Supporting Information for

Influence of Electroosmotic Flow on Stochastic Collisions at Ultramicroelectrodes

Scott N. Thorgaard, Sabrina Jenkins, and Anna R. Tarach*

*Grand Valley State University, Department of Chemistry, 1 Campus Drive, 348 Padnos Hall, Allendale MI, 49401, thorgaas@gvsu.edu

Supporting Information Contents:

Electronic supporting materials for this paper also include a movie showing correlated fluorescence microscopy of a collision experiment involving L. lactis. This file is available with the web version of the paper.

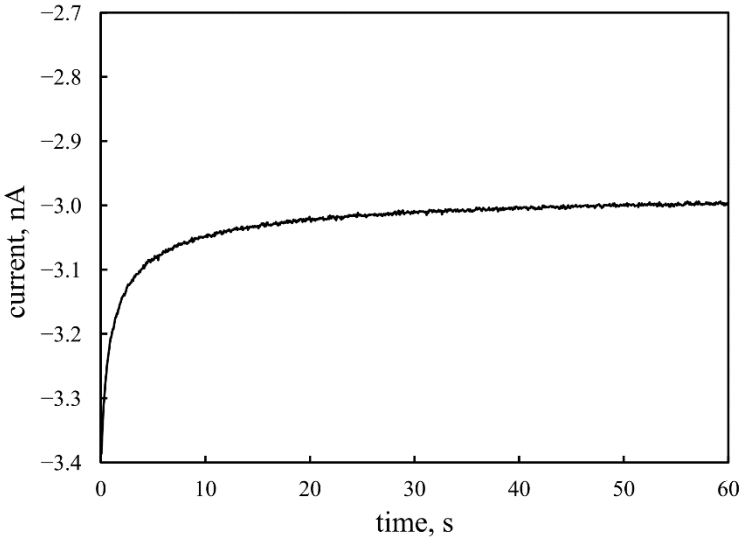


Figure S1. *i–t* curve recorded for a 5 µm radius Pt disk UME in 2 mM FcM with 0.1 mM KCl and no added bacteria. The UME potential was +0.47 V vs Ag/AgCl. All other details were as given in the experimental of the main paper.

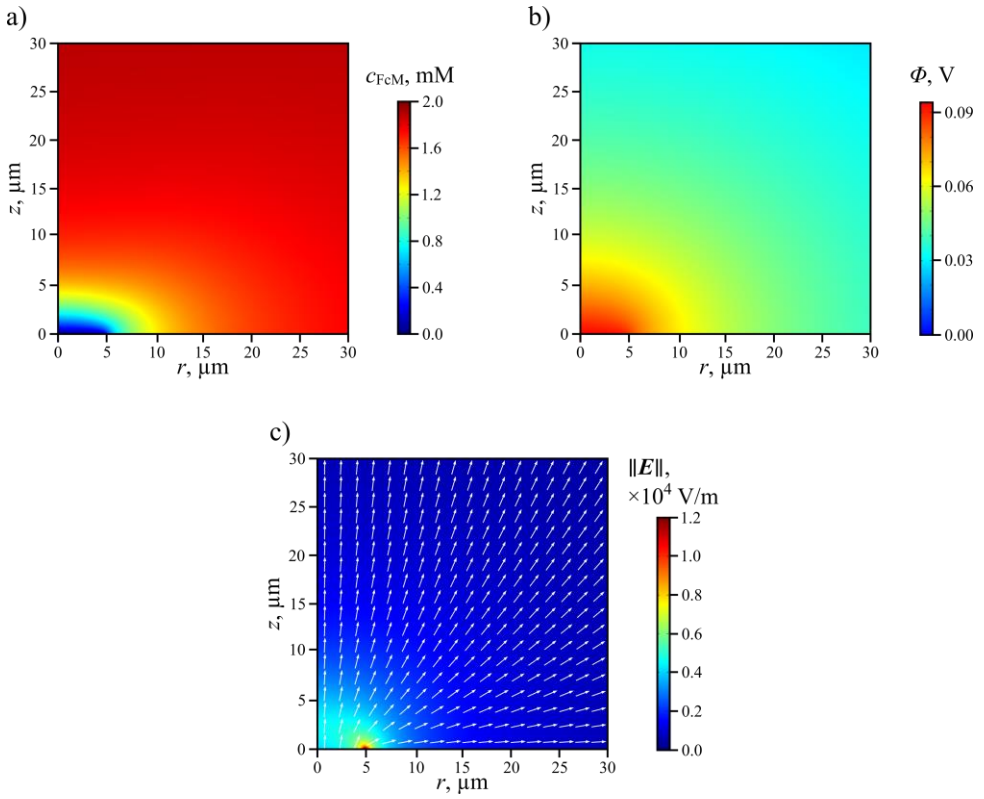


Figure S2. Model output for simulation of a 5 µm disk UME in 2 mM FcM with 0.035 mM KCl, under steady-state oxidation of FcM. For each plot, the center of the electrode disk occurs at r = 0 µm. a) Concentration of FcM. b) Solution electric potential. c) Electric field. The white arrows in the figure indicate directions of the electric field vectors, and the color map indicates the magnitude. The top of the color scale has been adjusted to highlight the electric field in the solution (electric field exactly at the electrode disk edge is larger than the top of the color scale).

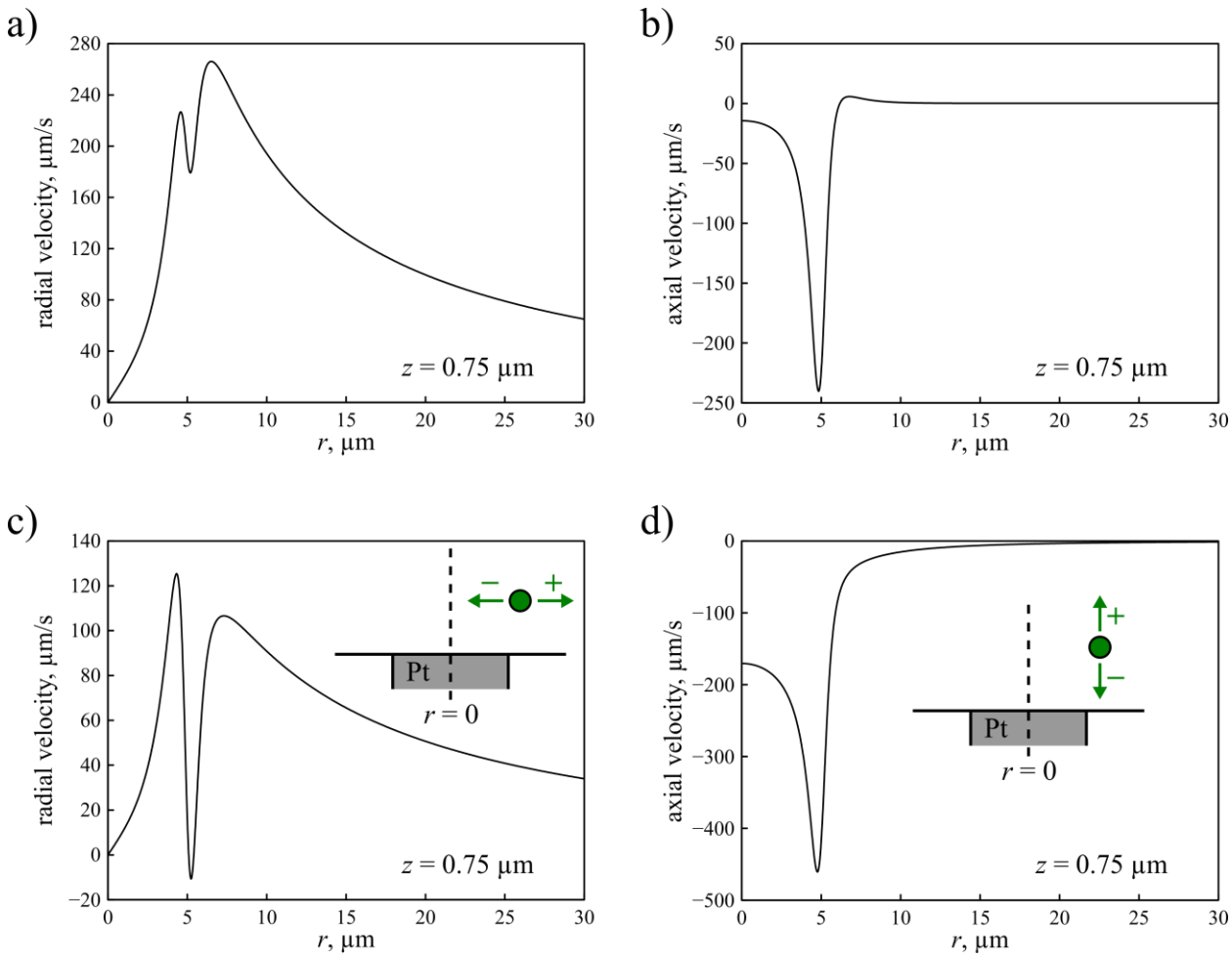


Figure S3. Velocities evaluated from the simulation shown in Figure 2 of the main paper. a) Radial component of solution velocity. b) Axial component of solution velocity. c) Radial component of expected velocity for *L. lactis* (sum of solution and electrophoretic velocities). d) Axial component of expected velocity for *L. lactis*. The center of the UME disk occurs at $r = 0$ μm in all plots. Velocities were evaluated along a line parallel to the electrode plane, with $z = 0.75$ μm.

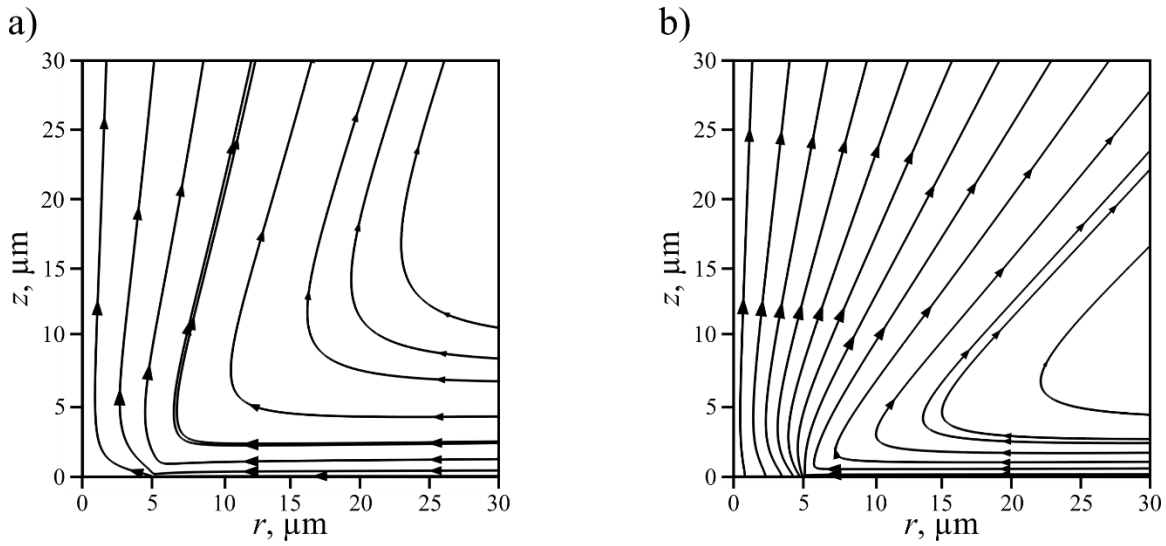


Figure S4. Simulated streamline plots for (a) solution velocity and (b) combined convection and EP velocity for *L. lactis* near a 5 µm radius disk UME in 2 mM A with 0.035 mM KCl, where A was an arbitrary redox species which could be reduced to A^-. These simulations were produced using the finite element model described in the main paper, but with the electrode reaction set to the reduction of A instead of FcM oxidation. Diffusion coefficients, electron transfer kinetics, and the magnitude of the electrode overpotential were set identical to the simulation shown in Figures 2 of the main paper. The sizes of the arrows along each streamline reflect the relative magnitudes of the velocities on a logarithmic scale.

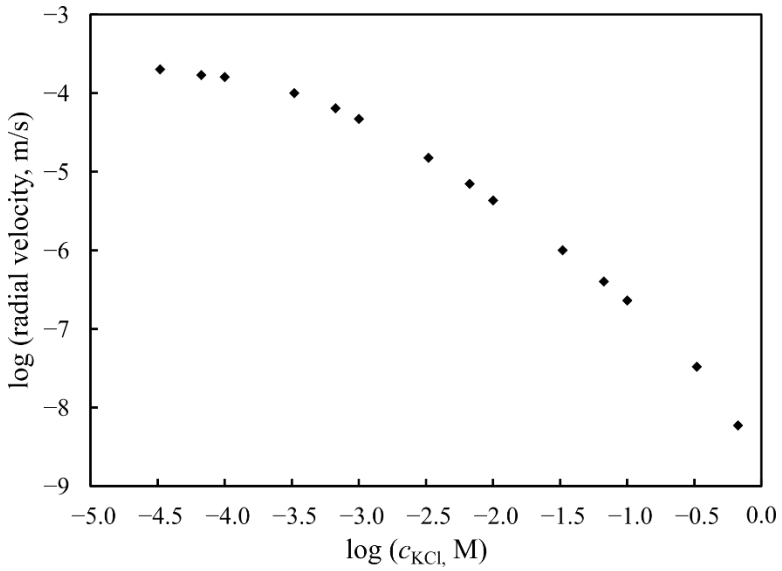


Figure S5. Logarithmic plot of simulated radial velocities from the finite element model as a function of the KCl concentration, with all other details identical to the simulation shown in Figure 2 of the main paper. Velocities (electroosmosis only; no consideration of bacteria electrophoresis) were evaluated from the Navier-Stokes simulation described in the main paper at the point r = 10 µm, z = 0.75 µm.

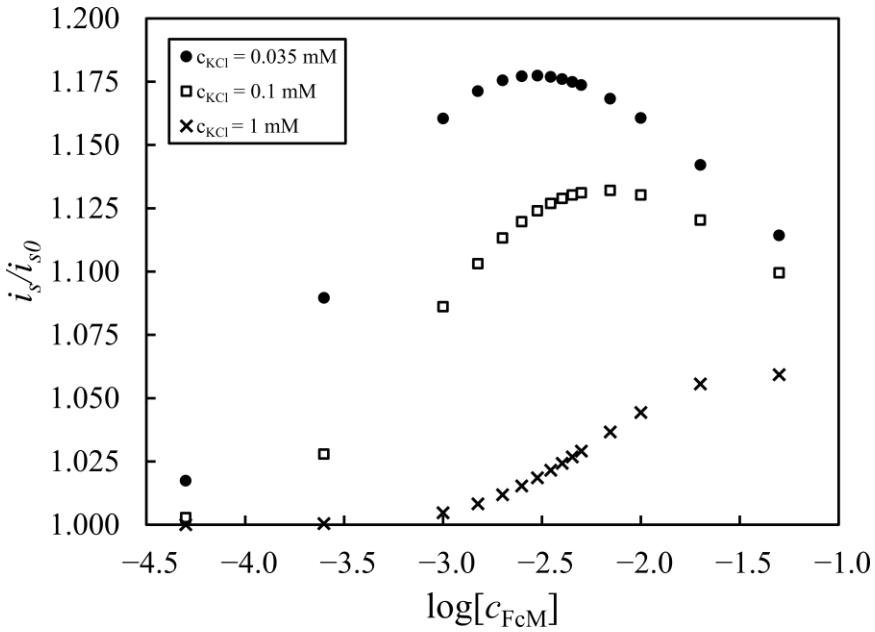


Figure S6. Enhancement of redox species transport by electroosmotic flow, evaluated from the finite element model. i_s/i_{s0} is the ratio of transport-limited steady-state current for FcM oxidation (i_s) at reduced ionic strength to steady-state current for FcM oxidation under fully supported (1 M KCl) conditions (i_{s0}). The supporting electrolyte was either 0.035 mM (circles), 0.1 mM (squares), or 1 mM (crosses) KCl.

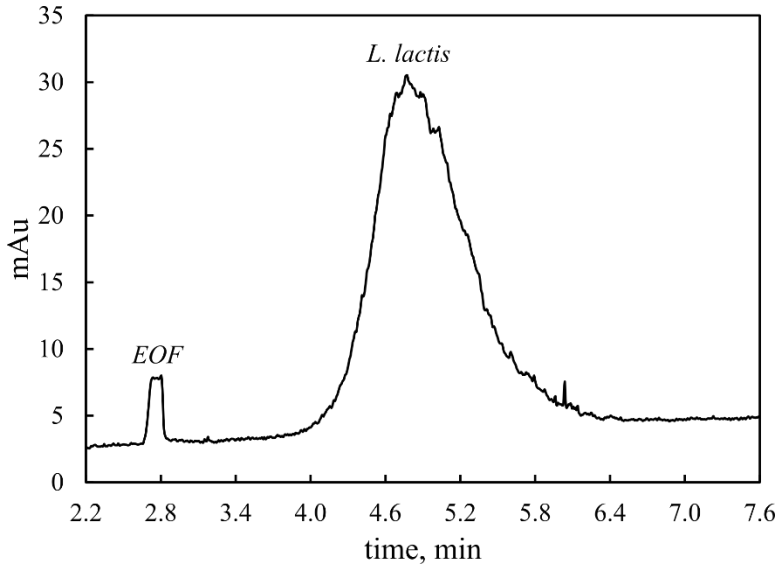


Figure S7. Capillary electropherogram for *L. lactis* in 2 mM FcM with 1 mM KCl. Band detection was performed by UV absorbance at a wavelength of 220 nm. The separation capillary surface was unmodified silica. The capillary had a length of 60.0 cm (detector at 50.0 cm) with an inner diameter of 101 µm. The separation voltage was 20.0 kV. The running solution was 2 mM FcM with 1 mM KCl, and the sample injection consisted of diluted *L. lactis* culture (washed as in the main paper) suspended in 2 mM FcM with 1 mM KCl and 1 mM DMSO. DMSO was added as a neutral species to mark the electroosmotic flow time (EOF peak in figure) for the separation. From a set of three replicate electropherograms, the mean zeta potential of *L. lactis* in 2 mM FcM with 1 mM KCl was determined to be −47.5 (± 0.6) mV.

