneg*tds.ntflux_cneg		current_anion
F_const*(tds.z_cpos*tds.ntflux_cpos+tds.z_cneg*tds.ntflux_cneg)/V_bias		conductance
F_const*tds.z_cpos*tds.ntflux_cpos/V_bias		conductance_cation
F_const*tds.z_cneg*tds.ntflux_cneg/V_bias		conductance_anion
u*nr+w*nz		current_water
(u*nr+w*nz)/V_bias		conductance_water

INTEGRATION SETTINGS

Description	Value
Integration order	4

5.1.2 average in pore

EXPRESSIONS

Expression	Unit	Description
is_inside_pore		pore_volume
cpos*is_inside_pore		total_cation
cneg*is_inside_pore		total_anion
tds.Dav_cpos*is_inside_pore		diffusion_coefficient_cation
tds.Dav_cneg*is_inside_pore		diffusion_coefficient_anion
mu_cpos*F_const*is_inside_pore		mobility_cation
mu_cneg*F_const*is_inside_pore		mobility_anion
es.epsilonrrr*is_inside_pore		permittivity
scd_ions*is_inside_pore		ion_charge_density

INTEGRATION SETTINGS

Description	Value
Integration order	4

5.1.3 average in pore surface

OUTPUT

Evaluated in	average in pore bulk (NaCl, ePNP-NS)

EXPRESSIONS

Expression	Unit	Description
is_inside_pore_bulk		pore_volume
cpos*is_inside_pore_bulk		total_cation
cneg*is_inside_pore_bulk		total_anion
tds.Dav_cpos*is_inside_pore_bulk		diffusion_coefficient_cation
tds.Dav_cneg*is_inside_pore_bulk		diffusion_coefficient_anion
mu_cpos*F_const*is_inside_pore_bulk		mobility_cation
mu_cneg*F_const*is_inside_pore_bulk		mobility_anion
es.epsilonrrr*is_inside_pore_bulk		permittivity
scd_ions*is_inside_pore_bulk		ion_charge_density

INTEGRATION SETTINGS

Description	Value
Integration order	4

5.1.4 average in pore bulk

OUTPUT

Evaluated in	average in pore bulk (NaCl, ePNP-NS)

EXPRESSIONS

Expression	Unit	Description
is_inside_pore_surface		pore_volume
cpos*is_inside_pore_surface		total_cation
cneg*is_inside_pore_surface		total_anion
tds.Dav_cpos*is_inside_pore_surface		diffusion_coefficient_cation
tds.Dav_cneg*is_inside_pore_surface		diffusion_coefficient_anion
mu_cpos*F_const*is_inside_pore_surface		mobility_cation
mu_cneg*F_const*is_inside_pore_surface		mobility_anion
es.epsilonrrr*is_inside_pore_surface		permittivity
scd_ions*is_inside_pore_surface		ion_charge_density

INTEGRATION SETTINGS

Description	Value
Integration order	4

5.1.5 Pore charge density

OUTPUT

Evaluated in	Table 33

DATA

Description	Value
Data set	Study 1: Demo/Solution 1

EXPRESSIONS

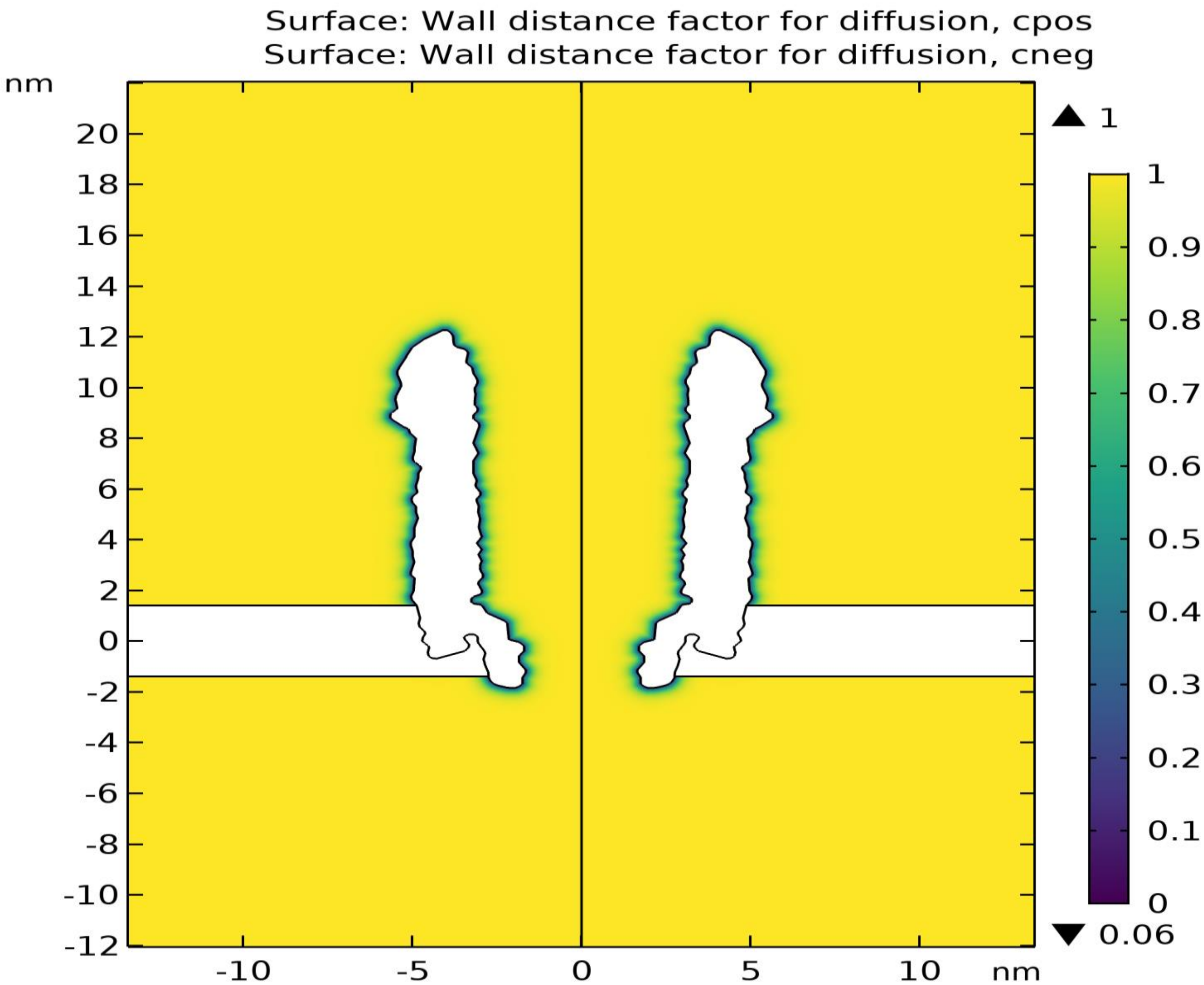
Expression	Unit	Description
if(r<0.01[nm],0,rhoq_pore(r,z)/(2*pi*r))	1	