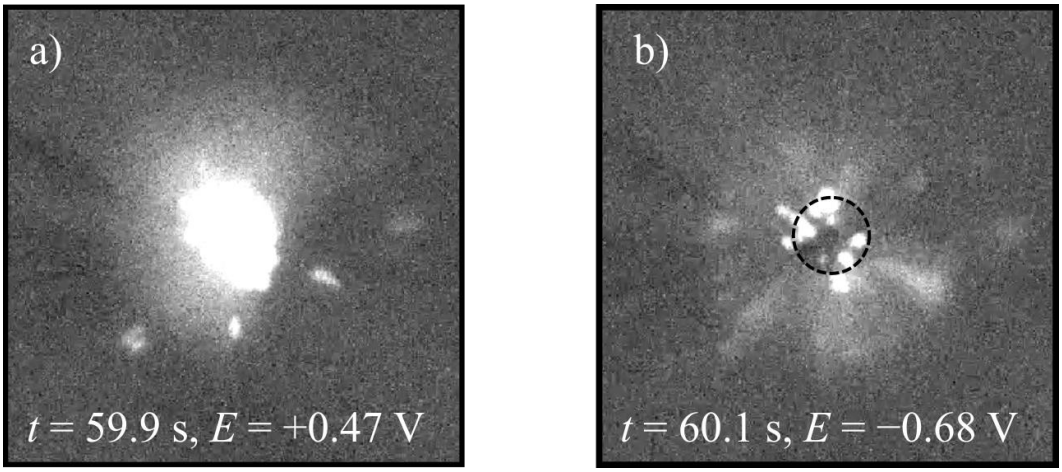


Figure S8. Correlated fluorescence microscopy images from a collision experiment involving *L. lactis.* The images were taken from the same experiment that produced Figure 4 in the main paper, and show the condition of the UME one movie frame before (a) and after (b) the electrode current was switched from negative (FcM oxidation at E = +0.47 V) to positive (oxygen reduction at E = −0.68 V). Before the potential step, the electrode was completely covered with *L. lactis* that had accumulated during the 60 s pulse at E = +0.47 V. After the potential step, most of the accumulated *L. lactis* were "blown off" of the electrode due to the change to convection near the electrode. The 5 µm radius disk UME is marked by a black dashed circle in b), and the numerous indistinct fluorescent objects surrounding the disk are *L. lactis* rapidly leaving the vicinity of the electrode, mostly normal to the electrode disk (out of the microscope focal plane).

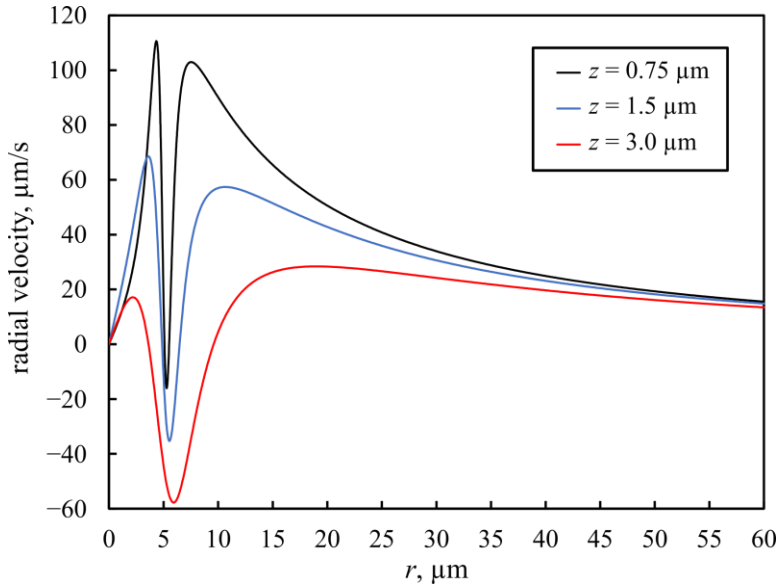


Figure S9. Radial velocities for *L. lactis* (including electrophoresis and convection due electroosmotic flow) from the finite element model for a 5 µm radius Pt UME in 2 mM FcM with 0.035 mM KCl, under steady-state oxidation of FcM. All details were identical Figure S3, c), except that the height of the line along which the radial velocities were evaluated was set to either 0.75 µm (black; same as Figure S3, c), 1.5 µm (blue), or 3.0 µm (red).

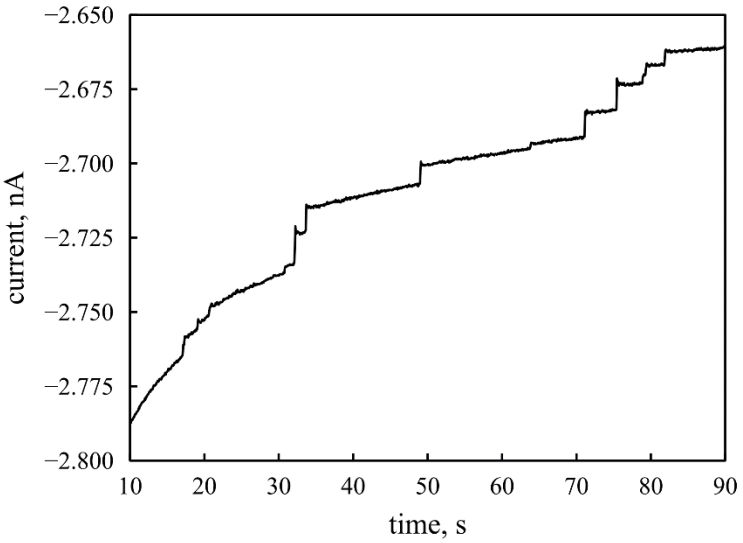


Figure S10. *i–t* curve for a collision experiment in a cell containing 2 mM FcM, 1 mM KCl, and 5.6 fM *L. lactis*, using a 5 µm radius Pt disk UME. The UME potential was +0.42 V vs Ag/AgCl. All other details were as given in the experimental of the main paper.

Appendix A: Development of Finite Element Model

A.1 Description of Model Physics

The geometry of the finite element model used in this work is shown in Figure S11. The model geometry was 2-D axisymmetric, with the electrode disk center placed at the origin. The model included coupled simulations to solve the Nernst-Planck and Navier-Stokes equations, and the boundary conditions for both parts of the model are summarized in Table 1. To simulate solution concentrations, the model solved the Nernst-Planck (1) and differential conservation (2) equations.[1]

$$\boldsymbol{J_i} = -D_i \nabla c_i - \frac{z_i F}{RT} D_i c_i \nabla \Phi + \boldsymbol{u} c_i \qquad (1)$$

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot \boldsymbol{J_i} \qquad (2)$$

Above, $\boldsymbol{J_i}$, D_i, c_i, and z_i are the flux, diffusion coefficient, concentration, and charge of species i, respectively. $\boldsymbol{u}$ is the solution velocity, Φ is the solution electric potential, and F, R, and T have their usual meanings. The model applied the approximation of electroneutrality (3),[2] which allowed values of the solution electric potential to be obtained from the Nernst-Planck equation.[3]

$$\sum_i z_i c_i = 0 \qquad (3)$$

The FcM, FcM^+, and K^+ concentrations were solved for using the Nernst-Planck equation, and the Cl^- concentration was established by electroneutrality. For the Nernst-Planck simulation, a flux boundary condition assuming Butler-Volmer kinetics was applied to the electrode surface to produce oxidation of FcM to FcM^+, with other species set to no flux at the electrode. No flux was assumed for all species at the glass insulation. A condition of fixed concentration was applied to the outer solution boundary. Charge conservation at the electrode

was implemented by treating it as a current source proportional to the flux of FcM, similar to the approach used in reference 3. The glass was assumed to be electrically insulating, and the outer boundary used a condition of fixed potential ($\Phi = 0$).

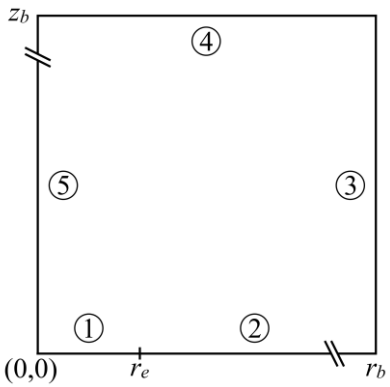


Figure S11. Geometry for the finite element model. The numbered boundaries are 1) Pt disk UME, 2) glass insulation, 3) and 4) outer solution boundary, 5) axis of symmetry. The electrode radius (r_e) was set to 5 µm, and the outer bounds of the simulation (r_b and z_b) were set to 1 mm.

Boundary	**Boundary conditions: Nernst-Planck, mass transport**	**Boundary conditions: Nernst-Planck; charge conservation**	**Boundary conditions: Navier-Stokes**
1 (Pt UME)	Flux (FcM oxidation)	Current source (FcM oxidation)	No slip
2 (glass)	No flux	Insulator	Electroosmotic velocity
3, 4 (outer bound)	Fixed concentration	Fixed potential (Φ = 0 V)	Open boundary

Table 1. Summary of boundary conditions for the finite element model. The numbering of the boundaries matches that in Figure S11.

To include electroosmotic flow occurring at the glass insulation, the model incorporated a coupled a simulation of the solution velocity using the Navier-Stokes equations. Assuming an incompressible flow, low Reynolds number, and constant solution viscosity, the Navier-Stokes equations are,[1]

$$\nabla \cdot \boldsymbol{u} = 0 \tag{4}$$

$$0 = -\nabla p + \mu \nabla^2 \boldsymbol{u} + \boldsymbol{f} \tag{5}$$

where p is the solution pressure, μ is the viscosity, and $\boldsymbol{f}$ is the external force. Electroosmotic flow was included by applying an electroosmotic velocity boundary condition to the glass surrounding the electrode. This applied a slip velocity to the solution touching the glass according to the expression,[4]

$$\boldsymbol{u} = \frac{\varepsilon_r \varepsilon_0 \zeta_g}{\mu} \boldsymbol{E}_t \tag{6}$$

Where ζ_g is the zeta potential of the glass, $\boldsymbol{E}_t$ is the electric field tangential to the surface, and ε_r and ε_0 are the relative and free space permittivities, respectively. The electric field was obtained from electric potential values in the coupled Nernst-Planck simulation. Because our model assumes electroneutrality rather than modelling the electrical double layer at the electrode, a no-slip boundary condition was used for the electrode surface. For elucidating the correlated microscopy in this work, we were primarily concerned with solution velocities at $r > 15$ μm. When an electroosmotic velocity condition was instead used for the UME, the solution velocities at these distances were found to be essentially independent of the zeta potential chosen for the electrode surface within a range of plausible values (Figure S12). Therefore, the no-slip condition, equivalent to assigning the UME a zeta potential of 0 V for the purposes of electroosmotic flow, was adequate for the needs of the model. An open boundary condition,

approximating a boundary in contact with a large volume of liquid (zero normal stress), was applied to outer solution boundary of the simulation.

Zeta potentials for glass and silica known to have a logarithmic dependence on the cation concentration in dilute binary electrolyte solutions.[5,6] Zeta potentials for bacteria also often exhibit a logarithmic dependence on the solution ionic strength.[7–9] When implementing the electroosmotic velocity condition for the glass surface, and also when determining electrophoretic velocities for *L. lactis*, we scaled zeta potentials throughout the model according to the expression below.

$$\zeta = \zeta_0 \frac{\log(c_{K+} + c_{FcM+})}{\log c_0} \qquad (7)$$

Where c_{K+} and c_{FcM+} are the local K^+ and FcM^+ concentrations, ζ_0 is a reference zeta potential, and c_0 is the cation concentration used for the reference zeta potential. A zeta potential of −47.5 (±0.6) mV was determined for *L. lactis* using capillary electrophoresis[10,11] measurements in 2 mM FcM with 1 mM KCl (Figure S7). The zeta potential for the glass in 1 mM KCl was set to −104 mV by adjusting its value to so that bacteria velocities in the model best matched the experimental data shown in Figure 5 of the main paper.

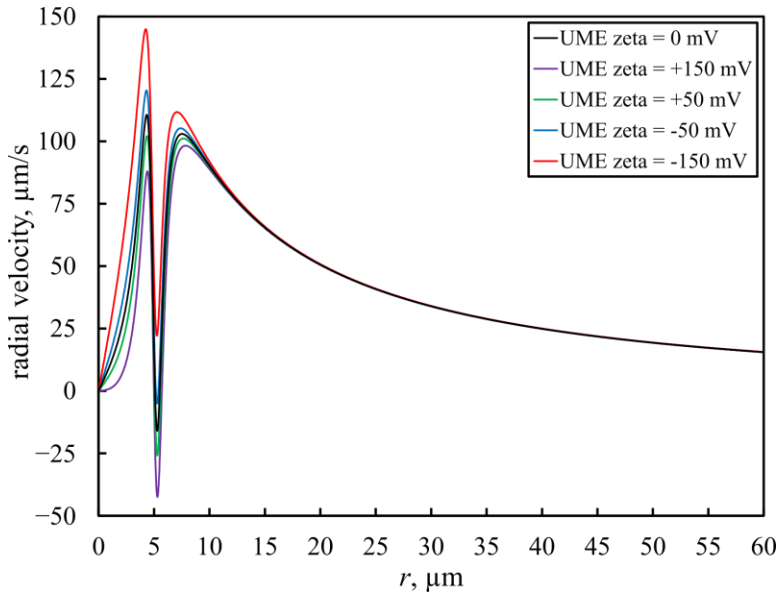


Figure S12. Radial velocities for *L. lactis* (including electrophoresis and convection due to electroosmotic flow) from the finite element model for a 5 µm radius Pt UME in 2 mM FcM with 0.035 mM KCl, under steady-state oxidation of FcM. Each curve shows the radial velocity evaluated with z = 0.75 µm. All model details were identical to the simulation which produced Figure S3, c), except instead of using a no-slip boundary condition for the electrode surface, an electroosmotic velocity condition was applied with the surface zeta potential set to either 0, +150, +50, −50, or −150 mV, as indicated in the legend. The black curve above overlaps exactly with radial velocities in Figure S3, c.

A.2 Other Parameters

The diffusion coefficient of FcM (7.5×10^{-9} m^2/s) was obtained by cyclic voltammetry using the instrumentation described in the main paper. The diffusion coefficient of ferrocenium methanol (FcM^+) was set equal to that of FcM. The diffusion coefficients of K^+ and Cl^- were obtained from literature values of their mobilities. The overpotential of the UME was set to

+0.23 V to match the applied overpotential used for the *L. lactis* collision experiments described in the main paper. The standard rate constant (k^0) and transfer coefficient (α) needed to implement Butler-Volmer kinetics at the UME were set to 0.01 m/s and 0.5, respectively, to reflect reversible electron transfer. Other physical parameters such as the viscosity of water were set to commonly available literature values.

A.3 Meshing of Simulation Domain

The simulation domain shown in Figure S11 was meshed using a series of nodes to prioritize dense elements in the most critical regions of the model. The elements immediately adjacent to the electrode disk edge were set to have a starting *(before refinement)* maximum size of 1 nm. The elements adjacent to the inside of the electrode disk, as well as a portion of the glass insulation extending 2.5 μm beyond the disk edge, were set to have a to have a starting maximum size of 20 nm. The glass insulation for 7.5 μm < r < 80 μm was set have a to have a starting maximum size of 0.5 μm. Finally, a refinement domain consisting of an 80 μm radius quarter-circle around the origin was used to further subdivide elements in the vicinity of the electrode using 2 refinements. Images of the mesh are shown in Figure S13, and additional meshing information is given in the COMSOL Model Report in Appendix B.

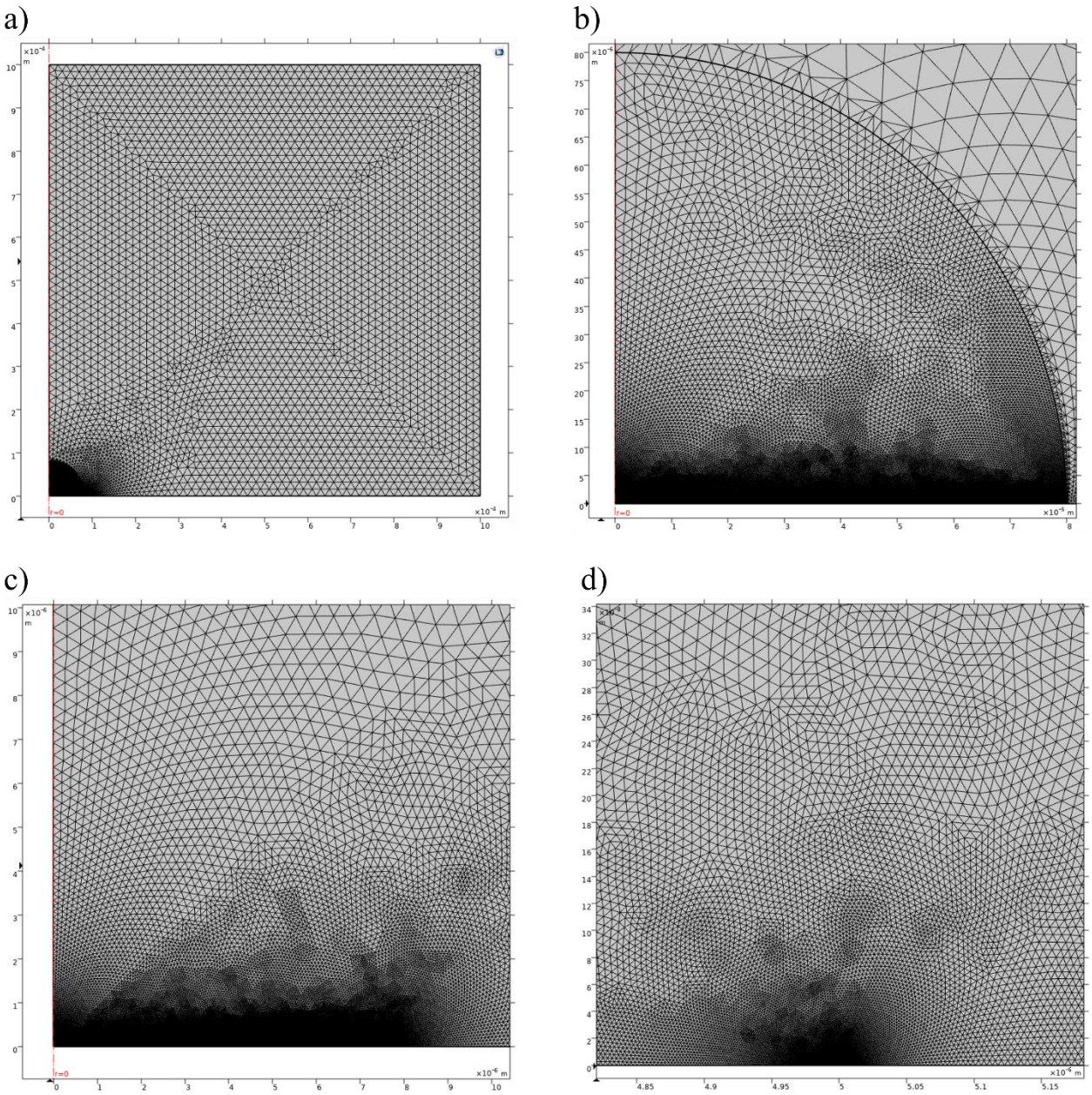


Figure S13. Images of the mesh used for the finite element model. a) Full domain. b) 80 µm wide refinement zone. c) Dense elements along the electrode surface and glass with $r < 7.5$ µm. d) Densest elements near the electrode disk edge at $r = 5$ µm.

References for Appendix A:

1) Newman, J.; Thomas-Aleya, K.E.; *Electrochemical Systems,* 3rd Ed. John Wiley & Sons: Hoboken, NJ, 2004.
2) Dickinson, E.J.F.; Limon-Petersen, J.G.; Compton, R.G. The electroneutrality approximation in electrochemistry *J. Solid State Electrochem.* **2011,** *15,* 1335–1345.
3) Boika, A.; Thorgaard, S.N.; Bard, A.J. Monitoring the Electrophoretic Migration and Adsorption of Single Insulating Nanoparticles at Ultramicroelectrodes *J. Phys. Chem. B* **2013,** *117,* 4371–4380.
4) Slater, G.W.; Tessier, F.; Kopecka, K. The Electroosmotic Flow, In *Microengineering in Biotechnology;* Hughes M.; Hoettges K., Eds. Humana Press: Totowa, NJ, 2009; pp. 121–134.
5) Kirby, B.J.; Hasselbrink, E.F. Zeta potential of microfluidic substrates: 1. Theory, experimental techniques, and effects on separations *Electrophoresis* **2004,** *25,* 187–202.
6) Scales, P.J.; Grieser, F.; Healy, T.W.; White L.R.; Chan, D.Y.C. Electrokinetics of the silica-solution interface: a flat plate streaming potential study *Langmuir,* **1992,** *8,* 965–972.
7) Rijnaarts, H.H.M.; Norde, W.; Lyklema, J.; Zehnder, A.J.B. DLVO and steric contributions to bacterial deposition in media of different ionic strengths *Colloid Surface B* **1999,** *14,* 179–195.
8) van der Wal, A.; Minor, M.; Norde, W.; Zehnder, A.J.B.; Lyklema, J. Electrokinetic Potential of Bacterial Cells *Langmuir,* **1997,** *13,* 165–171.
9) Abbott, A.; Rutter, P.R.; Berkeley, R.C.W. The Influence Of Ionic Strength, Ph And A Protein Layer On The Interaction Between Streptococcus Mutans And Glass Surfaces *J. Gen. Microbiol.* **1983,** *129,* 439–445.

10) Soni, K.A.; Balasubramanian, A.K.; Beskok, A.; Pillai, S.D. Zeta Potential of Selected Bacteria in Drinking Water When Dead, Starved, or Exposed to Minimal and Rich Culture Media *Curr. Microbiol.* **2008,** *56,* 93–97.

11) Pfetsch, A.; Welsch, T. Determination of the electrophoretic mobility of bacteria and their separation by capillary zone electrophoresis *Fresenius J. Anal. Chem.* **1997,** *359,* 198–201.

Appendix B: COMSOL Model Report

Contents:

1 Global Definitions

Date	Jul 3, 2020 1:15:00 PM

GLOBAL SETTINGS

Name	2020-07-03 003 EOF.mph
Path	C:\COMSOL Projects\2020-03 EOF at UME\2020-07-03_003 EOF.mph
Version	COMSOL Multiphysics 5.4 (Build: 388)
Unit system	SI

USED PRODUCTS

COMSOL Multiphysics
Electrochemistry Module

1.1 PARAMETERS

PARAMETERS 1

Name	Expression	Value	Description
zO	1	1	oxidized species charge
zRed	0	0	reduced species charge
zM	1	1	supporting cation charge
zA	-1	−1	supporting anion charge
E	0.23 [V]	0.23 V	applied potential
Ef	0 [V]	0 V	rxn formal potential
k0	0.01 [m/s]	0.01 m/s	standard rate constant
a	0.5	0.5	alpha (transfer coefficient)
f	(9.6485E4 [C])*(1/(8.3145 [J/K]))*(1/(298.15 [K]))	38.921 1/V	F/RT
cObulk	0[M]	0 mol/m^3	oxidized species bulk conc
cRbulk	0.002[M]	2 mol/m^3	reduced species bulk conc
cMAbulk	0.000035[M]	0.035 mol/m^3	supporting electrolyte bulk conc
cMbulk	cMAbulk	0.035 mol/m^3	supporting cation bulk conc
cAbulk	cMAbulk	0.035 mol/m^3	supporting anion bulk conc
F	(9.649E4 [C/mol])	96490 C/mol	Faraday constant
DR	7.5E-10[m^2/s]	7.5E−10 m^2/s	Diffusion coefficient of R (FcM)
DO	DR	7.5E−10 m^2/s	Diffusion coefficient of O (FcM+)

Name	Expression	Value	Description
DM	1.958e-9[m^2/s]	1.958E−9 m^2/s	Diffusion coefficient of M (K+)
DA	2.033e-9[m^2/s]	2.033E−9 m^2/s	Diffusion coefficient of A (Cl-)
re	5E-6 [m]	5E−6 m	UME disk radius
visc	0.0009544 [Pa*s]	9.544E−4 Pa·s	viscosity of water at 22 degC
epsilon0	8.8542E-12 [F/m]	8.8542E−12 F/m	Permittivity of free space
epsilonM	80	80	Relative permittivity
epsilon	epsilon0*epsilonM	7.0834E−10 F/m	Permittivities
zeta0	-0.104 [V]	−0.104 V	Reference zeta for glass in 1 mM KCl
zetabac0	-0.0475 [V]	−0.0475 V	Reference zeta for L. lactis in 1 mM KCl

2 Component 1

Date	May 17, 2019 2:19:00 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 Coordinate Systems

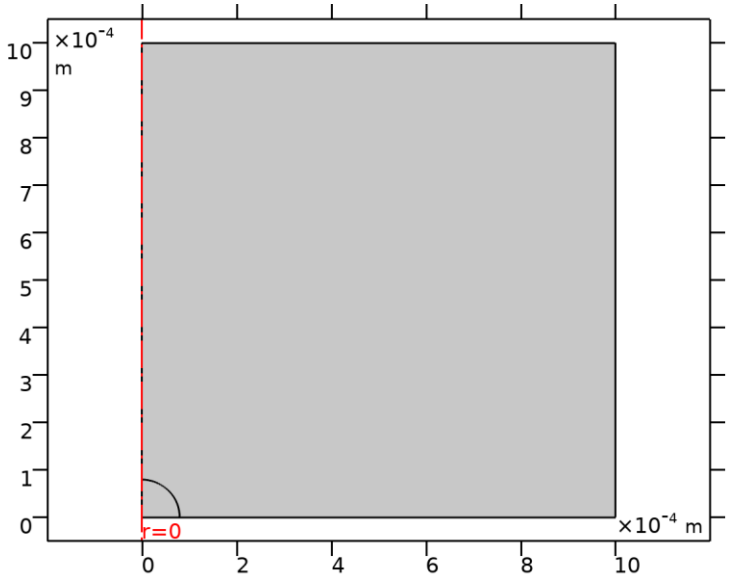
Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	to	n

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	m
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	2
Number of domains	2
Number of boundaries	9
Number of vertices	8

2.2.1 Square, Full simulation domain (sq1)

POSITION

Description	Value
Position	{0, 0}

SIZE

Description	Value
Side length	1E-3

2.2.2 Point, UME edge (pt2)

POINT

Description	Value
Point coordinate	{5.0E-6, 0}

2.2.3 Point, Marker for finer mesh elements (pt4)

POINT

Description	Value
Point coordinate	{7.500000000000001E-6, 0}

2.2.4 Circle, Refinement zone (c1)

POSITION

Description	Value
Position	{0, 0}

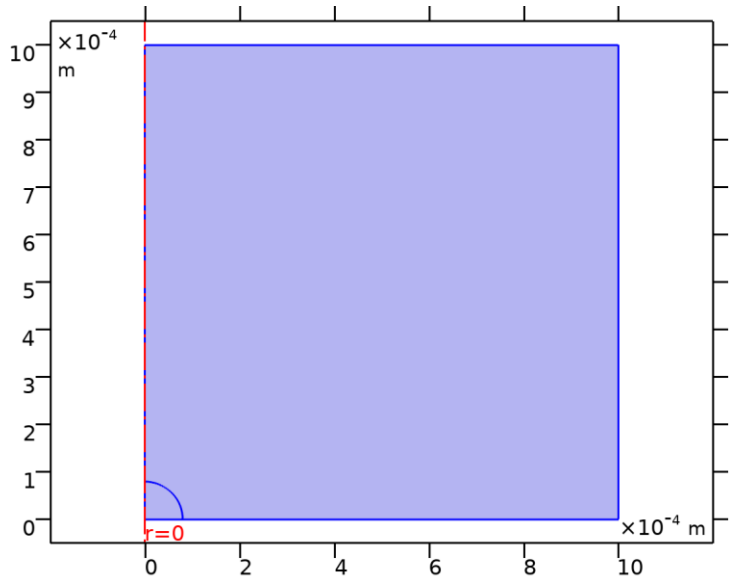
SIZE AND SHAPE

Description	Value
Radius	80E-6
Sector angle	90

2.3 TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK

USED PRODUCTS

COMSOL Multiphysics
Electrochemistry Module



Tertiary Current Distribution, Nernst-Planck

SELECTION

Geometric entity level	Domain
Selection	Domains 1–2

EQUATIONS

$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i$$
$$\nabla \cdot \mathbf{i}_l = F \sum_i z_i R_i + Q_l$$
$$\sum_i z_i c_i = 0$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla \phi_l$$
$$\mathbf{i}_l = F \sum_i z_i \mathbf{J}_i$$
$$\nabla \cdot \mathbf{i}_s = -F \sum_i z_i R_i + Q_s, \quad \mathbf{i}_s = -\sigma_s \nabla \phi_s$$
$$\phi_l = \mathrm{phi}, \quad \phi_s = \mathrm{phis}$$

2.3.1 Interface settings

Discretization

SETTINGS

Description	Value
Concentration	Quadratic
Electrolyte potential	Quadratic
Electric potential	Quadratic

Species

SETTINGS

Description	Value
Charge conservation model	Electroneutrality
From electroneutrality	cA

Advanced settings

SETTINGS

Description	Value
Convective term	Nonconservative form

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

2.3.2 Variables

Name	Expression	Unit	Description	Selection	Details
domflux.cOr	2*(tcd.dflux_cOr+tcd.mflux_cOr)*pi*r	mol/(m·s)	Domain flux, r component	Domains 1–2	
domflux.cOz	2*(tcd.dflux_cOz+tcd.mflux_cOz)*pi*r	mol/(m·s)	Domain flux, z component	Domains 1–2	
domflux.cRr	2*(tcd.dflux_cRr+tcd.mflux_cRr)*pi*r	mol/(m·s)	Domain flux, r component	Domains 1–2	
domflux.cRz	2*(tcd.dflux_cRz+tcd.mflux_cRz)*pi*r	mol/(m·s)	Domain flux, z component	Domains 1–2	
domflux.cMr	2*(tcd.dflux_cMr+tcd.mflux_cMr)*pi*r	mol/(m·s)	Domain flux, r component	Domains 1–2	
domflux.cMz	2*(tcd.dflux_cMz+tcd.mflux_cMz)*pi*r	mol/(m·s)	Domain flux, z component	Domains 1–2	
domflux.cAr	2*(tcd.dflux_cAr+tcd.mflux_cAr)*pi*r	mol/(m·s)	Domain flux, r component	Domains 1–2	
domflux.cAz	2*(tcd.dflux_cAz+tcd.mflux_cAz)*pi*r	mol/(m·s)	Domain flux, z component	Domains 1–2	
domflux.phir	2*tcd.Ilr*pi*r	A/m	Domain flux, r component	Domains 1–2	
domflux.phiz	2*tcd.Ilz*pi*r	A/m	Domain flux, z component	Domains 1–2	
domflux.phisr	2*tcd.Isr*pi*r	A/m	Domain flux, r component	Domains 1–2	
domflux.phisz	2*tcd.Isz*pi*r	A/m	Domain flux, z component	Domains 1–2	
tcd.bndflux_phil	if(r>0.001/sqrt(sqrt(mean(emetric2))),-	A/m^2	Boundary flux	Boundaries 1–8	

Name	Expression	Unit	Description	Selection	Details
	0.5*dflux_spatial(phi)/(pi*r),NaN)				
tcd.bndflux_phil	if(r>0.001/sqrt(sqrt(mean(emetric2))),0.25*(uflux_spatial(phi)-dflux_spatial(phi))/(pi*r),NaN)	A/m²	Boundary flux	Boundary 9	
tcd.nIl	tcd.bndflux_phil	A/m²	Normal electrolyte current density	Boundaries 2, 4–9	
tcd.nR	nR	1	Normal vector, R component	Boundary 9	
tcd.nPHI	0	1	Normal vector, PHI component	Boundary 9	
tcd.nZ	nZ	1	Normal vector, Z component	Boundary 9	
tcd.nR	dnR	1	Normal vector, R component	Boundaries 1–8	
tcd.nPHI	0	1	Normal vector, PHI component	Boundaries 1–8	
tcd.nZ	dnZ	1	Normal vector, Z component	Boundaries 1–8	
tcd.ndflux_cO	tcd.dflux_cOr*tcd.nrc+tcd.dflux_cOphi*tcd.nphic+tcd.dflux_cOz*tcd.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 2, 4–9	
tcd.ncflux_cO	tcd.cflux_cOr*tcd.nrc+tcd.cflux_cOphi*tcd.nphic+tcd.cflux_cOz*tcd.nzc	mol/(m²·s)	Normal convective flux	Boundaries 2, 4–9	
tcd.nmflux_cO	tcd.mflux_cOr*tcd.nrc+tcd.mflux_cOphi*tcd.nphic+tcd.mflux_cOz*tcd.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 2, 4–9	
tcd.ntflux_cO	tcd.bndFlux_cO+tcd.cflux_cOr*tcd.nrc+tcd.cflux_cOphi*tcd.nphic+tcd.cflux_cOz*tcd.nzc	mol/(m²·s)	Normal total flux	Boundaries 2, 4–9	
tcd.ndflux_cR	tcd.dflux_cRr*tcd.nrc+tcd.dflux_cRphi*t	mol/(m²·s)	Normal diffusive flux	Boundaries 2, 4–9	

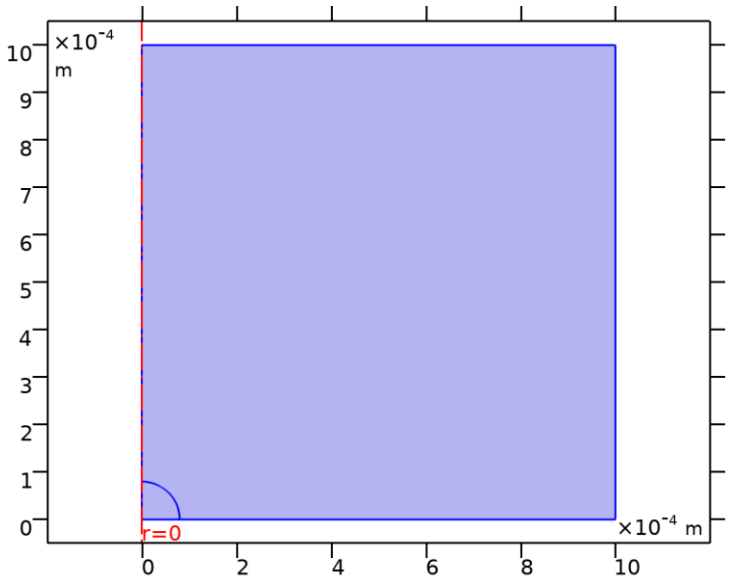
Name	Expression	Unit	Description	Selection	Details
	cd.nphic+tcd.dflux_cRz*tcd.nzc				
tcd.ncflux_cR	tcd.cflux_cRr*tcd.nrc+tcd.cflux_cRphi*tcd.nphic+tcd.cflux_cRz*tcd.nzc	mol/(m²·s)	Normal convective flux	Boundaries 2, 4–9	
tcd.nmflux_cR	tcd.mflux_cRr*tcd.nrc+tcd.mflux_cRphi*tcd.nphic+tcd.mflux_cRz*tcd.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 2, 4–9	
tcd.ntflux_cR	tcd.bndFlux_cR+tcd.cflux_cRr*tcd.nrc+tcd.cflux_cRphi*tcd.nphic+tcd.cflux_cRz*tcd.nzc	mol/(m²·s)	Normal total flux	Boundaries 2, 4–9	
tcd.ndflux_cM	tcd.dflux_cMr*tcd.nrc+tcd.dflux_cMphi*tcd.nphic+tcd.dflux_cMz*tcd.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 2, 4–9	
tcd.ncflux_cM	tcd.cflux_cMr*tcd.nrc+tcd.cflux_cMphi*tcd.nphic+tcd.cflux_cMz*tcd.nzc	mol/(m²·s)	Normal convective flux	Boundaries 2, 4–9	
tcd.nmflux_cM	tcd.mflux_cMr*tcd.nrc+tcd.mflux_cMphi*tcd.nphic+tcd.mflux_cMz*tcd.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 2, 4–9	
tcd.ntflux_cM	tcd.bndFlux_cM+tcd.cflux_cMr*tcd.nrc+tcd.cflux_cMphi*tcd.nphic+tcd.cflux_cMz*tcd.nzc	mol/(m²·s)	Normal total flux	Boundaries 2, 4–9	
tcd.ndflux_cA	tcd.dflux_cAr*tcd.nrc+tcd.dflux_cAphi*tcd.nphic+tcd.dflux_cAz*tcd.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 2, 4–9	
tcd.ncflux_cA	tcd.cflux_cAr*tcd.nrc+tcd.cflux_cAphi*tcd.nphic+tcd.cflux_cAz*tcd.nzc	mol/(m²·s)	Normal convective flux	Boundaries 2, 4–9	
tcd.nmflux_cA	tcd.mflux_cAr*tcd.nrc+tcd.mflux_cAphi	mol/(m²·s)	Normal electrophoretic flux	Boundaries 2, 4–9	

Name	Expression	Unit	Description	Selection	Details
	*tcd.nphic+tcd.mflux_cAz*tcd.nzc				
tcd.ntflux_cA	(tcd.cflux_cAr+tcd.mflux_cAr)*tcd.nrc+(tcd.cflux_cAphi+tcd.mflux_cAphi)*tcd.nphic+(tcd.cflux_cAz+tcd.mflux_cAz)*tcd.nzc+tcd.ndflux_cA	mol/(m²·s)	Normal total flux	Boundaries 2, 4–9	
tcd.bndFlux_cO	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cO)/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundaries 1–8	
tcd.bndFlux_cO	if(r>0.001/sqrt(sqrt(mean(emetric2))),0.25*(uflux_spatial(cO)-dflux_spatial(cO))/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundary 9	
tcd.bndFlux_cR	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cR)/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundaries 1–8	
tcd.bndFlux_cR	if(r>0.001/sqrt(sqrt(mean(emetric2))),0.25*(uflux_spatial(cR)-dflux_spatial(cR))/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundary 9	
tcd.bndFlux_cM	if(r>0.001/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cM)/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundaries 1–8	
tcd.bndFlux_cM	if(r>0.001/sqrt(sqrt(mean(emetric2))),0.25*(uflux_spatial(cM)-dflux_spatial(cM))/(pi*r),NaN)	mol/(m²·s)	Boundary flux	Boundary 9	
tcd.nr	nr	1	Normal vector, r component	Boundary 9	
tcd.nphi	0	1	Normal vector, phi component	Boundary 9	