INTEGRATION SETTINGS

Description	Value
Integration order	4
Compute volume integral	On

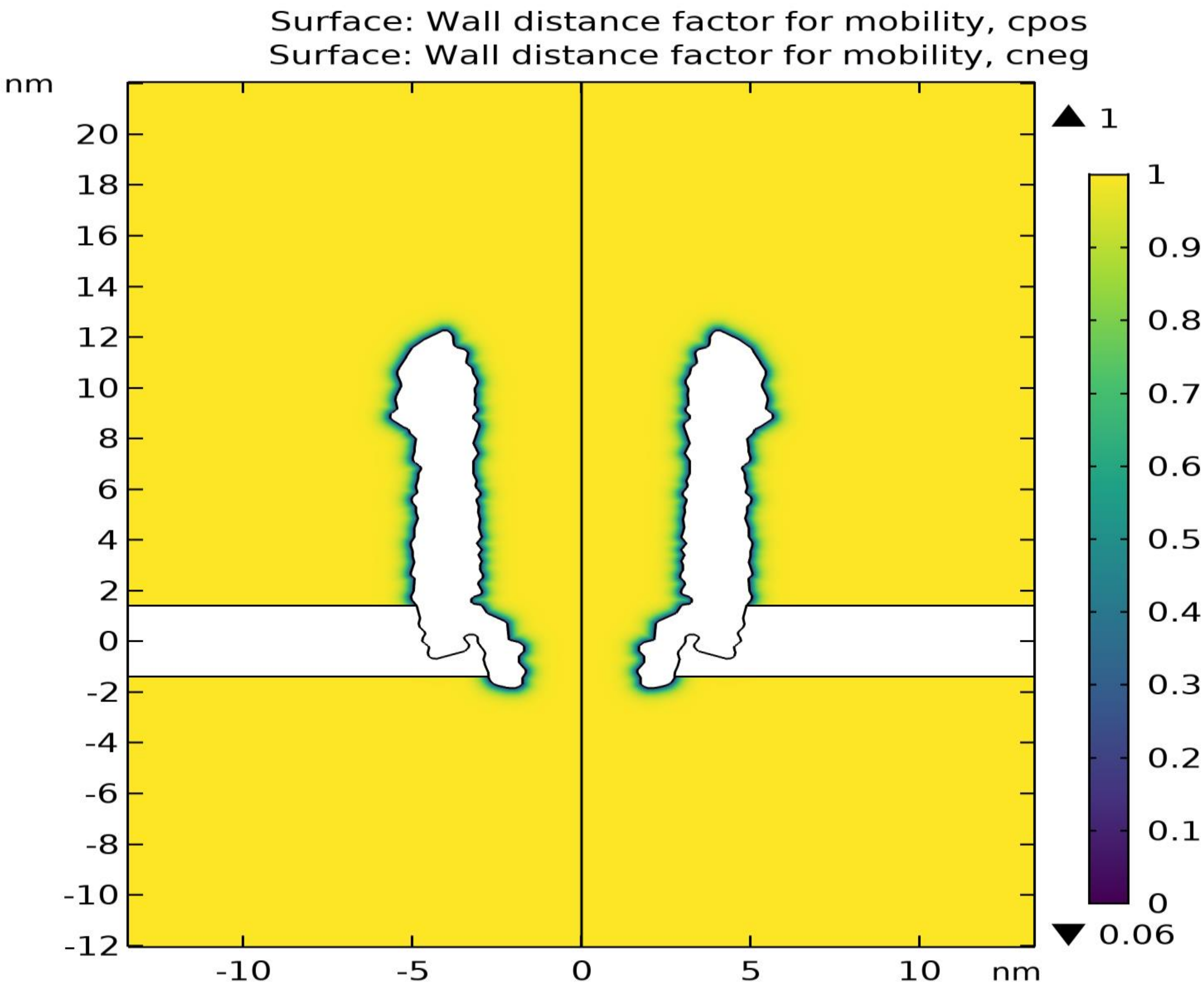
5.2 WALL DISTANCE CORRECTIONS

5.2.1 wdf diffusion: cpos (left) and cneg (right)



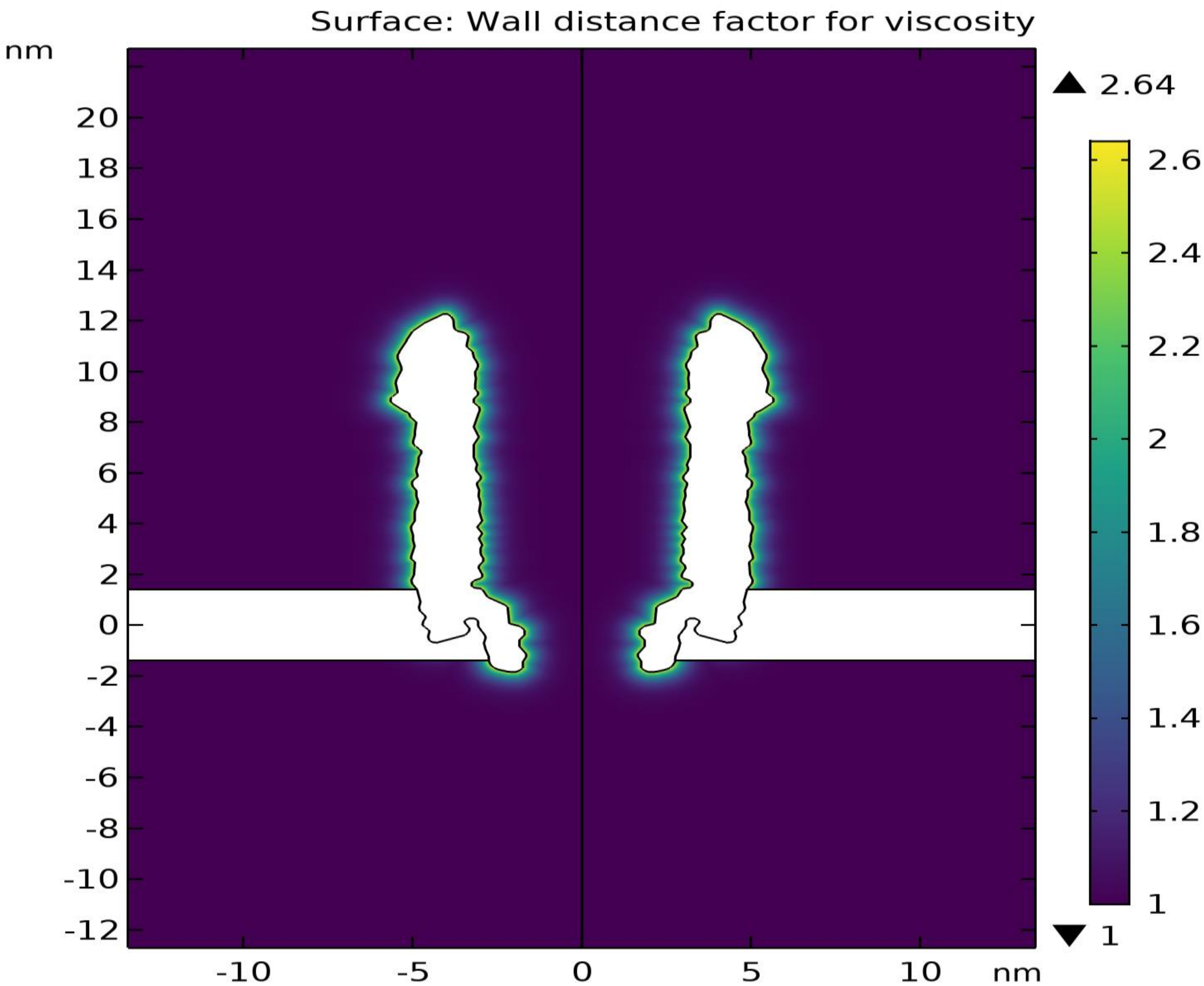
Surface: Wall distance factor for diffusion, cpos Surface: Wall distance factor for diffusion, cneg

5.2.2 wdf mobility: cpos (left) and cneg (right)



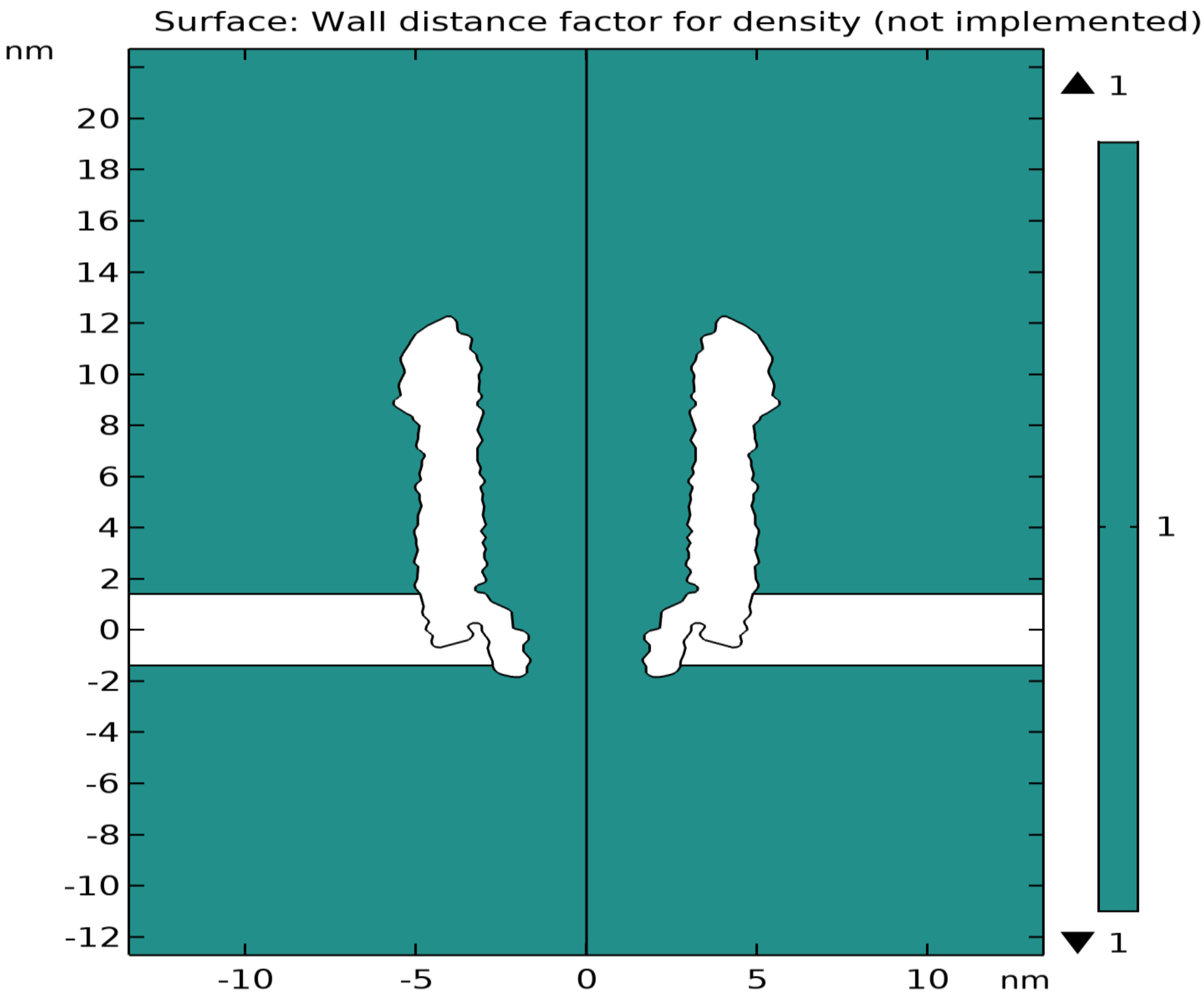
Surface: Wall distance factor for mobility, cpos Surface: Wall distance factor for mobility, cneg

5.2.3 wdf eta



Surface: Wall distance factor for viscosity

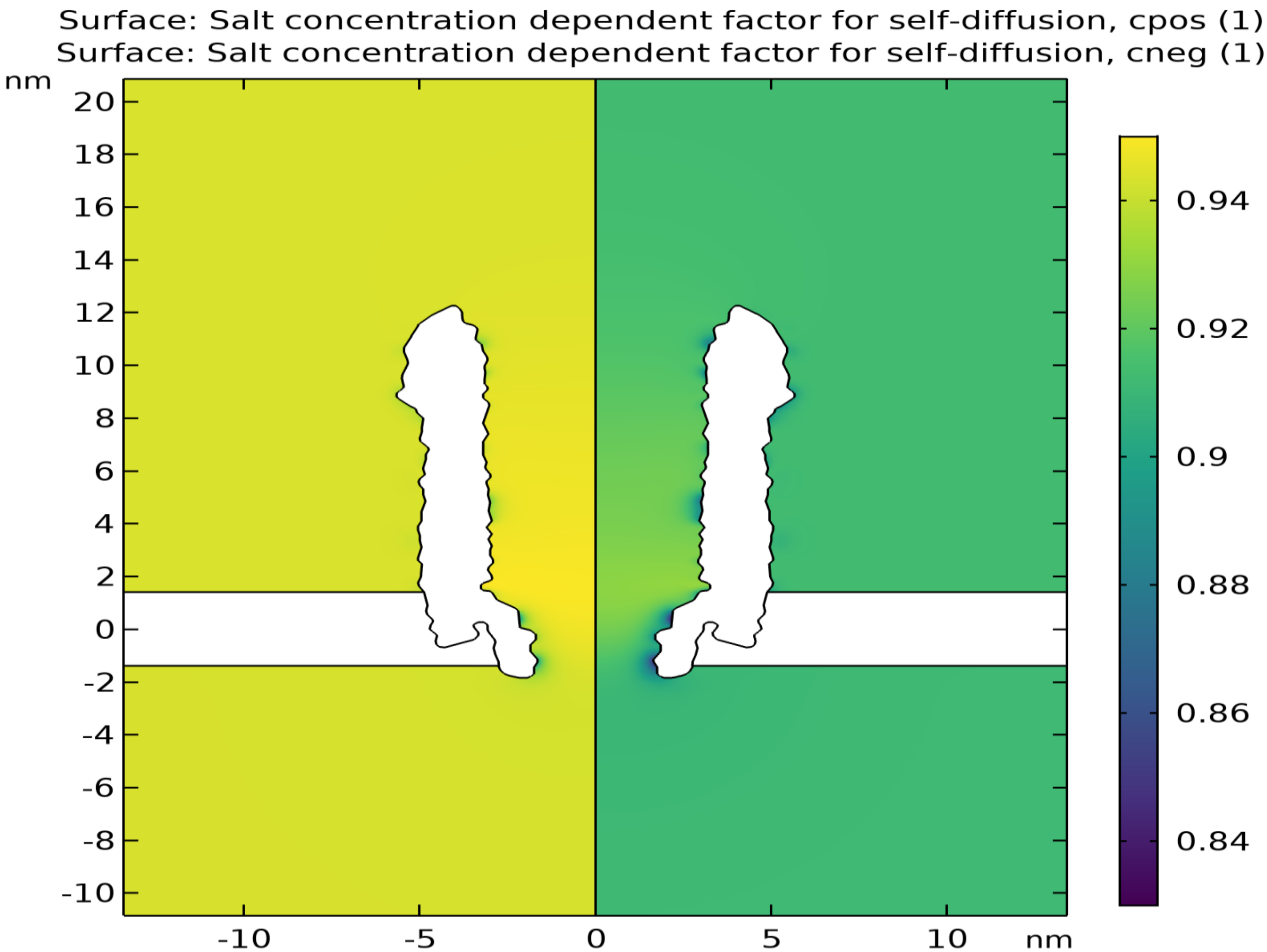
5.2.4 wdf rho



Surface: Wall distance factor for density (not implemented)

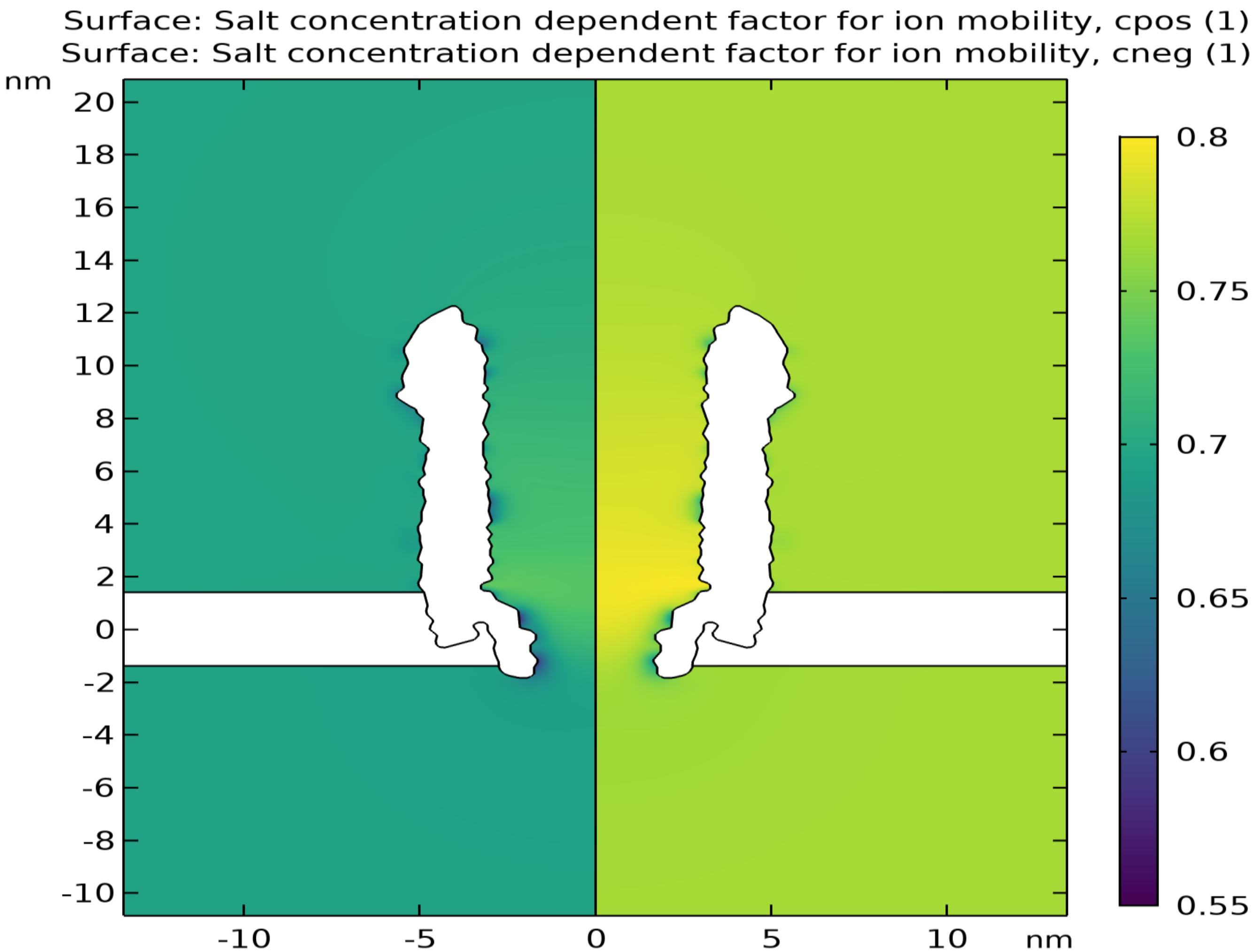
5.3 CONCENTRATION CORRECTIONS

5.3.1 cdf diffusion: cpos (left) and cneg (right)