Name	Expression	Unit	Description	Selection	Details
tcd.nz	nz	1	Normal vector, z component	Boundary 9	
tcd.nr	dnr	1	Normal vector, r component	Boundaries 1–8	
tcd.nphi	0	1	Normal vector, phi component	Boundaries 1–8	
tcd.nz	dnz	1	Normal vector, z component	Boundaries 1–8	
tcd.nrmesh	root.nrmesh	1	Normal vector (mesh), r component	Boundary 9	
tcd.nphimesh	0	1	Normal vector (mesh), phi component	Boundary 9	
tcd.nzmesh	root.nzmesh	1	Normal vector (mesh), z component	Boundary 9	
tcd.nrmesh	dnrmesh	1	Normal vector (mesh), r component	Boundaries 1–8	
tcd.nphimesh	0	1	Normal vector (mesh), phi component	Boundaries 1–8	
tcd.nzmesh	dnzmesh	1	Normal vector (mesh), z component	Boundaries 1–8	
tcd.nrc	root.nrc/tcd.ncLen	1	Normal vector, r component	Boundaries 1–9	
tcd.nphic	0	1	Normal vector, phi component	Boundaries 1–9	
tcd.nzc	root.nzc/tcd.ncLen	1	Normal vector, z component	Boundaries 1–9	
tcd.ncLen	sqrt(root.nrc^2+root.nzc^2+eps)	1	Help variable	Boundaries 1–9	
tcd.nil	0	A/m^2	Inward electrolyte current density	Domains 1–2	+ operation
tcd.nis	0	A/m^2	Inward electrode current density	Domains 1–2	+ operation
tcd.Qsi	0	A/m^3	Current source	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
tcd.R_cO	0	mol/(m³·s)	Total rate expression	Domains 1–2	+ operation
tcd.R_cR	0	mol/(m³·s)	Total rate expression	Domains 1–2	+ operation
tcd.R_cM	0	mol/(m³·s)	Total rate expression	Domains 1–2	+ operation
tcd.R_cA	0	mol/(m³·s)	Total rate expression	Domains 1–2	+ operation

2.3.3 Electrolyte 1



Electrolyte 1

SELECTION

Geometric entity level	Domain
Selection	Domains 1–2

EQUATIONS

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

$$\nabla \cdot \mathbf{i}_l = F \sum_i z_i R_i + Q_l$$

$$\sum_i z_i c_i = 0$$

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

$$\mathbf{i}_l = F \sum_i z_i \mathbf{J}_i$$

Diffusion

SETTINGS

Description	Value
Material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{DO, 0, 0}, {0, DO, 0}, {0, 0, DO}}
Diffusion coefficient	User defined
Diffusion coefficient	{{DR, 0, 0}, {0, DR, 0}, {0, 0, DR}}
Diffusion coefficient	User defined
Diffusion coefficient	{{DM, 0, 0}, {0, DM, 0}, {0, 0, DM}}
Diffusion coefficient	User defined
Diffusion coefficient	{{DA, 0, 0}, {0, DA, 0}, {0, 0, DA}}

Migration in electric field

SETTINGS

Description	Value
Mobility	Nernst - Einstein relation
Charge number	{zO, zRed, zM, zA}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model input

SETTINGS

Description	Value
Temperature	User defined
Temperature	293.15[K]

Variables

Name	Expression	Unit	Description	Selection	Details
cA	tcd.ctemp/(tcd.z_cA+eps)	mol/m³	Concentration	Domains 1–2	
tcd.Qh	-tcd.llr*phir-tcd.llz*phiz	W/m³	Total power dissipation density	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
tcd.llMag	sqrt(realdot(tcd.llr, tcd.llr)+realdot(tcd.llphi,tcd.llphi)+realdot(tcd.llz,tcd.llz))	A/m²	Electrolyte current density magnitude	Domains 1–2	
tcd.Qli	0	A/m³	Current source	Domains 1–2	+ operation
tcd.V	phi	V	Electric potential	Domains 1–2	
tcd.epsilon_p	1	1	Porosity	Domains 1–2	
tcd.D_cOrr	DO	m²/s	Diffusion coefficient, rr component	Domains 1–2	
tcd.D_cOphir	0	m²/s	Diffusion coefficient, phir component	Domains 1–2	
tcd.D_cOzr	0	m²/s	Diffusion coefficient, zr component	Domains 1–2	
tcd.D_cOrphi	0	m²/s	Diffusion coefficient, rphi component	Domains 1–2	
tcd.D_cOphiphi	DO	m²/s	Diffusion coefficient, phiphi component	Domains 1–2	
tcd.D_cOzphi	0	m²/s	Diffusion coefficient, zphi component	Domains 1–2	
tcd.D_cOrz	0	m²/s	Diffusion coefficient, rz component	Domains 1–2	
tcd.D_cOphiz	0	m²/s	Diffusion coefficient, phiz component	Domains 1–2	
tcd.D_cOzz	DO	m²/s	Diffusion coefficient, zz component	Domains 1–2	
tcd.D_cRrr	DR	m²/s	Diffusion coefficient, rr component	Domains 1–2	
tcd.D_cRphir	0	m²/s	Diffusion coefficient, phir component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.D_cRzr	0	m^2/s	Diffusion coefficient, zr component	Domains 1–2	
tcd.D_cRrphi	0	m^2/s	Diffusion coefficient, rphi component	Domains 1–2	
tcd.D_cRphiphi	DR	m^2/s	Diffusion coefficient, phiphi component	Domains 1–2	
tcd.D_cRzphi	0	m^2/s	Diffusion coefficient, zphi component	Domains 1–2	
tcd.D_cRrz	0	m^2/s	Diffusion coefficient, rz component	Domains 1–2	
tcd.D_cRphiz	0	m^2/s	Diffusion coefficient, phiz component	Domains 1–2	
tcd.D_cRzz	DR	m^2/s	Diffusion coefficient, zz component	Domains 1–2	
tcd.D_cMrr	DM	m^2/s	Diffusion coefficient, rr component	Domains 1–2	
tcd.D_cMphir	0	m^2/s	Diffusion coefficient, phir component	Domains 1–2	
tcd.D_cMzr	0	m^2/s	Diffusion coefficient, zr component	Domains 1–2	
tcd.D_cMrphi	0	m^2/s	Diffusion coefficient, rphi component	Domains 1–2	
tcd.D_cMphiphi	DM	m^2/s	Diffusion coefficient, phiphi component	Domains 1–2	
tcd.D_cMzphi	0	m^2/s	Diffusion coefficient, zphi component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.D_cMrz	0	m^2/s	Diffusion coefficient, rz component	Domains 1–2	
tcd.D_cMphiz	0	m^2/s	Diffusion coefficient, phiz component	Domains 1–2	
tcd.D_cMzz	DM	m^2/s	Diffusion coefficient, zz component	Domains 1–2	
tcd.D_cArr	DA	m^2/s	Diffusion coefficient, rr component	Domains 1–2	
tcd.D_cAphir	0	m^2/s	Diffusion coefficient, phir component	Domains 1–2	
tcd.D_cAzr	0	m^2/s	Diffusion coefficient, zr component	Domains 1–2	
tcd.D_cArphi	0	m^2/s	Diffusion coefficient, rphi component	Domains 1–2	
tcd.D_cAphiphi	DA	m^2/s	Diffusion coefficient, phiphi component	Domains 1–2	
tcd.D_cAzphi	0	m^2/s	Diffusion coefficient, zphi component	Domains 1–2	
tcd.D_cArz	0	m^2/s	Diffusion coefficient, rz component	Domains 1–2	
tcd.D_cAphiz	0	m^2/s	Diffusion coefficient, phiz component	Domains 1–2	
tcd.D_cAzz	DA	m^2/s	Diffusion coefficient, zz component	Domains 1–2	
tcd.z_cO	zO	1	Charge number	Domains 1–2	
tcd.z_cR	zRed	1	Charge number	Domains 1–2	
tcd.z_cM	zM	1	Charge number	Domains 1–2	
tcd.z_cA	zA	1	Charge number	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.Dav_cO	0.5*(tcd.D_cOrr+tcd.D_cOzz)	m^2/s	Average diffusion coefficient	Domains 1–2	
tcd.Dav_cR	0.5*(tcd.D_cRrr+tcd.D_cRzz)	m^2/s	Average diffusion coefficient	Domains 1–2	
tcd.Dav_cM	0.5*(tcd.D_cMrr+tcd.D_cMzz)	m^2/s	Average diffusion coefficient	Domains 1–2	
tcd.Dav_cA	0.5*(tcd.D_cArr+tcd.D_cAzz)	m^2/s	Average diffusion coefficient	Domains 1–2	
tcd.tflux_cOr	tcd.dflux_cOr+tcd.cflux_cOr+tcd.mflux_cOr	$mol/(m^2·s)$	Total flux, r component	Domains 1–2	+ operation
tcd.tflux_cOphi	tcd.dflux_cOphi+tcd.cflux_cOphi+tcd.mflux_cOphi	$mol/(m^2·s)$	Total flux, phi component	Domains 1–2	+ operation
tcd.tflux_cOz	tcd.dflux_cOz+tcd.cflux_cOz+tcd.mflux_cOz	$mol/(m^2·s)$	Total flux, z component	Domains 1–2	+ operation
tcd.dfluxMag_cO	sqrt(tcd.dflux_cOr^2+tcd.dflux_cOphi^2+tcd.dflux_cOz^2)	$mol/(m^2·s)$	Diffusive flux magnitude	Domains 1–2	
tcd.tfluxMag_cO	sqrt(tcd.tflux_cOr^2+tcd.tflux_cOphi^2+tcd.tflux_cOz^2)	$mol/(m^2·s)$	Total flux magnitude	Domains 1–2	
tcd.mflux_cOr	tcd.z_cO*F_const*cO*(-tcd.um_cOrr*d(tcd.V,r)-tcd.um_cOrz*d(tcd.V,z))	$mol/(m^2·s)$	Electrophoretic flux, r component	Domains 1–2	
tcd.mflux_cOphi	tcd.z_cO*F_const*cO*(-tcd.um_cOphir*d(tcd.V,r)-tcd.um_cOphiz*d(tcd.V,z))	$mol/(m^2·s)$	Electrophoretic flux, phi component	Domains 1–2	
tcd.mflux_cOz	tcd.z_cO*F_const*cO*(-tcd.um_cOzr*d(tcd.V,r)-tcd.um_cOzz*d(tcd.V,z))	$mol/(m^2·s)$	Electrophoretic flux, z component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.tflux_cRr	tcd.dflux_cRr+tcd.cflux_cRr+tcd.mflux_cRr	mol/(m²·s)	Total flux, r component	Domains 1–2	+ operation
tcd.tflux_cRphi	tcd.dflux_cRphi+tcd.cflux_cRphi+tcd.mflux_cRphi	mol/(m²·s)	Total flux, phi component	Domains 1–2	+ operation
tcd.tflux_cRz	tcd.dflux_cRz+tcd.cflux_cRz+tcd.mflux_cRz	mol/(m²·s)	Total flux, z component	Domains 1–2	+ operation
tcd.dfluxMag_cR	sqrt(tcd.dflux_cRr^2+tcd.dflux_cRphi^2+tcd.dflux_cRz^2)	mol/(m²·s)	Diffusive flux magnitude	Domains 1–2	
tcd.tfluxMag_cR	sqrt(tcd.tflux_cRr^2+tcd.tflux_cRphi^2+tcd.tflux_cRz^2)	mol/(m²·s)	Total flux magnitude	Domains 1–2	
tcd.mflux_cRr	tcd.z_cR*F_const*cR*(-tcd.um_cRrr*d(tcd.V,r)-tcd.um_cRrz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, r component	Domains 1–2	
tcd.mflux_cRphi	tcd.z_cR*F_const*cR*(-tcd.um_cRphir*d(tcd.V,r)-tcd.um_cRphiz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, phi component	Domains 1–2	
tcd.mflux_cRz	tcd.z_cR*F_const*cR*(-tcd.um_cRzr*d(tcd.V,r)-tcd.um_cRzz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, z component	Domains 1–2	
tcd.tflux_cMr	tcd.dflux_cMr+tcd.cflux_cMr+tcd.mflux_cMr	mol/(m²·s)	Total flux, r component	Domains 1–2	+ operation
tcd.tflux_cMphi	tcd.dflux_cMphi+tcd.cflux_cMphi+tcd.mflux_cMphi	mol/(m²·s)	Total flux, phi component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
tcd.tflux_cMz	tcd.dflux_cMz+tcd.cflux_cMz+tcd.mflux_cMz	mol/(m²·s)	Total flux, z component	Domains 1–2	+ operation
tcd.dfluxMag_cM	sqrt(tcd.dflux_cMr^2+tcd.dflux_cMphi^2+tcd.dflux_cMz^2)	mol/(m²·s)	Diffusive flux magnitude	Domains 1–2	
tcd.tfluxMag_cM	sqrt(tcd.tflux_cMr^2+tcd.tflux_cMphi^2+tcd.tflux_cMz^2)	mol/(m²·s)	Total flux magnitude	Domains 1–2	
tcd.mflux_cMr	tcd.z_cM*F_const*cM*(-tcd.um_cMrr*d(tcd.V,r)-tcd.um_cMrz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, r component	Domains 1–2	
tcd.mflux_cMphi	tcd.z_cM*F_const*cM*(-tcd.um_cMphir*d(tcd.V,r)-tcd.um_cMphiz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, phi component	Domains 1–2	
tcd.mflux_cMz	tcd.z_cM*F_const*cM*(-tcd.um_cMzr*d(tcd.V,r)-tcd.um_cMzz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, z component	Domains 1–2	
tcd.tflux_cAr	tcd.dflux_cAr+tcd.cflux_cAr+tcd.mflux_cAr	mol/(m²·s)	Total flux, r component	Domains 1–2	+ operation
tcd.tflux_cAphi	tcd.dflux_cAphi+tcd.cflux_cAphi+tcd.mflux_cAphi	mol/(m²·s)	Total flux, phi component	Domains 1–2	+ operation
tcd.tflux_cAz	tcd.dflux_cAz+tcd.cflux_cAz+tcd.mflux_cAz	mol/(m²·s)	Total flux, z component	Domains 1–2	+ operation
tcd.dfluxMag_cA	sqrt(tcd.dflux_cAr^2+tcd.dflux_cAphi^2+tcd.dflux_cAz^2)	mol/(m²·s)	Diffusive flux magnitude	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.tfluxMag_cA	sqrt(tcd.tflux_cAr^2+tcd.tflux_cAphi^2+tcd.tflux_cAz^2)	mol/(m²·s)	Total flux magnitude	Domains 1–2	
tcd.mflux_cAr	tcd.z_cA*F_const*cA*(-tcd.um_cArr*d(tcd.V,r)-tcd.um_cArz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, r component	Domains 1–2	
tcd.mflux_cAphi	tcd.z_cA*F_const*cA*(-tcd.um_cAphir*d(tcd.V,r)-tcd.um_cAphiz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, phi component	Domains 1–2	
tcd.mflux_cAz	tcd.z_cA*F_const*cA*(-tcd.um_cAzr*d(tcd.V,r)-tcd.um_cAzz*d(tcd.V,z))	mol/(m²·s)	Electrophoretic flux, z component	Domains 1–2	
tcd.u	model.input.u1	m/s	Velocity field, r component	Domains 1–2	Meta
tcd.v	model.input.u2	m/s	Velocity field, phi component	Domains 1–2	Meta
tcd.w	model.input.u3	m/s	Velocity field, z component	Domains 1–2	Meta
tcd.cflux_cOr	cO*tcd.u	mol/(m²·s)	Convective flux, r component	Domains 1–2	
tcd.cflux_cOphi	cO*tcd.v	mol/(m²·s)	Convective flux, phi component	Domains 1–2	
tcd.cflux_cOz	cO*tcd.w	mol/(m²·s)	Convective flux, z component	Domains 1–2	
tcd.cfluxMag_cO	sqrt(tcd.cflux_cOr^2+tcd.cflux_cOphi^2+tcd.cflux_cOz^2)	mol/(m²·s)	Convective flux magnitude	Domains 1–2	
tcd.cflux_cRr	cR*tcd.u	mol/(m²·s)	Convective flux, r component	Domains 1–2	
tcd.cflux_cRphi	cR*tcd.v	mol/(m²·s)	Convective flux, phi component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.cflux_cRz	cR*tcd.w	mol/(m²·s)	Convective flux, z component	Domains 1–2	
tcd.cfluxMag_cR	sqrt(tcd.cflux_cRr^2+tcd.cflux_cRphi^2+tcd.cflux_cRz^2)	mol/(m²·s)	Convective flux magnitude	Domains 1–2	
tcd.cflux_cMr	cM*tcd.u	mol/(m²·s)	Convective flux, r component	Domains 1–2	
tcd.cflux_cMphi	cM*tcd.v	mol/(m²·s)	Convective flux, phi component	Domains 1–2	
tcd.cflux_cMz	cM*tcd.w	mol/(m²·s)	Convective flux, z component	Domains 1–2	
tcd.cfluxMag_cM	sqrt(tcd.cflux_cMr^2+tcd.cflux_cMphi^2+tcd.cflux_cMz^2)	mol/(m²·s)	Convective flux magnitude	Domains 1–2	
tcd.cflux_cAr	cA*tcd.u	mol/(m²·s)	Convective flux, r component	Domains 1–2	
tcd.cflux_cAphi	cA*tcd.v	mol/(m²·s)	Convective flux, phi component	Domains 1–2	
tcd.cflux_cAz	cA*tcd.w	mol/(m²·s)	Convective flux, z component	Domains 1–2	
tcd.cfluxMag_cA	sqrt(tcd.cflux_cAr^2+tcd.cflux_cAphi^2+tcd.cflux_cAz^2)	mol/(m²·s)	Convective flux magnitude	Domains 1–2	
tcd.um_cOrr	tcd.D_cOrr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rr component	Domains 1–2	
tcd.um_cOphir	tcd.D_cOphir/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phir component	Domains 1–2	
tcd.um_cOzr	tcd.D_cOzr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zr component	Domains 1–2	
tcd.um_cOrphi	tcd.D_cOrphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rphi component	Domains 1–2	
tcd.um_cOphiphi	tcd.D_cOphiphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiphi component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.um_cOzphi	tcd.D_cOzphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zphi component	Domains 1–2	
tcd.um_cOrz	tcd.D_cOrz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rz component	Domains 1–2	
tcd.um_cOphiz	tcd.D_cOphiz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiz component	Domains 1–2	
tcd.um_cOzz	tcd.D_cOzz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zz component	Domains 1–2	
tcd.um_cRrr	tcd.D_cRrr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rr component	Domains 1–2	
tcd.um_cRphir	tcd.D_cRphir/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phir component	Domains 1–2	
tcd.um_cRzr	tcd.D_cRzr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zr component	Domains 1–2	
tcd.um_cRrphi	tcd.D_cRrphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rphi component	Domains 1–2	
tcd.um_cRphiphi	tcd.D_cRphiphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiphi component	Domains 1–2	
tcd.um_cRzphi	tcd.D_cRzphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zphi component	Domains 1–2	
tcd.um_cRrz	tcd.D_cRrz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rz component	Domains 1–2	
tcd.um_cRphiz	tcd.D_cRphiz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiz component	Domains 1–2	
tcd.um_cRzz	tcd.D_cRzz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zz component	Domains 1–2	
tcd.um_cMrr	tcd.D_cMrr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rr component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.um_cMphir	tcd.D_cMphir/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phir component	Domains 1–2	
tcd.um_cMzr	tcd.D_cMzr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zr component	Domains 1–2	
tcd.um_cMrphi	tcd.D_cMrphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rphi component	Domains 1–2	
tcd.um_cMphiphi	tcd.D_cMphiphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiphi component	Domains 1–2	
tcd.um_cMzphi	tcd.D_cMzphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zphi component	Domains 1–2	
tcd.um_cMrz	tcd.D_cMrz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rz component	Domains 1–2	
tcd.um_cMphiz	tcd.D_cMphiz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiz component	Domains 1–2	
tcd.um_cMzz	tcd.D_cMzz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zz component	Domains 1–2	
tcd.um_cArr	tcd.D_cArr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rr component	Domains 1–2	
tcd.um_cAphir	tcd.D_cAphir/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phir component	Domains 1–2	
tcd.um_cAzr	tcd.D_cAzr/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zr component	Domains 1–2	
tcd.um_cArphi	tcd.D_cArphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rphi component	Domains 1–2	
tcd.um_cAphiphi	tcd.D_cAphiphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiphi component	Domains 1–2	
tcd.um_cAzphi	tcd.D_cAzphi/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zphi component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.um_cArz	tcd.D_cArz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, rz component	Domains 1–2	
tcd.um_cAphiz	tcd.D_cAphiz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, phiz component	Domains 1–2	
tcd.um_cAzz	tcd.D_cAzz/(R_const*tcd.ice1.minput_temperature)	s·mol/kg	Mobility, zz component	Domains 1–2	
tcd.dflux_cOr	-tcd.D_cOrr*tcd.grad_cOr-tcd.D_cOrphi*tcd.grad_cOphi-tcd.D_cOrz*tcd.grad_cOz	mol/(m²·s)	Diffusive flux, r component	Domains 1–2	
tcd.dflux_cOphi	-tcd.D_cOphir*tcd.grad_cOr-tcd.D_cOphiphi*tcd.grad_cOphi-tcd.D_cOphiz*tcd.grad_cOz	mol/(m²·s)	Diffusive flux, phi component	Domains 1–2	
tcd.dflux_cOz	-tcd.D_cOzr*tcd.grad_cOr-tcd.D_cOzphi*tcd.grad_cOphi-tcd.D_cOzz*tcd.grad_cOz	mol/(m²·s)	Diffusive flux, z component	Domains 1–2	
tcd.grad_cOr	cOr	mol/m⁴	Concentration gradient, r component	Domains 1–2	
tcd.grad_cOphi	0	mol/m⁴	Concentration gradient, phi component	Domains 1–2	
tcd.grad_cOz	cOz	mol/m⁴	Concentration gradient, z component	Domains 1–2	
tcd.ctemp	-cO*tcd.z_cO-cR*tcd.z_cR-cM*tcd.z_cM	mol/m³	Concentration	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
tcd.dflux_cRr	-tcd.D_cRrr*tcd.grad_cRr-tcd.D_cRrphi*tcd.grad_cRphi-tcd.D_cRrz*tcd.grad_cRz	mol/(m²·s)	Diffusive flux, r component	Domains 1–2	
tcd.dflux_cRphi	-tcd.D_cRphir*tcd.grad_cRr-tcd.D_cRphiphi*tcd.grad_cRphi-tcd.D_cRphiz*tcd.grad_cRz	mol/(m²·s)	Diffusive flux, phi component	Domains 1–2	
tcd.dflux_cRz	-tcd.D_cRzr*tcd.grad_cRr-tcd.D_cRzphi*tcd.grad_cRphi-tcd.D_cRzz*tcd.grad_cRz	mol/(m²·s)	Diffusive flux, z component	Domains 1–2	
tcd.grad_cRr	cRr	mol/m⁴	Concentration gradient, r component	Domains 1–2	
tcd.grad_cRphi	0	mol/m⁴	Concentration gradient, phi component	Domains 1–2	
tcd.grad_cRz	cRz	mol/m⁴	Concentration gradient, z component	Domains 1–2	
tcd.dflux_cMr	-tcd.D_cMrr*tcd.grad_cMr-tcd.D_cMrphi*tcd.grad_cMphi-tcd.D_cMrz*tcd.grad_cMz	mol/(m²·s)	Diffusive flux, r component	Domains 1–2	
tcd.dflux_cMphi	-tcd.D_cMphir*tcd.grad_cMr-tcd.D_cMphiphi*tcd.grad_cMphi-tcd.D_cMphiz*tcd.grad_cMz	mol/(m²·s)	Diffusive flux, phi component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.dflux_cMz	-tcd.D_cMzr*tcd.grad_cMr-tcd.D_cMzphi*tcd.grad_cMphi-tcd.D_cMzz*tcd.grad_cMz	mol/(m²·s)	Diffusive flux, z component	Domains 1–2	
tcd.grad_cMr	cMr	mol/m⁴	Concentration gradient, r component	Domains 1–2	
tcd.grad_cMphi	0	mol/m⁴	Concentration gradient, phi component	Domains 1–2	
tcd.grad_cMz	cMz	mol/m⁴	Concentration gradient, z component	Domains 1–2	
tcd.dflux_cAr	-tcd.D_cArr*tcd.grad_cAr-tcd.D_cArphi*tcd.grad_cAphi-tcd.D_cArz*tcd.grad_cAz	mol/(m²·s)	Diffusive flux, r component	Domains 1–2	
tcd.dflux_cAphi	-tcd.D_cAphir*tcd.grad_cAr-tcd.D_cAphiphi*tcd.grad_cAphi-tcd.D_cAphiz*tcd.grad_cAz	mol/(m²·s)	Diffusive flux, phi component	Domains 1–2	
tcd.dflux_cAz	-tcd.D_cAzr*tcd.grad_cAr-tcd.D_cAzphi*tcd.grad_cAphi-tcd.D_cAzz*tcd.grad_cAz	mol/(m²·s)	Diffusive flux, z component	Domains 1–2	
tcd.grad_cAr	d(cA,r)	mol/m⁴	Concentration gradient, r component	Domains 1–2	
tcd.grad_cAphi	0	mol/m⁴	Concentration gradient, phi component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
tcd.grad_cAz	d(cA,z)	mol/m^4	Concentration gradient, z component	Domains 1–2	
tcd.cbf_cO	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–9	
tcd.cbf_cR	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–9	
tcd.cbf_cM	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–9	
tcd.kappa0rr	cO*tcd.um_cOrr*(tcd.z_cO*F_const)^2+cR*tcd.um_cRrr*(tcd.z_cR*F_const)^2+cM*tcd.um_cMrr*(tcd.z_cM*F_const)^2+cA*tcd.um_cArr*(tcd.z_cA*F_const)^2	S/m	Electrolyte conductivity, rr component	Domains 1–2	+ operation
tcd.kappa0phir	cO*tcd.um_cOphir*(tcd.z_cO*F_const)^2+cR*tcd.um_cRphir*(tcd.z_cR*F_const)^2+cM*tcd.um_cMphir*(tcd.z_cM*F_const)^2+cA*tcd.um_cAphir*(tcd.z_cA*F_const)^2	S/m	Electrolyte conductivity, phir component	Domains 1–2	+ operation
tcd.kappa0zr	cO*tcd.um_cOzr*(tcd.z_cO*F_const)^2+cR*tcd.um_cRzr*(tcd.z_cR*F_const)^2+cM*tcd.um_cMzr*(tcd.z_cM*F_const)^2+cA*tcd.um_cAzr*(tcd.z_cA*F_const)^2	S/m	Electrolyte conductivity, zr component	Domains 1–2	+ operation
tcd.kappa0rphi	cO*tcd.um_cOrphi*(tcd.z_cO*F_const)^2+cR*tcd.um_cRrphi*(tcd.z_cR*F_const)^2+cM*tcd.um_cMrphi*(tcd.z_cM*F_const)^2+cA	S/m	Electrolyte conductivity, rphi component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
	tcd.um_cArphi(tcd.z_cA*F_const)^2				
tcd.kappa0phiphi	cO*tcd.um_cOphiphi*(tcd.z_cO*F_const)^2+cR*tcd.um_cRphiphi*(tcd.z_cR*F_const)^2+cM*tcd.um_cMphiphi*(tcd.z_cM*F_const)^2+cA*tcd.um_cAphiphi*(tcd.z_cA*F_const)^2	S/m	Electrolyte conductivity, phiphi component	Domains 1–2	+ operation
tcd.kappa0zphi	cO*tcd.um_cOzphi*(tcd.z_cO*F_const)^2+cR*tcd.um_cRzphi*(tcd.z_cR*F_const)^2+cM*tcd.um_cMzphi*(tcd.z_cM*F_const)^2+cA*tcd.um_cAzphi*(tcd.z_cA*F_const)^2	S/m	Electrolyte conductivity, zphi component	Domains 1–2	+ operation
tcd.kappa0rz	cO*tcd.um_cOrz*(tcd.z_cO*F_const)^2+cR*tcd.um_cRrz*(tcd.z_cR*F_const)^2+cM*tcd.um_cMrz*(tcd.z_cM*F_const)^2+cA*tcd.um_cArz*(tcd.z_cA*F_const)^2	S/m	Electrolyte conductivity, rz component	Domains 1–2	+ operation
tcd.kappa0phiz	cO*tcd.um_cOphiz*(tcd.z_cO*F_const)^2+cR*tcd.um_cRphiz*(tcd.z_cR*F_const)^2+cM*tcd.um_cMphiz*(tcd.z_cM*F_const)^2+cA*tcd.um_cAphiz*(tcd.z_cA*F_const)^2	S/m	Electrolyte conductivity, phiz component	Domains 1–2	+ operation
tcd.kappa0zz	cO*tcd.um_cOzz*(tcd.z_cO*F_const)^2+cR*tcd.um_cRzz*(tcd.z_cR*F_const)	S/m	Electrolyte conductivity, zz component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
	^2+cM*tcd.um_cMzz*(tcd.z_cM*F_const)^2+cA*tcd.um_cAzz*(tcd.z_cA*F_const)^2				
tcd.Il0r	F_const*(tcd.z_cO*(-tcd.D_cOrr*tcd.grad_cOr-tcd.D_cOrphi*tcd.grad_cOphi-tcd.D_cOrz*tcd.grad_cOz+tcd.z_cO*F_const*cO*(-tcd.um_cOrr*phir-tcd.um_cOrz*phiz))+tcd.z_cR*(-tcd.D_cRrr*tcd.grad_cRr-tcd.D_cRrphi*tcd.grad_cRphi-tcd.D_cRrz*tcd.grad_cRz+tcd.z_cR*F_const*cR*(-tcd.um_cRrr*phir-tcd.um_cRrz*phiz))+tcd.z_cM*(-tcd.D_cMrr*tcd.grad_cMr-tcd.D_cMrphi*tcd.grad_cMphi-tcd.D_cMrz*tcd.grad_cMz+tcd.z_cM*F_const*cM*(-tcd.um_cMrr*phir-tcd.um_cMrz*phiz))+tcd.z_cA*(-tcd.D_cArr*tcd.grad_cAr-tcd.D_cArphi*tcd.grad_cAphi-tcd.D_cArz*tcd.grad_cAz+tcd.z_cA*F_const*cA*(-tcd.um_cArr*phir-	A/m²	Electrolyte current density vector, r component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
	tcd.um_cArz*phiz)))				
tcd.Il0phi	F_const*(tcd.z_cO*(-tcd.D_cOphir*tcd.grad_cOr-tcd.D_cOphiphi*tcd.grad_cOphi-tcd.D_cOphiz*tcd.grad_cOz+tcd.z_cO*F_const*cO*(-tcd.um_cOphir*phir-tcd.um_cOphiz*phiz))+tcd.z_cR*(-tcd.D_cRphir*tcd.grad_cRr-tcd.D_cRphiphi*tcd.grad_cRphi-tcd.D_cRphiz*tcd.grad_cRz+tcd.z_cR*F_const*cR*(-tcd.um_cRphir*phir-tcd.um_cRphiz*phiz))+tcd.z_cM*(-tcd.D_cMphir*tcd.grad_cMr-tcd.D_cMphiphi*tcd.grad_cMphi-tcd.D_cMphiz*tcd.grad_cMz+tcd.z_cM*F_const*cM*(-tcd.um_cMphir*phir-tcd.um_cMphiz*phiz))+tcd.z_cA*(-tcd.D_cAphir*tcd.grad_cAr-tcd.D_cAphiphi*tcd.grad_cAphi-tcd.D_cAphiz*tcd.grad_cAz+tcd.z_cA*F_const*cA*(-tcd.um_cAphir*phir-	A/m^2	Electrolyte current density vector, phi component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
	tcd.um_cAphiz*phiz)))				
tcd.Il0z	F_const*(tcd.z_cO*(-tcd.D_cOzr*tcd.grad_cOr-tcd.D_cOzphi*tcd.grad_cOphi-tcd.D_cOzz*tcd.grad_cOz+tcd.z_cO*F_const*cO*(-tcd.um_cOzr*phir-tcd.um_cOzz*phiz))+tcd.z_cR*(-tcd.D_cRzr*tcd.grad_cRr-tcd.D_cRzphi*tcd.grad_cRphi-tcd.D_cRzz*tcd.grad_cRz+tcd.z_cR*F_const*cR*(-tcd.um_cRzr*phir-tcd.um_cRzz*phiz))+tcd.z_cM*(-tcd.D_cMzr*tcd.grad_cMr-tcd.D_cMzphi*tcd.grad_cMphi-tcd.D_cMzz*tcd.grad_cMz+tcd.z_cM*F_const*cM*(-tcd.um_cMzr*phir-tcd.um_cMzz*phiz))+tcd.z_cA*(-tcd.D_cAzr*tcd.grad_cAr-tcd.D_cAzphi*tcd.grad_cAphi-tcd.D_cAzz*tcd.grad_cAz+tcd.z_cA*F_const*cA*(-tcd.um_cAzr*phir-tcd.um_cAzz*phiz)))	A/m²	Electrolyte current density vector, z component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
tcd.kapparr	tcd.kappa0rr	S/m	Electrolyte conductivity, rr component	Domains 1–2	
tcd.kappaphir	tcd.kappa0phir	S/m	Electrolyte conductivity, phir component	Domains 1–2	
tcd.kappazr	tcd.kappa0zr	S/m	Electrolyte conductivity, zr component	Domains 1–2	
tcd.kapparphi	tcd.kappa0rphi	S/m	Electrolyte conductivity, rphi component	Domains 1–2	
tcd.kappaphiphi	tcd.kappa0phiphi	S/m	Electrolyte conductivity, phiphi component	Domains 1–2	
tcd.kappazphi	tcd.kappa0zphi	S/m	Electrolyte conductivity, zphi component	Domains 1–2	
tcd.kapparz	tcd.kappa0rz	S/m	Electrolyte conductivity, rz component	Domains 1–2	
tcd.kappaphiz	tcd.kappa0phiz	S/m	Electrolyte conductivity, phiz component	Domains 1–2	
tcd.kappazz	tcd.kappa0zz	S/m	Electrolyte conductivity, zz component	Domains 1–2	
tcd.Ilr	tcd.Il0r	A/m^2	Electrolyte current density vector, r component	Domains 1–2	
tcd.Ilphi	tcd.Il0phi	A/m^2	Electrolyte current density vector, phi component	Domains 1–2	
tcd.Ilz	tcd.Il0z	A/m^2	Electrolyte current density vector, z component	Domains 1–2	
tcd.Res_cO	-tcd.D_cOrr*cOrr-tcd.D_cOrz*cOrz-tcd.D_cOzr*cOzr-	$mol/(m^3 \cdot s)$	Equation residual	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
	tcd.D_cOzz*cOzz+d(cO*tcd.z_cO*F_const*(-tcd.um_cOrr*phir-tcd.um_cOrz*phiz),r)+if(abs(r)<0.001*h_spatial,d(cO*tcd.z_cO*F_const*(-tcd.um_cOrr*phir-tcd.um_cOrz*phiz),r),cO*tcd.z_cO*F_const*(-tcd.um_cOrr*phir-tcd.um_cOrz*phiz)/r)+d(cO*tcd.z_cO*F_const*(-tcd.um_cOzr*phir-tcd.um_cOzz*phiz),z)+tcd.u*cOr+tcd.w*cOz-tcd.R_cO				
tcd.Res_cR	-tcd.D_cRrr*cRrr-tcd.D_cRrz*cRrz-tcd.D_cRzr*cRzr-tcd.D_cRzz*cRzz+d(cR*tcd.z_cR*F_const*(-tcd.um_cRrr*phir-tcd.um_cRrz*phiz),r)+if(abs(r)<0.001*h_spatial,d(cR*tcd.z_cR*F_const*(-tcd.um_cRrr*phir-tcd.um_cRrz*phiz),r),cR*tcd.z_cR*F_const*(-tcd.um_cRrr*phir-tcd.um_cRrz*phiz)/r)+d(cR*tcd.z_cR*F_const*(-tcd.um_cRzr*phir-tcd.um_cRzz*phiz),z)+tcd.u*cRr+tcd.w*cRz-tcd.R_cR	mol/(m³·s)	Equation residual	Domains 1–2	
tcd.Res_cM	-tcd.D_cMrr*cMrr-tcd.D_cMrz*cMrz-tcd.D_cMzr*cMzr-	mol/(m³·s)	Equation residual	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
	tcd.D_cMzz*cMzz +d(cM*tcd.z_cM*F _const*(- tcd.um_cMrr*phir- tcd.um_cMrz*phiz) ,r)+if(abs(r)<0.001 *h_spatial,d(cM*tc d.z_cM*F_const*(- tcd.um_cMrr*phir- tcd.um_cMrz*phiz) ,r),cM*tcd.z_cM*F_ const*(- tcd.um_cMrr*phir- tcd.um_cMrz*phiz) /r)+d(cM*tcd.z_cM *F_const*(- tcd.um_cMzr*phir- tcd.um_cMzz*phiz),z)+tcd.u*cMr+tc d.w*cMz-tcd.R_cM				