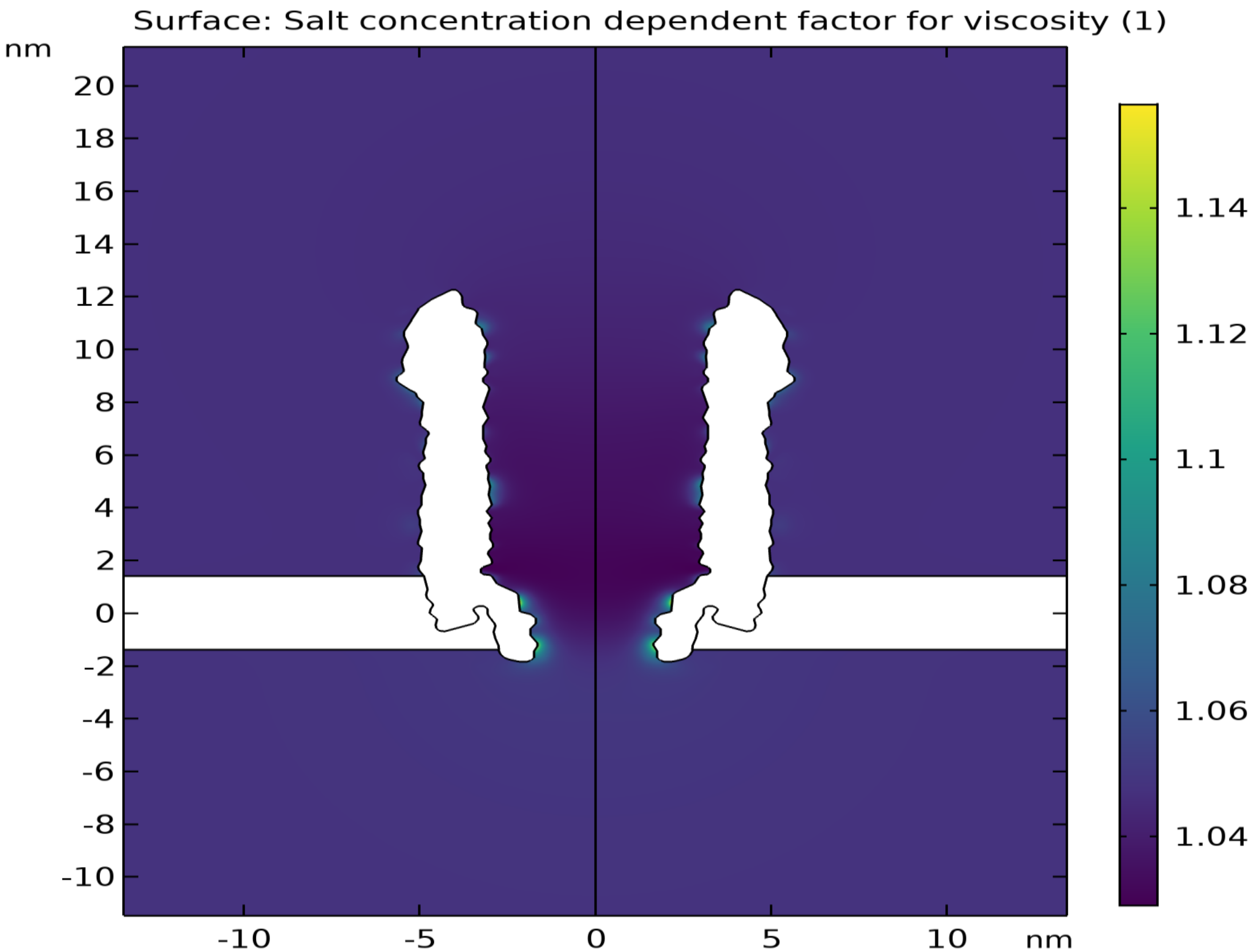
Surface: Salt concentration dependent factor for self-diffusion, cpos (1) Surface: Salt concentration dependent factor for self-diffusion, cneg (1)

5.3.2 cdf mobility: cpos (left) and cneg (right)



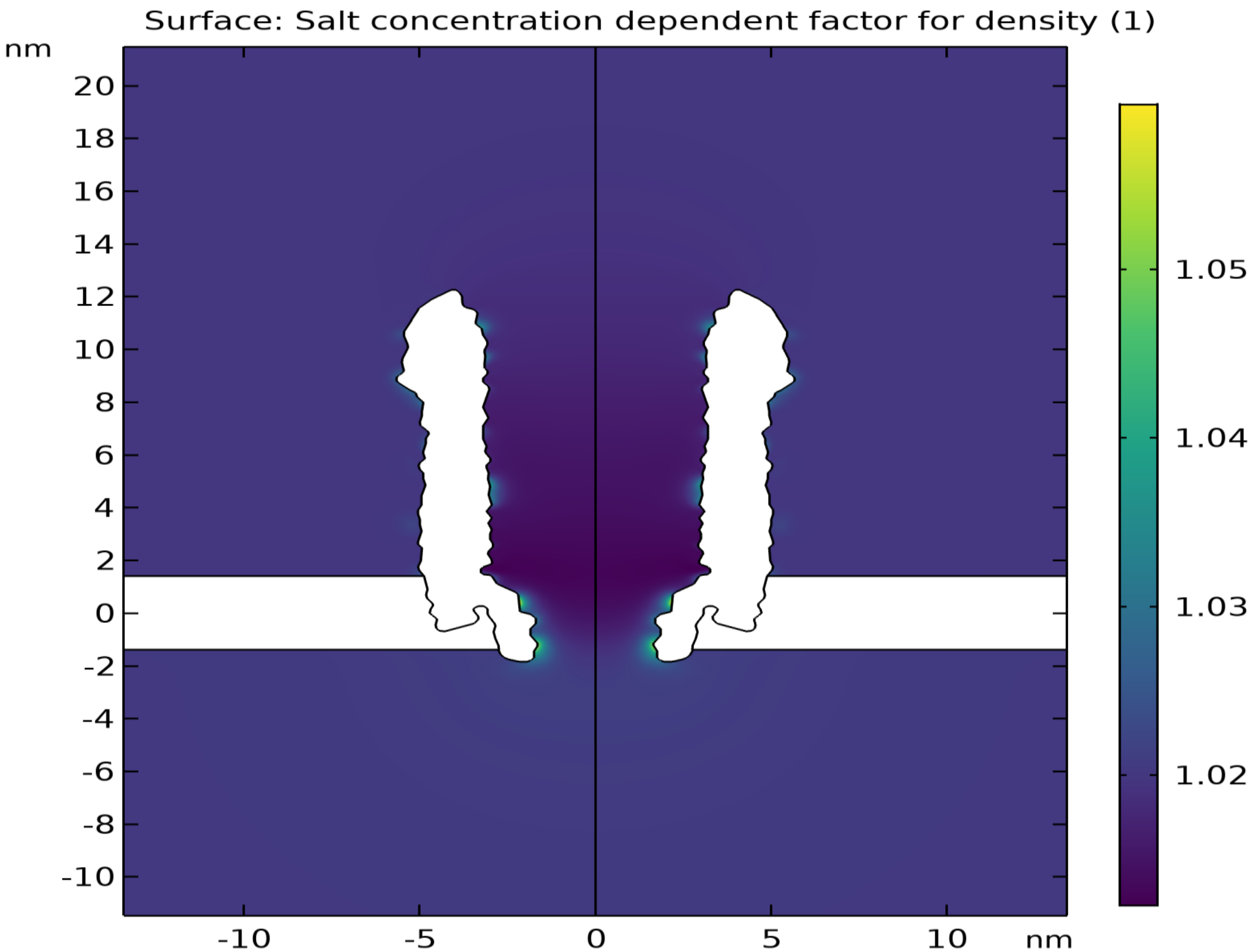
Surface: Salt concentration dependent factor for ion mobility, cpos (1) Surface: Salt concentration dependent factor for ion mobility, cneg (1)