Shape functions

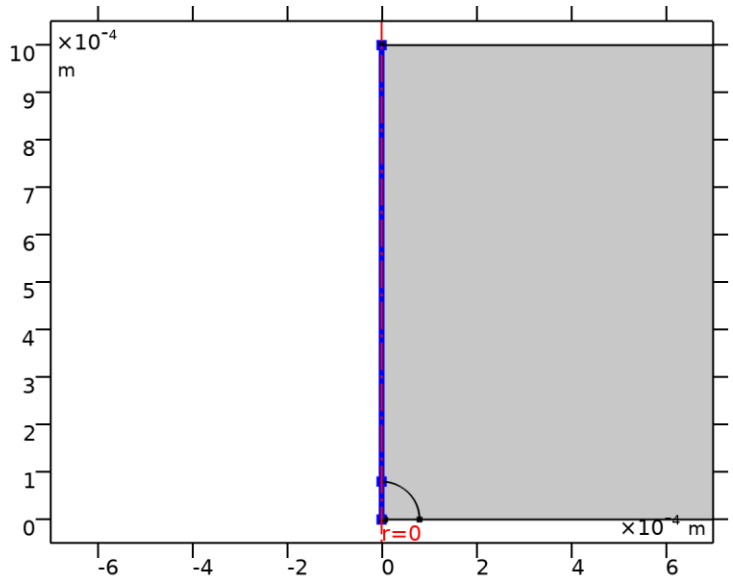
Name	Shape function	Unit	Description	Shape frame	Selection
cO	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domains 1–2
cR	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domains 1–2
cM	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domains 1–2
phi	Lagrange (Quadratic)	V	Electrolyte potential	Spatial	Domains 1–2

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(tcd.Ilr*test(phir)+tcd.Ilz*test(phiz)+tcd.Qli*test(phi))*pi*r	4	Spatial	Domains 1–2
- 2*(tcd.u*cOr+tcd.w*cOz)*test(c O)*(isScalingSystemDomain== 0)*pi*r	4	Spatial	Domains 1–2
2*tcd.cbf_cO*test(cO)*pi*r	4	Spatial	Boundaries 1–9

Weak expression	Integration order	Integration frame	Selection
-2*(tcd.u*cRr+tcd.w*cRz)*test(cR)*(isScalingSystemDomain==0)*pi*r	4	Spatial	Domains 1–2
2*tcd.cbf_cR*test(cR)*pi*r	4	Spatial	Boundaries 1–9
-2*(tcd.u*cMr+tcd.w*cMz)*test(cM)*(isScalingSystemDomain==0)*pi*r	4	Spatial	Domains 1–2
2*tcd.cbf_cM*test(cM)*pi*r	4	Spatial	Boundaries 1–9
2*tcd.z_cO*F_const*cO*((-tcd.um_cOrr*d(tcd.V,r)-tcd.um_cOrz*d(tcd.V,z))*test(cOr)+(-tcd.um_cOzr*d(tcd.V,r)-tcd.um_cOzz*d(tcd.V,z))*test(cOz))*pi*r	4	Spatial	Domains 1–2
2*tcd.z_cR*F_const*cR*((-tcd.um_cRrr*d(tcd.V,r)-tcd.um_cRrz*d(tcd.V,z))*test(cRr)+(-tcd.um_cRzr*d(tcd.V,r)-tcd.um_cRzz*d(tcd.V,z))*test(cRz))*pi*r	4	Spatial	Domains 1–2
2*tcd.z_cM*F_const*cM*((-tcd.um_cMrr*d(tcd.V,r)-tcd.um_cMrz*d(tcd.V,z))*test(cMr)+(-tcd.um_cMzr*d(tcd.V,r)-tcd.um_cMzz*d(tcd.V,z))*test(cMz))*pi*r	4	Spatial	Domains 1–2
2*(tcd.dflux_cOr*test(cOr)+tcd.dflux_cOz*test(cOz))*pi*r	4	Spatial	Domains 1–2
2*(tcd.dflux_cRr*test(cRr)+tcd.dflux_cRz*test(cRz))*pi*r	4	Spatial	Domains 1–2
2*(tcd.dflux_cMr*test(cMr)+tcd.dflux_cMz*test(cMz))*pi*r	4	Spatial	Domains 1–2
2*tcd.streamline*(isScalingSystemDomain==0)*pi*r	4	Spatial	Domains 1–2
2*tcd.crosswind*(isScalingSystemDomain==0)*pi*r	6	Spatial	Domains 1–2

2.3.4 Axial Symmetry 1

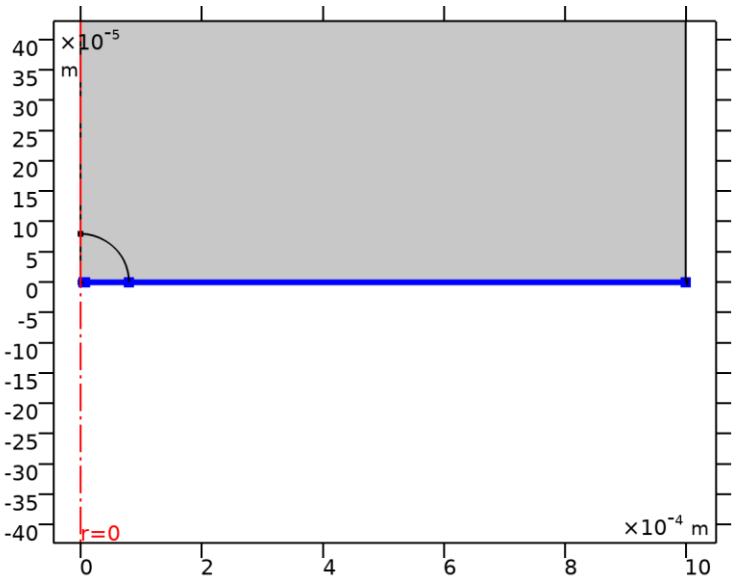


Axial Symmetry 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1, 3

2.3.5 No Flux 1



No Flux 1

SELECTION

Geometric entity level	Boundary

Selection	Boundaries 5–7

EQUATIONS

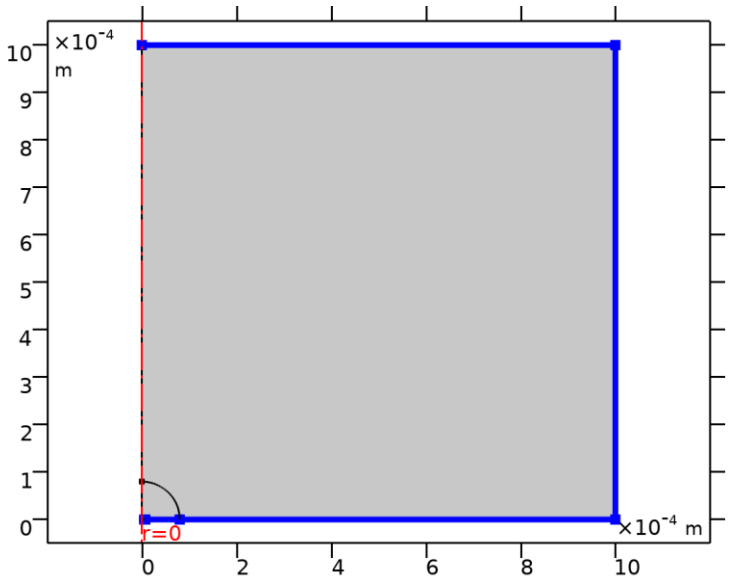
$$-\mathbf{n} \cdot \mathbf{J}_i = 0$$

Convection

SETTINGS

Description	Value
Include	Off

2.3.6 Insulation 1



Insulation 1

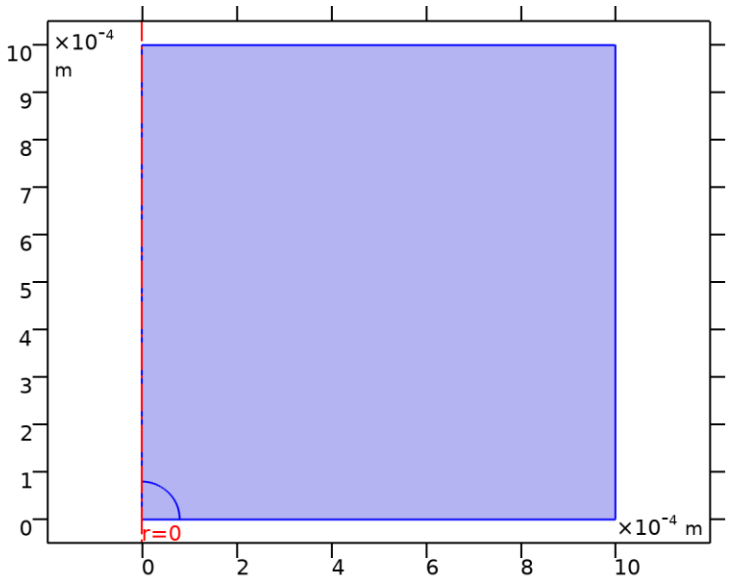
SELECTION

Geometric entity level	Boundary
Selection	Boundaries 4–8

EQUATIONS

$$-\mathbf{n} \cdot \mathbf{i}_l = 0, \quad -\mathbf{n} \cdot \mathbf{i}_s = 0$$

2.3.7 Initial Values 1



Initial Values 1

SELECTION

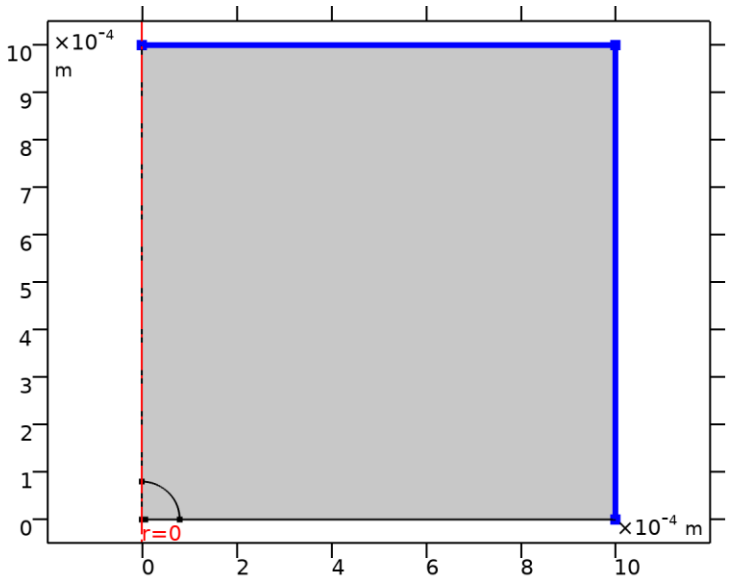
Geometric entity level	Domain
Selection	Domains 1–2

Initial values

SETTINGS

Description	Value
Concentration	{cObulk, cRbulk, cMbulk, cAbulk}
Electrolyte potential	0
Electric potential	0

2.3.8 Electrolyte Potential 1



Electrolyte Potential 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 4, 8

EQUATIONS

$$\phi_l = \phi_{l,bnd}$$

Electrolyte potential

SETTINGS

Description	Value
Boundary electrolyte potential	0[V]

Constraint settings

SETTINGS

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

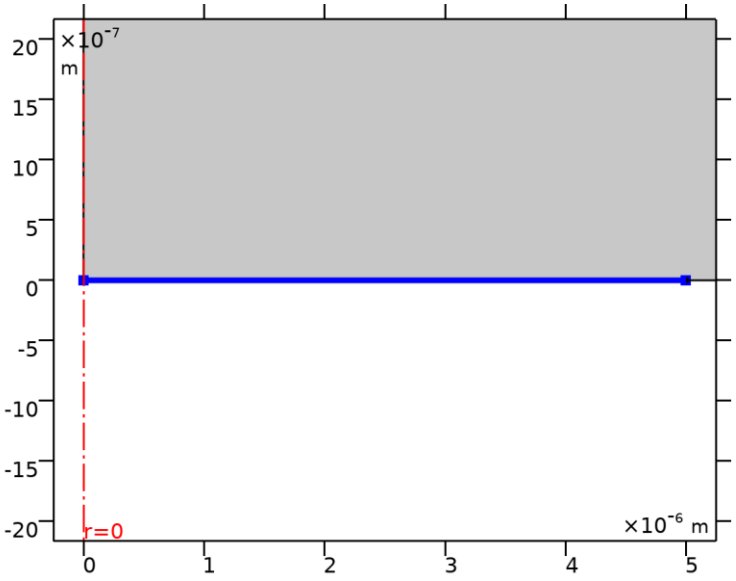
Variables

Name	Expression	Unit	Description	Selection
tcd.philbnd	0[V]	V	Boundary electrolyte potential	Boundaries 4, 8

Constraints

Constraint	Constraint force	Shape function	Selection	Details
tcd.philbnd-phi	test(tcd.philbnd-phi)	Lagrange (Quadratic)	Boundaries 4, 8	Elemental

2.3.9 Electrolyte Current Density 1



Electrolyte Current Density 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 2

EQUATIONS

$$-\mathbf{n}\cdot\mathbf{i}_l = i_{n,l}$$

Electrolyte current density

SETTINGS

Description	Value
	Inward electrolyte current density
	(zRed*F*(-DR*cRz - zRed*DR*f*cR*phiz) + zO*F*(-DO*cOz - zO*DO*f*cO*phiz))

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

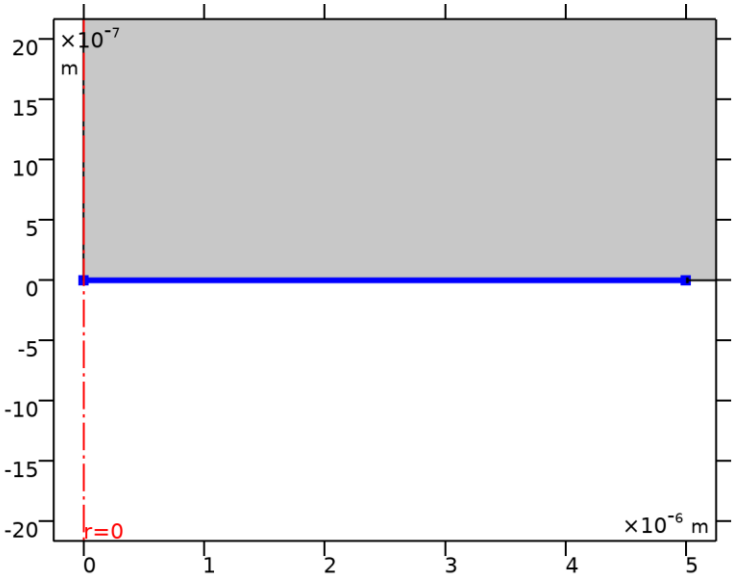
Variables

Name	Expression	Unit	Description	Selection	Details
tcd.nil	F*(zRed*DR*(-cRz-zRed*f*cR*phiz)+zO*DO*(-cOz-zO*f*cO*phiz))	A/m^2	Inward electrolyte current density	Boundary 2	+ operation
tcd.nil_icd1	F*(zRed*DR*(-cRz-zRed*f*cR*phiz)+zO*DO*(-cOz-zO*f*cO*phiz))	A/m^2	Inward electrolyte current density	Boundary 2	

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*tcd.nil_icd1*test(phi)*pi*R	4	Material	Boundary 2

2.3.10 Flux 1



Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 2

EQUATIONS

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

Inward flux

SETTINGS

Description	Value
Species cO	On
Species cR	On
Species cM	On
Species cA	Off
Inward flux	{-k0*exp(-a*f*(E-Ef))*cO + k0*exp((1 - a)*f*(E-Ef))*cR, k0*exp(-a*f*(E-Ef))*cO - k0*exp((1 - a)*f*(E-Ef))*cR, 0, 0}

Convection

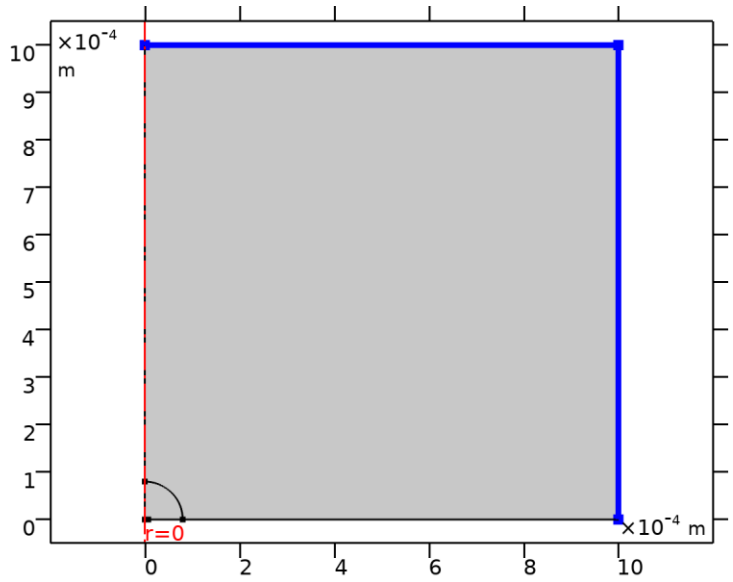
SETTINGS

Description	Value
Include	Off

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*k0*(-exp(-a*f*(E-Ef))*cO+exp((1-a)*f*(E-Ef))*cR)*test(cO)*pi*R	4	Material	Boundary 2
2*k0*(exp(-a*f*(E-Ef))*cO-exp((1-a)*f*(E-Ef))*cR)*test(cR)*pi*R	4	Material	Boundary 2
0	4	Material	Boundary 2

2.3.11 Concentration 1



Concentration 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 4, 8

EQUATIONS

$c_i = c_{0,i}$

Concentration

SETTINGS

Description	Value
Species cO	On
Species cR	On
Species cM	On
Species cA	On
Concentration	{cObulk, cRbulk, cMbulk, cAbulk}

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
tcd.c0_cO	cObulk	mol/m³	Concentration	Boundaries 4, 8
tcd.c0_cR	cRbulk	mol/m³	Concentration	Boundaries 4, 8
tcd.c0_cM	cMbulk	mol/m³	Concentration	Boundaries 4, 8

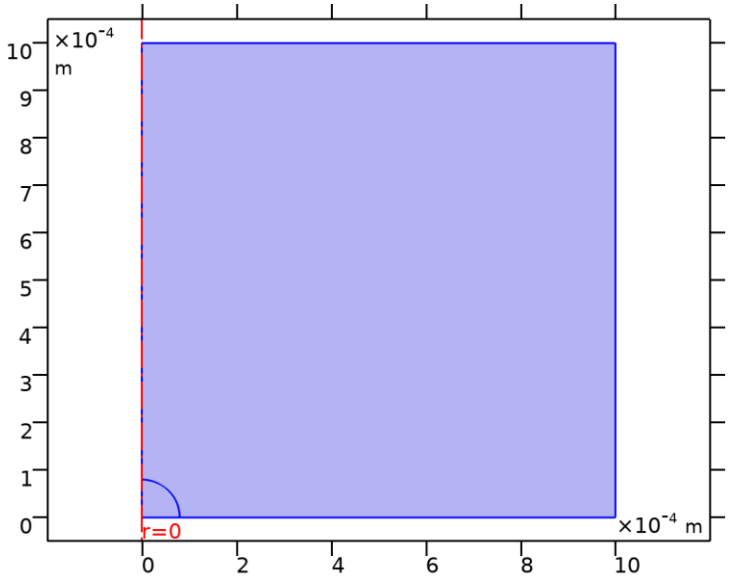
Constraints

Constraint	Constraint force	Shape function	Selection	Details
-cO+tcd.c0_cO	test(-cO+tcd.c0_cO)	Lagrange (Quadratic)	Boundaries 4, 8	Elemental
-cR+tcd.c0_cR	test(-cR+tcd.c0_cR)	Lagrange (Quadratic)	Boundaries 4, 8	Elemental
-cM+tcd.c0_cM	test(-cM+tcd.c0_cM)	Lagrange (Quadratic)	Boundaries 4, 8	Elemental

2.4 CREEPING FLOW

USED PRODUCTS

COMSOL Multiphysics
Electrochemistry Module



Creeping Flow

SELECTION

Geometric entity level	Domain
Selection	Domains 1–2

EQUATIONS

$$0 = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F}$$

$$\rho\nabla\cdot(\mathbf{u})=0$$
$$\mathbf{K}=\mu\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathsf{T}}\right)$$

2.4.1 Interface settings

Discretization

SETTINGS

Description	Value
Discretization of fluids	P1 + P1

Physical model

SETTINGS

Description	Value
Neglect inertial term (Stokes flow)	On
Compressibility	Incompressible flow
Enable porous media domains	Off
Reference temperature	User defined
Reference temperature	293.15[K]
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

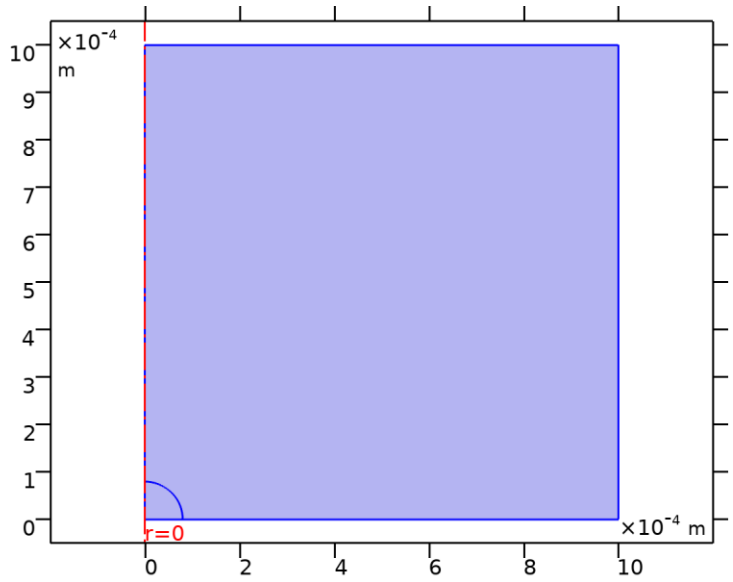
Description	Value
Use pseudo time stepping for stationary equation form	Automatic from physics
CFL number expression	Automatic

2.4.2 Variables

Name	Expression	Unit	Description	Selection	Details
spf.Tref	model.input.Tref	K	Reference temperature	Global	Meta
spf.dz	1	m	Thickness	Domains 1–2	
spf.pref	1[atm]	Pa	Reference pressure level	Domains 1–2	
spf.pA	p+spf.pref	Pa	Absolute pressure	Domains 1–2	
spf.hasWF	0		Help variable	Boundaries 1–8	
spf.hasWF_u	0		Help variable	Boundary 9	
spf.hasWF_d	0		Help variable	Boundary 9	
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	Domains 1–2	
spf.locCFL	CFLCMP	1	Local CFL number	Domains 1–2	
spf.geometryLengthScale	2.5E-4	m	Geometry length scale	Domains 1–2	
spf.time_step_inv	max(sqrt(emetric_spatial(u,w)*2^gmg_level^2),spf.nu/spf.geometryLengthScale^2)	Hz	Inverse time step	Domains 1–2	
spf.tsti	nojac(spf.time_step_inv/spf.locCFL)	1/s	Help variable	Domains 1–2	
spf.nr	nr	1	Normal vector, r component	Boundary 9	

Name	Expression	Unit	Description	Selection	Details
spf.nphi	0	1	Normal vector, phi component	Boundary 9	
spf.nz	nz	1	Normal vector, z component	Boundary 9	
spf.nr	dnr	1	Normal vector, r component	Boundaries 1–8	
spf.nphi	0	1	Normal vector, phi component	Boundaries 1–8	
spf.nz	dnz	1	Normal vector, z component	Boundaries 1–8	
spf.nrmesh	root.nrmesh	1	Normal vector, r component	Boundary 9	
spf.nphimesh	0	1	Normal vector, phi component	Boundary 9	
spf.nzmesh	root.nzmesh	1	Normal vector, z component	Boundary 9	
spf.nrmesh	dnrmesh	1	Normal vector, r component	Boundaries 1–8	
spf.nphimesh	0	1	Normal vector, phi component	Boundaries 1–8	
spf.nzmesh	dnzmesh	1	Normal vector, z component	Boundaries 1–8	

2.4.3 Fluid Properties 1



Fluid Properties 1

SELECTION

Geometric entity level	Domain
Selection	Domains 1–2

EQUATIONS

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

Fluid properties

SETTINGS

Description	Value
Density	User defined
Density	997.8
Dynamic viscosity	User defined
Dynamic viscosity	visc

Variables

Name	Expression	Unit	Description	Selection	Details
spf.rho	material.rho	kg/m³	Density	Domains 1–2	Meta
spf.mu	material.mu	Pa·s	Dynamic viscosity	Domains 1–2	Meta

Name	Expression	Unit	Description	Selection	Details
spf.Trho	spf.fp1.minput_temperature	K	Temperature for density evaluation	Domains 1–2	
spf.prho	spf.fp1.minput_pressure	Pa	Pressure for the evaluation of density	Domains 1–2	
spf.rhoref	subst(material.rho,spf.fp1.minput_temperature,spf.Tref,spf.fp1.minput_pressure,spf.pref)	kg/m³	Reference density	Domains 1–2	Meta
spf.mumat	material.mu	Pa·s	Dynamic viscosity	Domains 1–2	Meta
spf.srijrr	ur	1/s	Strain rate tensor, rr component	Domains 1–2	
spf.srijphir	0	1/s	Strain rate tensor, phir component	Domains 1–2	
spf.srijzr	0.5*(wr+uz)	1/s	Strain rate tensor, zr component	Domains 1–2	
spf.srijrphi	0	1/s	Strain rate tensor, rphi component	Domains 1–2	
spf.srijphiphi	if(abs(r)<0.001*h_spatial,ur,u/r)	1/s	Strain rate tensor, phiphi component	Domains 1–2	
spf.srijzphi	0	1/s	Strain rate tensor, zphi component	Domains 1–2	
spf.srijrz	0.5*(uz+wr)	1/s	Strain rate tensor, rz component	Domains 1–2	
spf.srijphiz	0	1/s	Strain rate tensor, phiz component	Domains 1–2	
spf.srijzz	wz	1/s	Strain rate tensor, zz component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
spf.srijmeanrr	0.5*root.comp1.spf.elemint(2*ur)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, rr component	Domains 1–2	
spf.srijmeanphir	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, phir component	Domains 1–2	
spf.srijmeanzr	0.5*root.comp1.spf.elemint(wr+uz)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zr component	Domains 1–2	
spf.srijmeanrphi	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, rphi component	Domains 1–2	
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	Domains 1–2	
spf.srijmeanzphi	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zphi component	Domains 1–2	
spf.srijmeanrz	0.5*root.comp1.spf.elemint(uz+wr)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, rz component	Domains 1–2	
spf.srijmeanphiz	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, phiz component	Domains 1–2	
spf.srijmeanzz	0.5*root.comp1.spf.elemint(2*wz)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zz component	Domains 1–2	
spf.rrijrr	0	1/s	Rotation rate tensor, rr component	Domains 1–2	

Name	Expression	Unit	Description	Selection	Details
spf.rrijphir	0	1/s	Rotation rate tensor, phir component	Domains 1–2	
spf.rrijzr	0.5*(wr-uz)	1/s	Rotation rate tensor, zr component	Domains 1–2	
spf.rrijrphi	0	1/s	Rotation rate tensor, rphi component	Domains 1–2	
spf.rrijphiphi	0	1/s	Rotation rate tensor, phiphi component	Domains 1–2	
spf.rrijzphi	0	1/s	Rotation rate tensor, zphi component	Domains 1–2	
spf.rrijrz	0.5*(uz-wr)	1/s	Rotation rate tensor, rz component	Domains 1–2	
spf.rrijphiz	0	1/s	Rotation rate tensor, phiz component	Domains 1–2	
spf.rrijzz	0	1/s	Rotation rate tensor, zz component	Domains 1–2	
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.srijzphi^2+2*spf.srijzz^2+eps)	1/s	Shear rate	Domains 1–2	
spf.divu	ur+if(abs(r)<0.001*h_spatial,ur,u/r)+wz	1/s	Divergence of velocity field	Domains 1–2	
spf.Fr	0	N/m³	Volume force, r component	Domains 1–2	+ operation
spf.Fphi	0	N/m³	Volume force, phi component	Domains 1–2	+ operation
spf.Fz	0	N/m³	Volume force, z component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
spf.U	sqrt(u^2+w^2)	m/s	Velocity magnitude	Domains 1–2	
spf.vorticityr	0	1/s	Vorticity field, r component	Domains 1–2	
spf.vorticityphi	-wr+uz	1/s	Vorticity field, phi component	Domains 1–2	
spf.vorticityz	0	1/s	Vorticity field, z component	Domains 1–2	
spf.vort_magn	sqrt(spf.vorticityr^2+spf.vorticityphi^2+spf.vorticityz^2)	1/s	Vorticity magnitude	Domains 1–2	
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	Domains 1–2	
spf.nu	spf.mu/spf.rho	m^2/s	Kinematic viscosity	Domains 1–2	
spf.betaT	0	1/Pa	Isothermal compressibility coefficient	Domains 1–2	
spf.Qm	0	$kg/(m^3·s)$	Source term	Domains 1–2	+ operation
spf.Fgtotr	0	N/m^3	Gravity force, r component	Domains 1–2	+ operation
spf.Fgtotphi	0	N/m^3	Gravity force, phi component	Domains 1–2	+ operation
spf.Fgtotz	0	N/m^3	Gravity force, z component	Domains 1–2	+ operation
spf.mu_eff	spf.mu+spf.muT	Pa·s	Dynamic viscosity	Domains 1–2	
spf.muT	0	Pa·s	Turbulent dynamic viscosity	Domains 1–2	
spf.T_stressr	spf.K_stressr-p*spf.nrmesh	N/m^2	Total stress, r component	Boundaries 1–9	+ operation
spf.T_stressphi	spf.K_stressphi-p*spf.nphimesh	N/m^2	Total stress, phi component	Boundaries 1–9	+ operation
spf.T_stressz	spf.K_stressz-p*spf.nzmesh	N/m^2	Total stress, z component	Boundaries 1–9	+ operation

Name	Expression	Unit	Description	Selection	Details
spf.K_stressr	spf.mu_eff*(2*ur*spf.nrmesh+(uz+wr)*spf.nzmesh)	N/m²	Viscous stress, r component	Boundaries 1–9	+ 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 1–9	+ operation
spf.K_stressz	spf.mu_eff*((wr+uz)*spf.nrmesh+2*wz*spf.nzmesh)	N/m²	Viscous stress, z component	Boundaries 1–9	+ operation
spf.K_stress_tensorrr	2*spf.mu_eff*ur	N/m²	Viscous stress tensor, rr component	Domains 1–2	+ operation
spf.K_stress_tensorphir	0	N/m²	Viscous stress tensor, phir component	Domains 1–2	+ operation
spf.K_stress_tensorzr	spf.mu_eff*(wr+uz)	N/m²	Viscous stress tensor, zr component	Domains 1–2	+ operation
spf.K_stress_tensorrphi	0	N/m²	Viscous stress tensor, rphi component	Domains 1–2	+ 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	Domains 1–2	+ operation
spf.K_stress_tensorzphi	0	N/m²	Viscous stress tensor, zphi component	Domains 1–2	+ operation
spf.K_stress_tensorrz	spf.mu_eff*(uz+wr)	N/m²	Viscous stress tensor, rz component	Domains 1–2	+ operation
spf.K_stress_tensorphiz	0	N/m²	Viscous stress tensor, phiz component	Domains 1–2	+ operation
spf.K_stress_tensorzz	2*spf.mu_eff*wz	N/m²	Viscous stress tensor, zz component	Domains 1–2	+ operation
spf.K_stress_tensor_testrr	2*spf.mu_eff*test(ur)	N/m²	Viscous stress tensor test, rr component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
spf.K_stress_tensor_testphir	0	N/m²	Viscous stress tensor test, phir component	Domains 1–2	+ operation
spf.K_stress_tensor_testzr	spf.mu_eff*(test(wr)+test(uz))	N/m²	Viscous stress tensor test, zr component	Domains 1–2	+ operation
spf.K_stress_tensor_testrphi	0	N/m²	Viscous stress tensor test, rphi component	Domains 1–2	+ 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	Domains 1–2	+ operation
spf.K_stress_tensor_testzphi	0	N/m²	Viscous stress tensor test, zphi component	Domains 1–2	+ operation
spf.K_stress_tensor_testrz	spf.mu_eff*(test(uz)+test(wr))	N/m²	Viscous stress tensor test, rz component	Domains 1–2	+ operation
spf.K_stress_tensor_testphiz	0	N/m²	Viscous stress tensor test, phiz component	Domains 1–2	+ operation
spf.K_stress_tensor_testzz	2*spf.mu_eff*test(wz)	N/m²	Viscous stress tensor test, zz component	Domains 1–2	+ operation
spf.upwind_helpr	-d(r,TIME)	m/s	Upwind term, r component	Domains 1–2	+ operation
spf.upwind_helpphi	0	m/s	Upwind term, phi component	Domains 1–2	+ operation
spf.upwind_helpz	-d(z,TIME)	m/s	Upwind term, z component	Domains 1–2	+ operation
spf.tau_vdrr	2*spf.mu*spf.srijrr	Pa	Viscous stress tensor, rr component	Domains 1–2	+ operation
spf.tau_vdphir	2*spf.mu*spf.srijphir	Pa	Viscous stress tensor, phir component	Domains 1–2	+ operation
spf.tau_vdzr	2*spf.mu*spf.srijzr	Pa	Viscous stress tensor, zr component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
spf.tau_vdrphi	2*spf.mu*spf.srijrphi	Pa	Viscous stress tensor, rphi component	Domains 1–2	+ operation
spf.tau_vdphiphi	2*spf.mu*spf.srijphiphi	Pa	Viscous stress tensor, phiphi component	Domains 1–2	+ operation
spf.tau_vdzphi	2*spf.mu*spf.srijzphi	Pa	Viscous stress tensor, zphi component	Domains 1–2	+ operation
spf.tau_vdrz	2*spf.mu*spf.srijrz	Pa	Viscous stress tensor, rz component	Domains 1–2	+ operation
spf.tau_vdphiz	2*spf.mu*spf.srijphiz	Pa	Viscous stress tensor, phiz component	Domains 1–2	+ operation
spf.tau_vdzz	2*spf.mu*spf.srijzz	Pa	Viscous stress tensor, zz component	Domains 1–2	+ 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	Domains 1–2	+ operation
spf.epsilon_p	1	1	Porosity	Domains 1–2	
spf.Fst_tensorrr	0	N/m²	Surface tension force, rr component	Domains 1–2	+ operation
spf.Fst_tensorphir	0	N/m²	Surface tension force, phir component	Domains 1–2	+ operation
spf.Fst_tensorzr	0	N/m²	Surface tension force, zr component	Domains 1–2	+ operation
spf.Fst_tensorrphi	0	N/m²	Surface tension force, rphi component	Domains 1–2	+ operation
spf.Fst_tensorphiphi	0	N/m²	Surface tension force, phiphi component	Domains 1–2	+ operation

Name	Expression	Unit	Description	Selection	Details
spf.Fst_tensorzphi	0	N/m²	Surface tension force, zphi component	Domains 1–2	+ operation
spf.Fst_tensorrz	0	N/m²	Surface tension force, rz component	Domains 1–2	+ operation
spf.Fst_tensorphiz	0	N/m²	Surface tension force, phiz component	Domains 1–2	+ operation
spf.Fst_tensorzz	0	N/m²	Surface tension force, zz component	Domains 1–2	+ operation
spf.continuityEquation	spf.rho*spf.divu	kg/(m³·s)	Continuity equation	Domains 1–2	
spf.contCoeff	spf.rho	kg/m³	Help variable	Domains 1–2	
spf.res_u	pr-(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	Domains 1–2	
spf.res_v	-spf.Fphi	N/m³	Equation residual	Domains 1–2	
spf.res_w	pz-(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	Domains 1–2	
spf.res_p	spf.rho*spf.divu	kg/(m³·s)	Pressure equation residual	Domains 1–2	

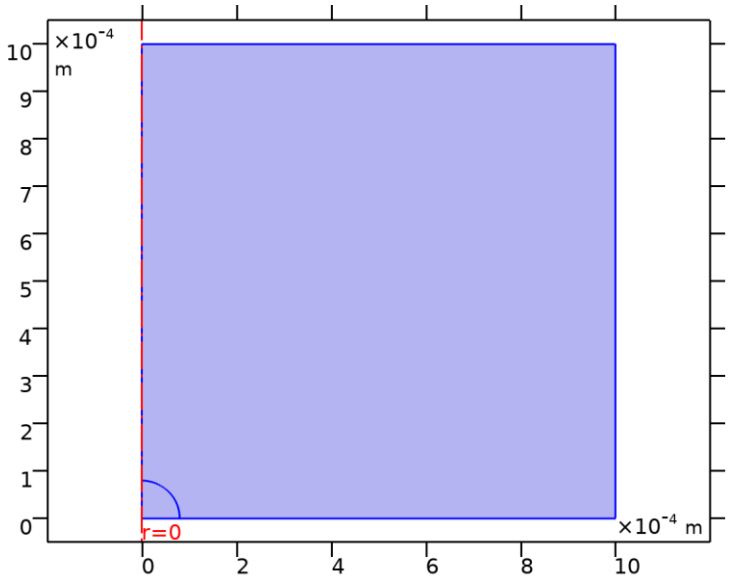
Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
u	Lagrange (Linear)	m/s	Velocity field, r component	Spatial	Domains 1–2
w	Lagrange (Linear)	m/s	Velocity field, z component	Spatial	Domains 1–2
p	Lagrange (Linear)	Pa	Pressure	Spatial	Domains 1–2