5.3.3 cdf eta



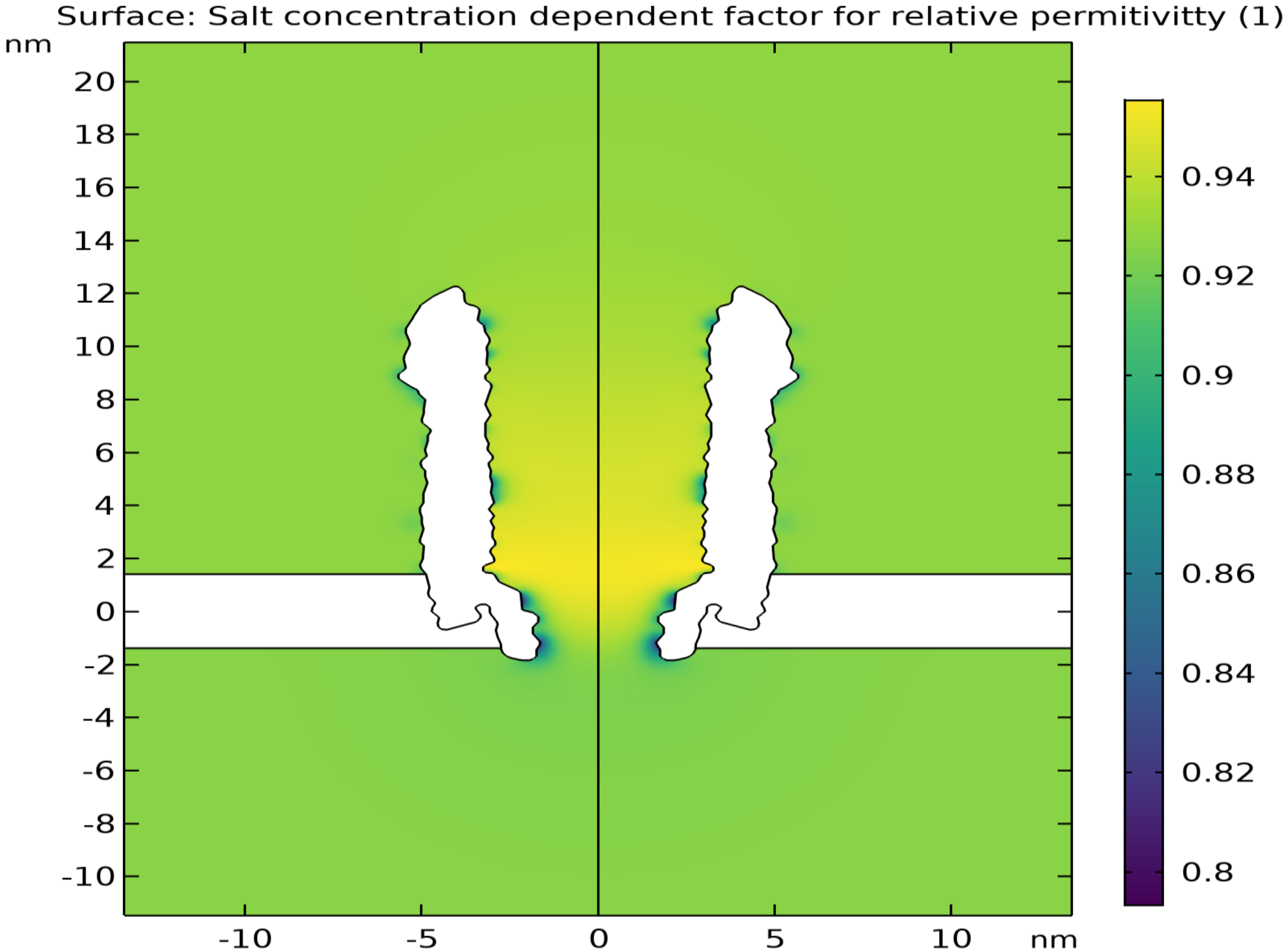
Surface: Salt concentration dependent factor for viscosity (1)

5.3.4 cdf rho



Surface: Salt concentration dependent factor for density (1)

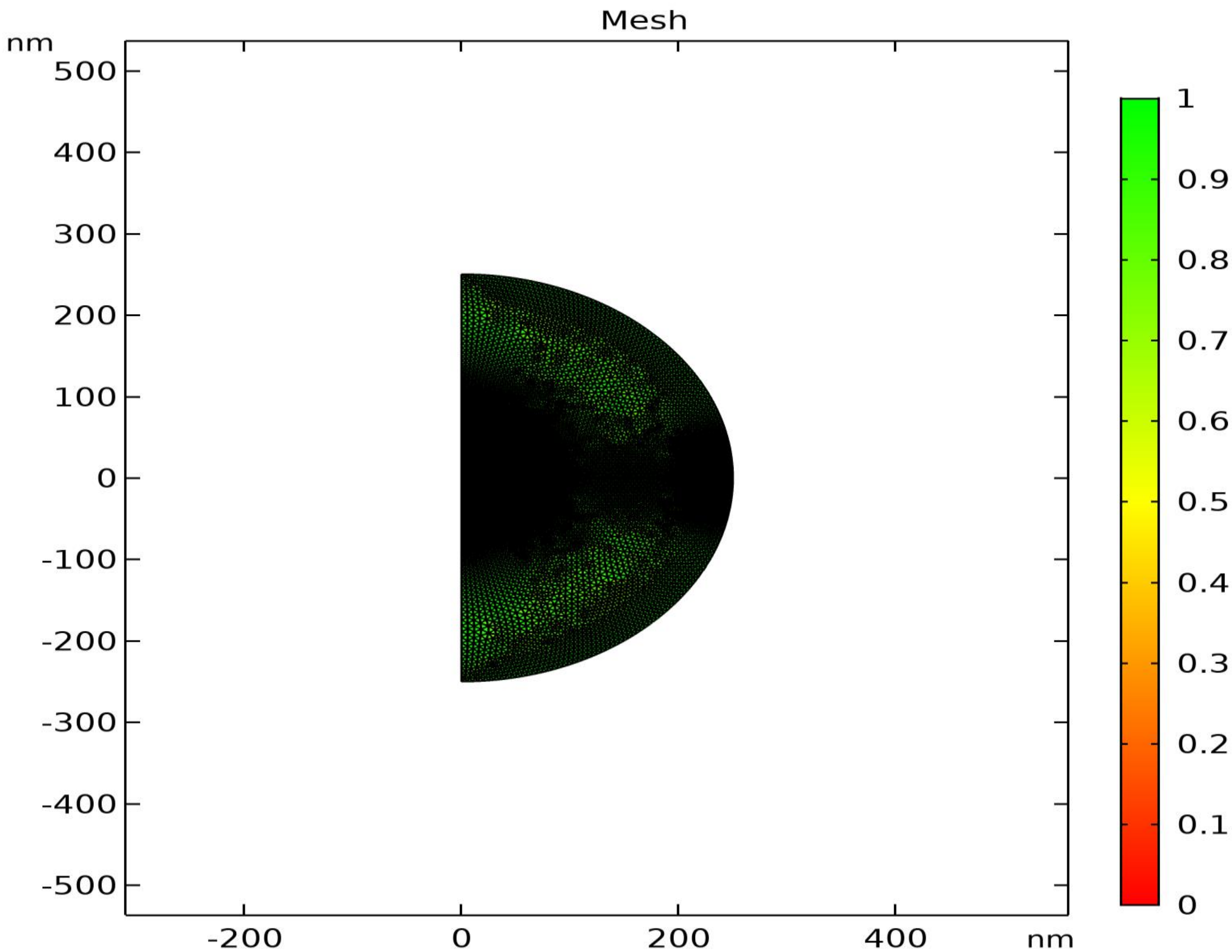
5.3.5 cdf epsr_w



Surface: Salt concentration dependent factor for relative permitivitty (1)

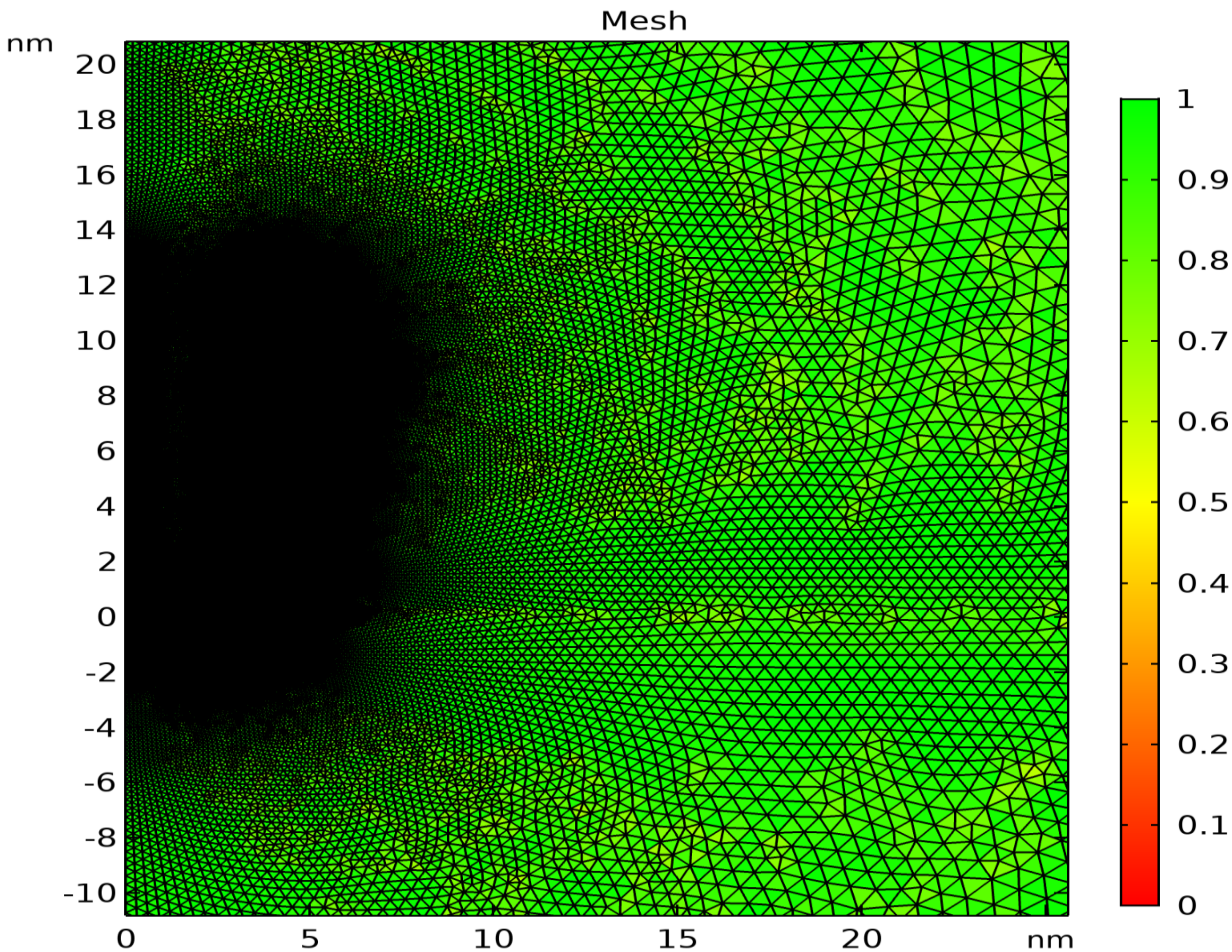
5.4 MESH QUALITY

5.4.1 Mesh skewness quality (full)



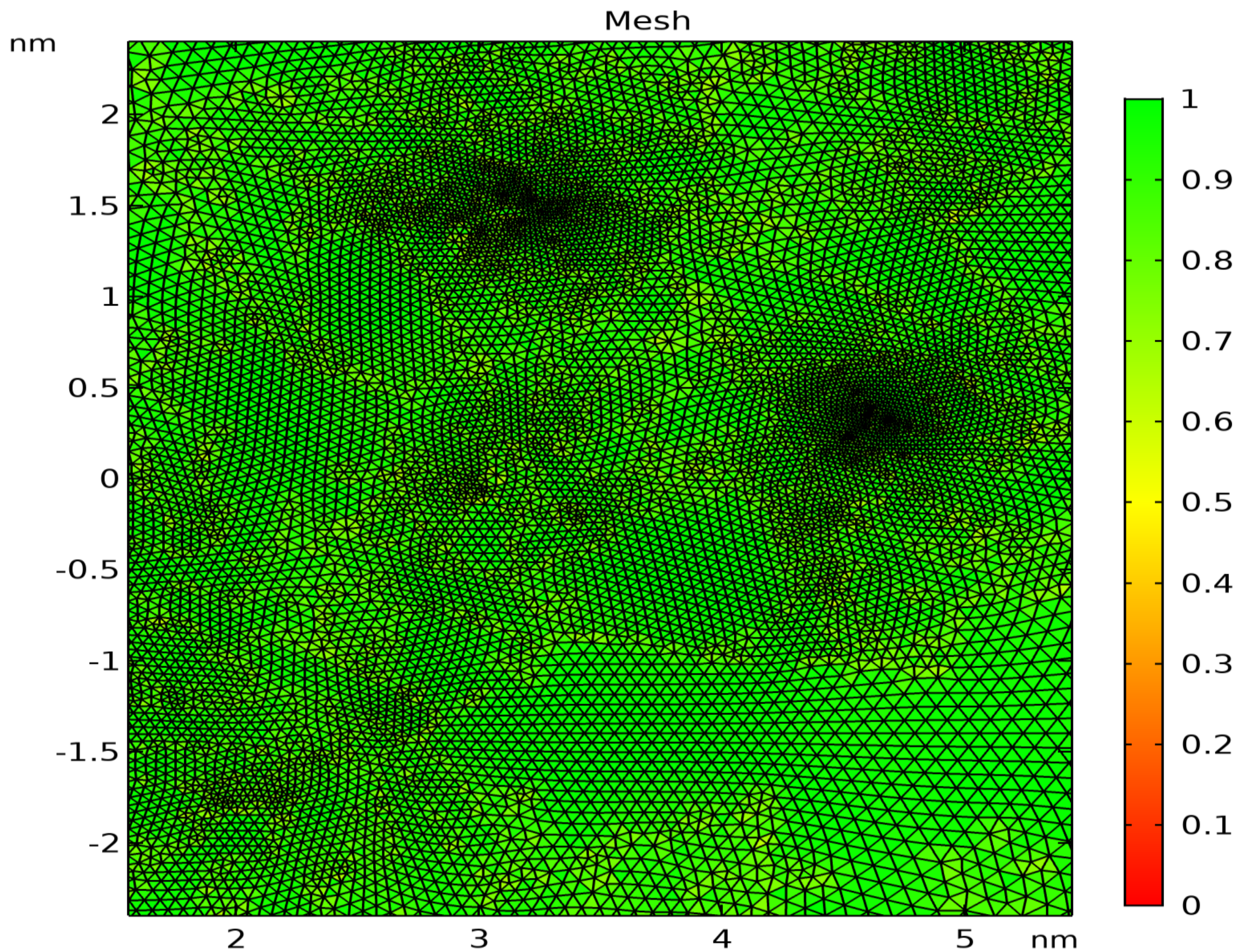
Mesh

5.4.2 Mesh skewness quality (pore)



Mesh

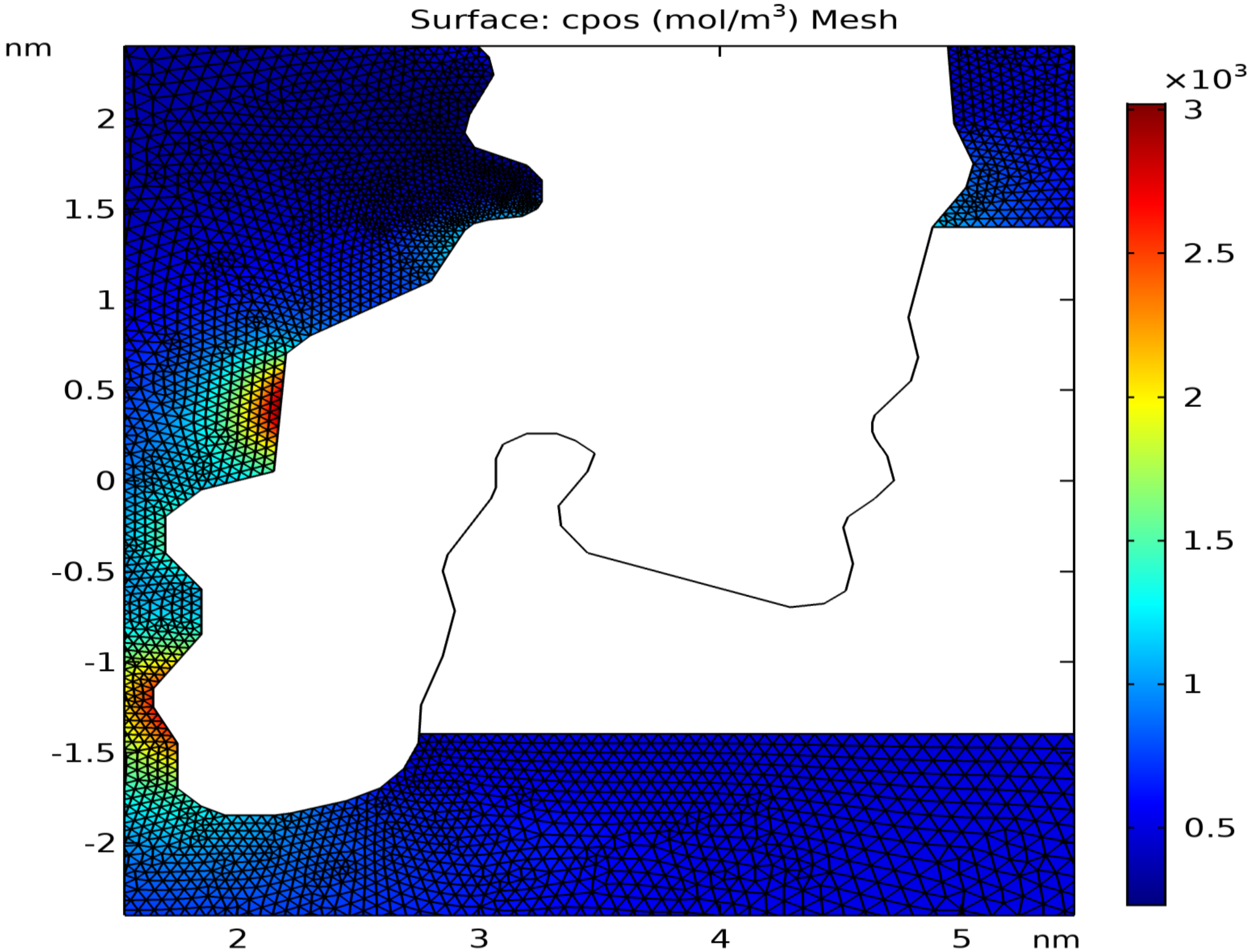
5.4.3 Mesh skewness quality (constriction)



Mesh

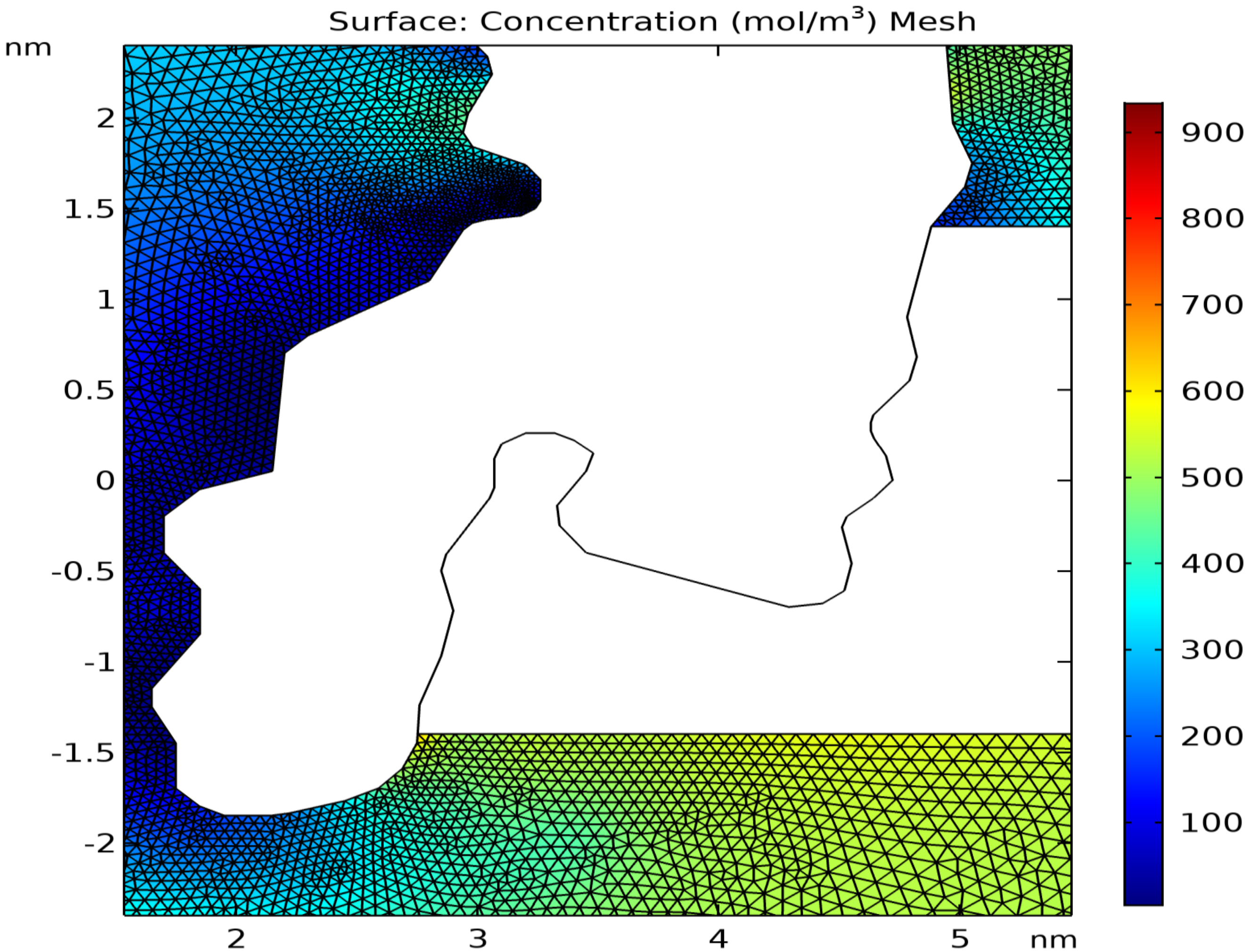
5.5 ELECTRICAL DOUBLE LAYER

5.5.1 Mesh cpos concentration (constriction)



Surface: cpos (mol/m^3) Mesh

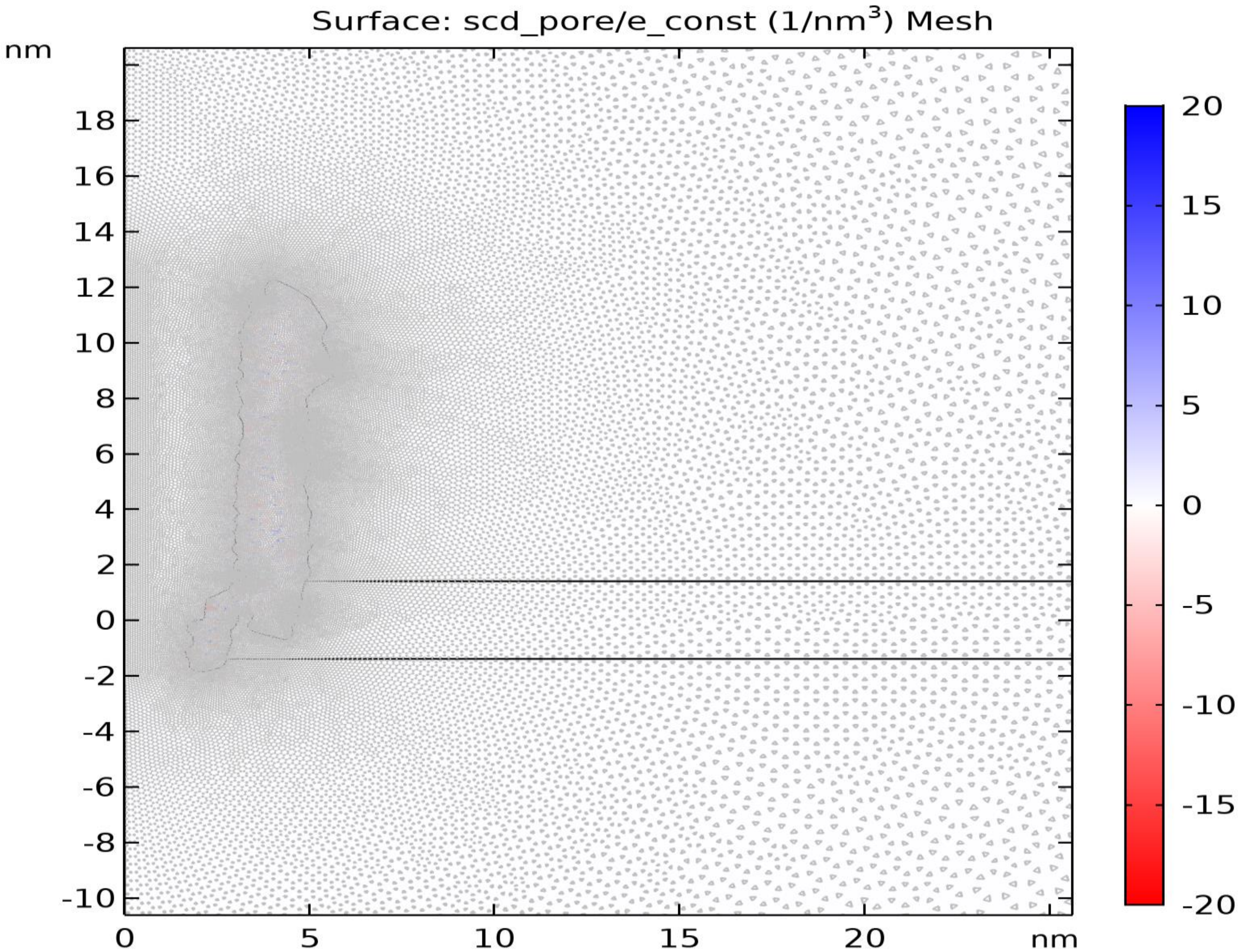
5.5.2 Mesh cneg concentration (constriction)



Surface: Concentration (mol/m^3) Mesh

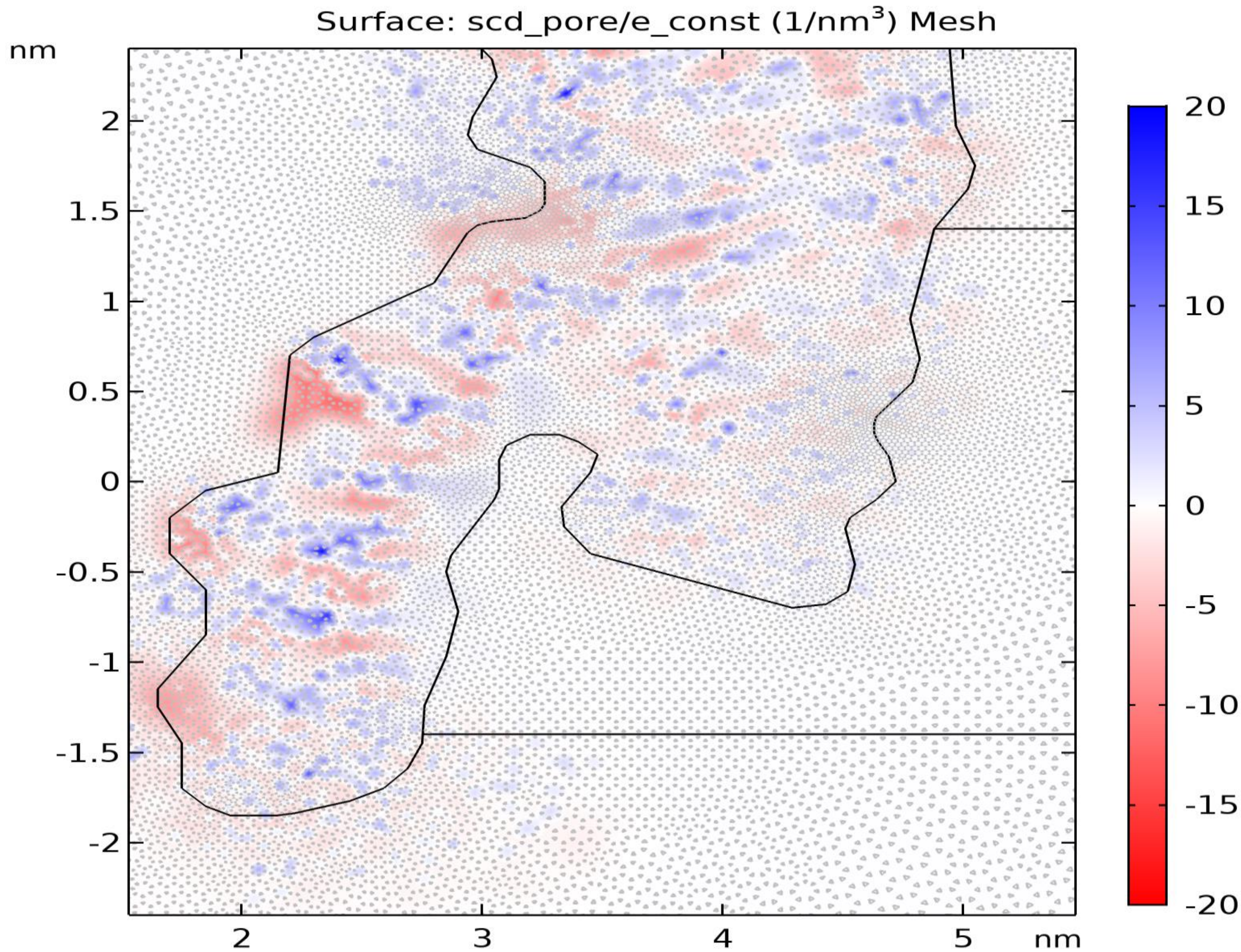
5.6 PORE CHARGE DENSITY

5.6.1 Mesh scd_pore (pore)



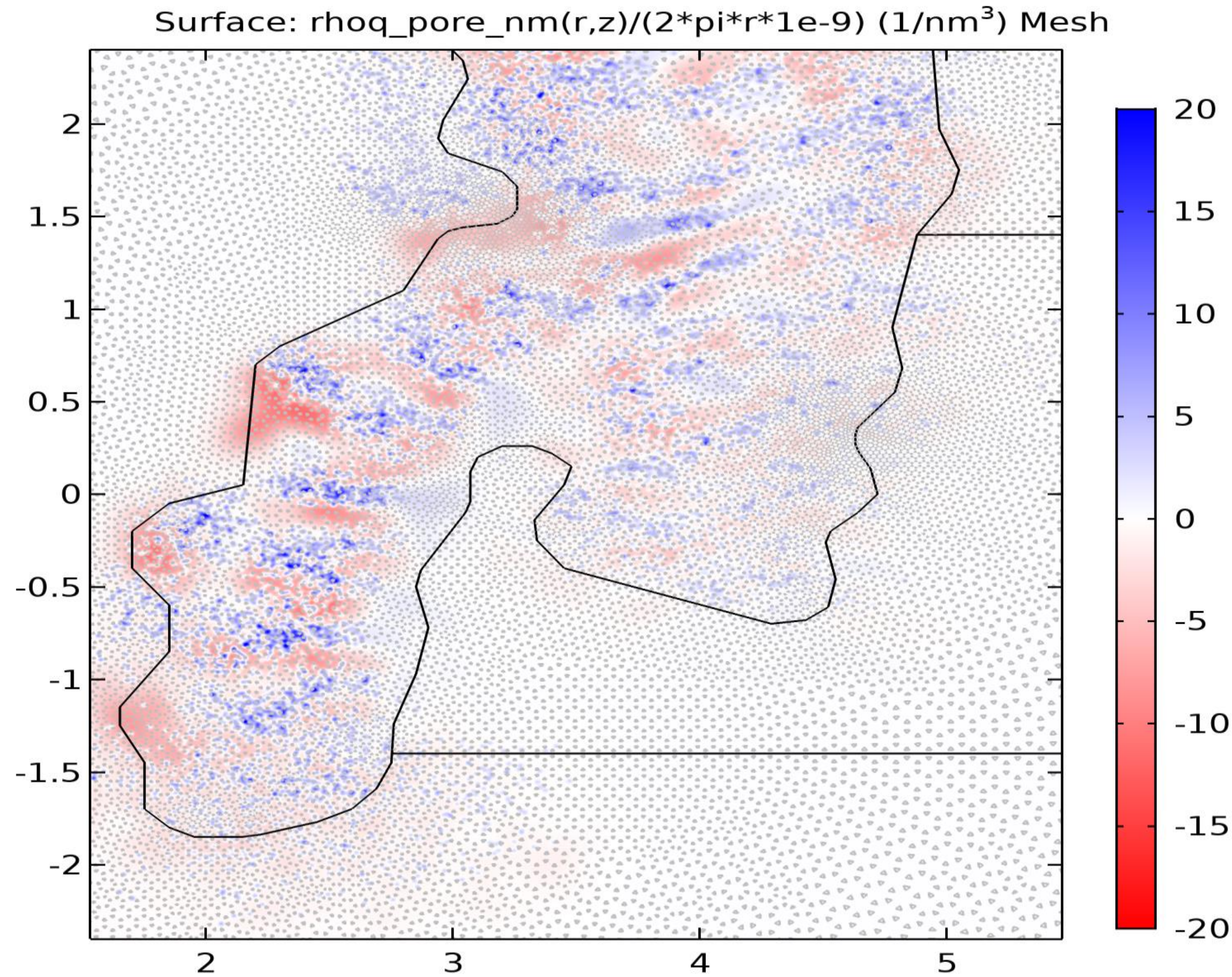
Surface: scd_pore/e_const (1/nm^3) Mesh

5.6.2 Mesh scd_pore (constriction)



Surface: scd_pore/e_const (1/nm^3*) Mesh*

5.6.3 Mesh scd_pore as gridded (constriction)



*Surface: rhoq_pore_nm(r,z)/(2*pi*r*1e-9) (1/nm^3) Mesh*