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-spf.K_stress_tensorzz)*test(wz))*pi*r	2	Spatial	Domains 1–2
2*(spf.Fr*test(u)+spf.Fz*test(w))*pi*r	2	Spatial	Domains 1–2
-2*spf.continuityEquation*test(p)*pi*r	2	Spatial	Domains 1–2
2*spf.streamlinens*pi*r	2	Spatial	Domains 1–2
2*(spf.usePseudoTimeStepping>0)*spf.rho*spf.tsti*(-(u-nojac(u))*test(u)-(w-nojac(w))*test(w))*pi*r	2	Spatial	Domains 1–2

2.4.4 Initial Values 1



Initial Values 1

SELECTION

Geometric entity level	Domain
Selection	Domains 1–2

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

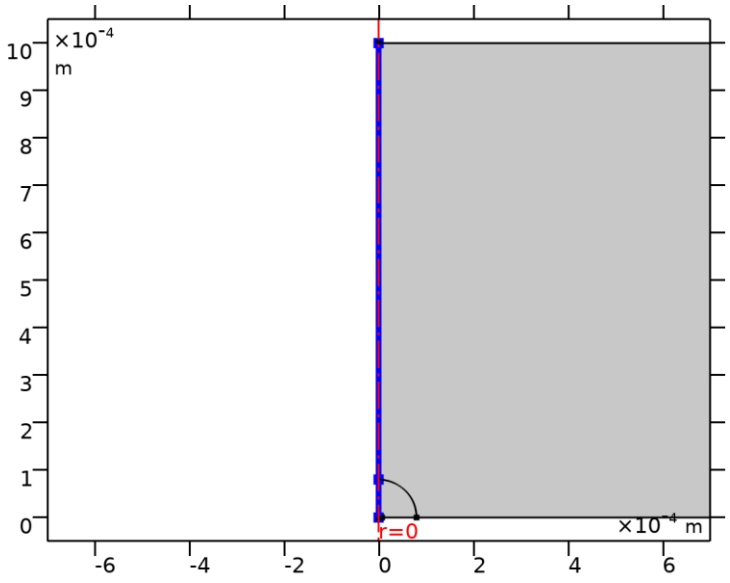
SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection
spf.u_initr	0	m/s	Velocity field, r component	Domains 1–2
spf.u_initphi	0	m/s	Velocity field, phi component	Domains 1–2
spf.u_initz	0	m/s	Velocity field, z component	Domains 1–2
spf.p_init	0	Pa	Pressure	Domains 1–2

2.4.5 Axial Symmetry 1



Axial Symmetry 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1, 3

Constraint settings

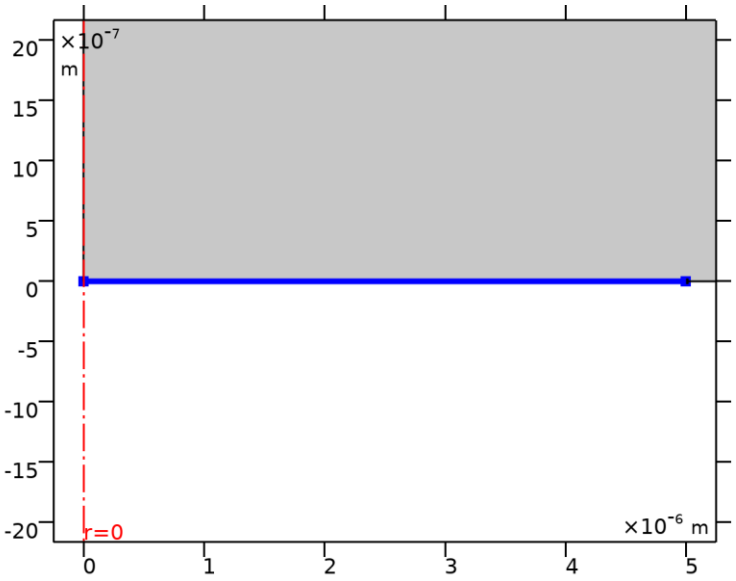
SETTINGS

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, 3	Elemental

2.4.6 Wall 1



Wall 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 2

EQUATIONS

$$u = 0$$

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

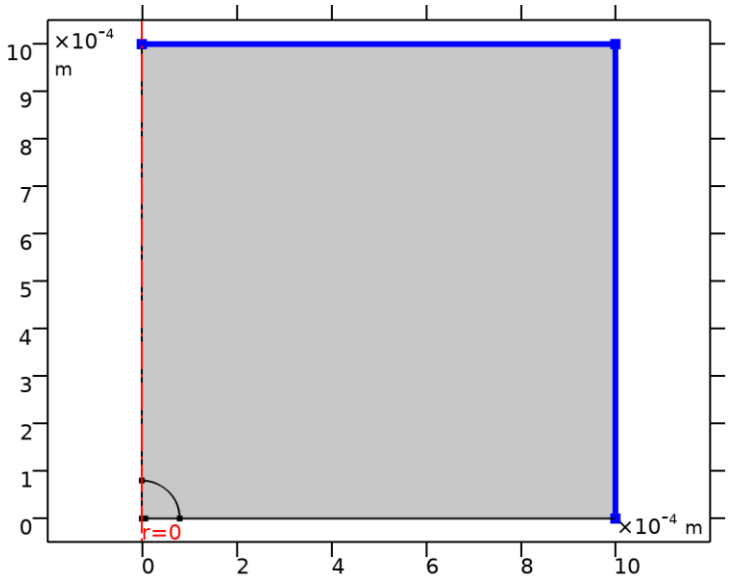
Variables

Name	Expression	Unit	Description	Selection	Details
spf.ubndr	0	m/s	Velocity at boundary, r component	Boundary 2	+ operation
spf.ubndphi	0	m/s	Velocity at boundary, phi component	Boundary 2	+ operation
spf.ubndz	0	m/s	Velocity at boundary, z component	Boundary 2	+ operation
spf.uLeakager	0	m/s	Leakage velocity, r component	Boundary 2	+ operation
spf.uLeakagephi	0	m/s	Leakage velocity, phi component	Boundary 2	+ operation
spf.uLeakagez	0	m/s	Leakage velocity, z component	Boundary 2	+ operation
spf.noSlipWall	1	1	Help variable	Boundary 2	

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-u+spf.ubndr+spf.uLeakager	test(-u)	Lagrange (Linear)	Boundary 2	Elemental
spf.ubndphi+spf.uLeakagephi	0		Boundary 2	Elemental
-w+spf.ubndz+spf.uLeakagez	test(-w)	Lagrange (Linear)	Boundary 2	Elemental

2.4.7 Open Boundary 1



Open Boundary 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 4, 8

EQUATIONS

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

Boundary condition

SETTINGS

Description	Value
Boundary condition	Normal stress
Normal stress	0

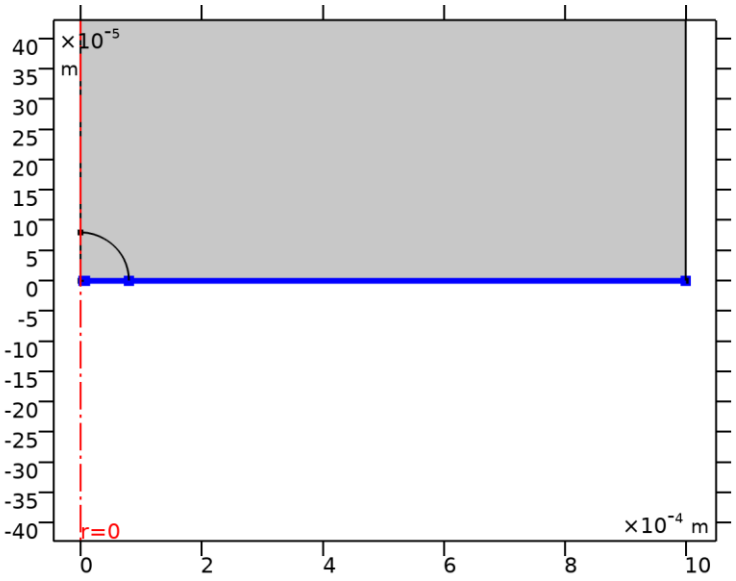
Variables

Name	Expression	Unit	Description	Selection
spf.f0	0	N/m²	Normal stress	Boundaries 4, 8

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 4, 8

2.4.8 Wall, Glass insulation



Wall, Glass insulation

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 5–7

EQUATIONS

$$\mathbf{u} = \mu_{eo}\mathbf{E}_t$$

$$\mu_{eo} = -\frac{\epsilon_r\epsilon_0\zeta}{\mu}, \quad \mathbf{E}_t = \mathbf{E} - (\mathbf{E}\cdot\mathbf{n})\mathbf{n}$$

Boundary condition

SETTINGS

Description	Value
Wall condition	Electroosmotic velocity

Description	Value
Electric field	User defined
Electric field	{-phir, 0, -phiz}
Electroosmotic mobility	Built - in expression
Zeta potential	zeta0*(log((cM + cO)/(1[M]))/(log(0.001)))
Relative permittivity	80

Wall movement

SETTINGS

Description	Value
Translational velocity	Automatic from frame
Sliding wall	Off

Variables

Name	Expression	Unit	Description	Selection	Details
spf.ubndr	spf.ueor	m/s	Velocity at boundary, r component	Boundaries 5–7	+ operation
spf.ubndphi	spf.ueophi	m/s	Velocity at boundary, phi component	Boundaries 5–7	+ operation
spf.ubndz	spf.ueoz	m/s	Velocity at boundary, z component	Boundaries 5–7	+ operation
spf.uLeakager	0	m/s	Leakage velocity, r component	Boundaries 5–7	+ operation
spf.uLeakagephi	0	m/s	Leakage velocity, phi component	Boundaries 5–7	+ operation
spf.uLeakagez	0	m/s	Leakage velocity, z component	Boundaries 5–7	+ operation
spf.u_herer	u	m/s	Intermediate variable, r component	Boundaries 5–7	
spf.u_herephi	0	m/s	Intermediate variable, phi component	Boundaries 5–7	

Name	Expression	Unit	Description	Selection	Details
spf.u_herez	w	m/s	Intermediate variable, z component	Boundaries 5–7	
spf.u_therer	spf.ubndr+spf.uLeakager	m/s	Intermediate variable, r component	Boundaries 5–7	
spf.u_therephi	spf.ubndphi+spf.uLeakagephi	m/s	Intermediate variable, phi component	Boundaries 5–7	
spf.u_therez	spf.ubndz+spf.uLeakagez	m/s	Intermediate variable, z component	Boundaries 5–7	
spf.KStressn_avr	spf.K_stress_tensorrr*spf.nrmesh+spf.K_stress_tensorrphi*spf.nphimesh+spf.K_stress_tensorrz*spf.nzmesh	N/m^2	Average viscous stress, r component	Boundaries 5–7	
spf.KStressn_avphi	spf.K_stress_tensorphir*spf.nrmesh+spf.K_stress_tensorphiphi*spf.nphimesh+spf.K_stress_tensorphiz*spf.nzmesh	N/m^2	Average viscous stress, phi component	Boundaries 5–7	
spf.KStressn_avz	spf.K_stress_tensorzr*spf.nrmesh+spf.K_stress_tensorzphi*spf.nphimesh+spf.K_stress_tensorzz*spf.nzmesh	N/m^2	Average viscous stress, z component	Boundaries 5–7	
spf.KStressTestn_avr	spf.K_stress_tensor_testrr*spf.nrmesh+spf.K_stress_tensor_testrphi*spf.nphimesh+spf.K_stress_tensor_testrz*spf.nzmesh	N/m^2	Average viscous stress, r component	Boundaries 5–7	
spf.KStressTestn_avphi	spf.K_stress_tensor_testphir*spf.nrmesh+spf.K_stress_tensor_testphiphi*spf.nphimesh+spf.K_stress_tensor_testphiz*spf.nzmesh	N/m^2	Average viscous stress, phi component	Boundaries 5–7	

Name	Expression	Unit	Description	Selection	Details
spf.KStressTestn_avz	spf.K_stress_tensor_testzr*spf.nrmesh+spf.K_stress_tensor_testzphi*spf.nphimesh+spf.K_stress_tensor_testzz*spf.nzmesh	N/m²	Average viscous stress, z component	Boundaries 5–7	
spf.ujumpr	spf.u_herer-spf.u_therer	m/s	Velocity jump, r component	Boundaries 5–7	
spf.ujumpphi	spf.u_herephi-spf.u_therephi	m/s	Velocity jump, phi component	Boundaries 5–7	
spf.ujumpz	spf.u_herez-spf.u_therez	m/s	Velocity jump, z component	Boundaries 5–7	
spf.meshVol	meshvol_spatial	m		Boundaries 5–7	
spf.meshVolInt	down(meshvol_spatial)	m²	Volume of interior mesh element	Boundaries 5–7	
spf.c_here	24*nojac(down(spf.mu))*spf.meshVol/spf.meshVolInt	Pa·s/m	Intermediate variable	Boundaries 5–7	
spf.sigma_dg_ns	4*spf.c_here	Pa·s/m		Boundaries 5–7	
spf.rhoFace	down(spf.rho)	kg/m³	Density face value	Boundaries 5–7	
spf.contCoeffFace	down(spf.contCoeff)	kg/m³	Help variable	Boundaries 5–7	
spf.umxTnFace	(spf.upwind_helpr*spf.nrmesh+spf.upwind_helpphi*spf.nphimesh+spf.upwind_helpz*spf.nzmesh<0)*(spf.upwind_helpr*spf.nrmesh+spf.upwind_helpphi*spf.nphimesh+spf.upwind_helpz*spf.nzmesh)	m/s	Relative velocity on face	Boundaries 5–7	
spf.upwind_ns	spf.rhoFace*spf.umxTnFace*(spf.ujumpr*test(spf.u_herer)+spf.ujumpphi*test(spf.u_herephi)+spf.ujumpz*test(spf.u_herez))	W/m²	Upwind term	Boundaries 5–7	

Name	Expression	Unit	Description	Selection	Details
spf.upwindCont	spf.contCoeffFace*(spf.ujumpr*spf.nrmesh+spf.ujumpphi*spf.nphimesh+spf.ujumpz*spf.nzmesh)*test(p)	$kg^2/(m^3 \cdot s^3)$	Upwind term for continuity equation	Boundaries 5–7	
spf.pFace	p	Pa	Pressure face value	Boundaries 5–7	
spf.consFlux	spf.pFace*(-test(spf.u_herer)*spf.nrmesh-test(spf.u_herephi)*spf.nphimesh-test(spf.u_herez)*spf.nzmesh)	W/m^2	Conservative flux	Boundaries 5–7	+ operation
spf.zeta	zeta0*log((cM+cO)/1[M])/log(0.001)	V	Zeta potential	Boundaries 5–7	
spf.epsilonr	80	1	Relative permittivity	Boundaries 5–7	
spf.Er	model.input.E1	V/m	Electric field, r component	Boundaries 5–7	Meta
spf.Ephi	model.input.E2	V/m	Electric field, phi component	Boundaries 5–7	Meta
spf.Ez	model.input.E3	V/m	Electric field, z component	Boundaries 5–7	Meta
spf.mueo	-spf.zeta*epsilon0_const*spf.epsilonr/spf.mu	$m^2/(V \cdot s)$	Electroosmotic mobility	Boundaries 5–7	
spf.ueor	(spf.Er-spf.nrmesh*(spf.nrmesh*spf.Er+spf.nphimesh*spf.Ephi+spf.nzmesh*spf.Ez))*spf.mueo	m/s	Electroosmotic velocity, r component	Boundaries 5–7	
spf.ueophi	(spf.Ephi-spf.nphimesh*(spf.nrmesh*spf.Er+spf.nphimesh*spf.Ephi+spf.nzmesh*spf.Ez))*spf.mueo	m/s	Electroosmotic velocity, phi component	Boundaries 5–7	

Name	Expression	Unit	Description	Selection	Details
spf.ueoz	(spf.Ez-spf.nzmesh*(spf.nrmesh*spf.Er+spf.nphimesh*spf.Ephi+spf.nzmesh*spf.Ez))*spf.mueo	m/s	Electroosmotic velocity, z component	Boundaries 5–7	

Weak expressions

Weak expression	Integration order	Integration frame	Selection
2*(spf.KStressn_avr*test(spf.u_herer)+spf.KStressn_avphi*test(spf.u_herephi)+spf.KStressn_avz*test(spf.u_herez)+spf.KStressTestn_avr*spf.ujumpr+spf.KStressTestn_avphi*spf.ujumpphi+spf.KStressTestn_avz*spf.ujumpz-spf.sigma_dg_ns*spf.ujumpr*test(spf.u_herer)-spf.sigma_dg_ns*spf.ujumpphi*test(spf.u_herephi)-spf.sigma_dg_ns*spf.ujumpz*test(spf.u_herez)+spf.upwind_ns+spf.upwindCont+spf.consFlux)*pi*r	2	Spatial	Boundaries 5–7

2.5 MULTIPHYSICS

2.5.1 Flow Coupling 1

USED PRODUCTS

COMSOL Multiphysics

Coupled interfaces

SETTINGS

Description	Value
Source	Creeping Flow (spf)
Destination	Tertiary Current Distribution, Nernst - Planck (tcd)

Variables

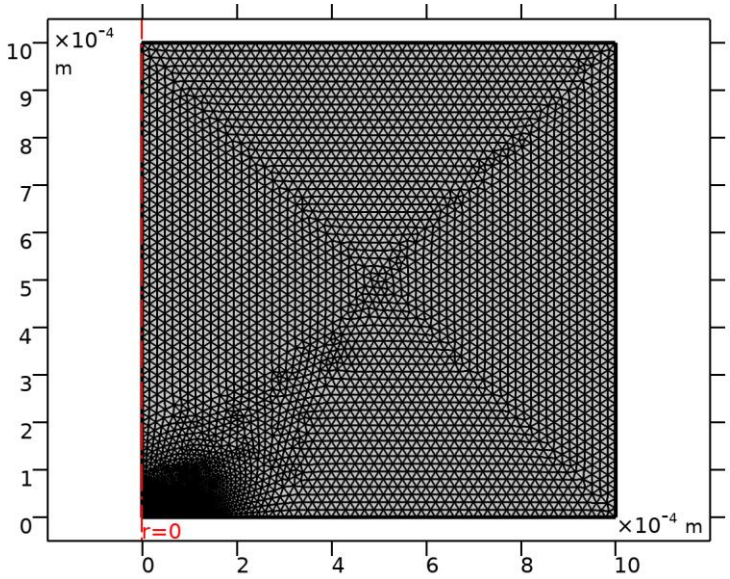
Name	Expression	Unit	Description	Selection
fc1.uR	spatial.invF11*u+spatial.invF31*w	m/s	Velocity field, R component	Global

Name	Expression	Unit	Description	Selection
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

2.6 MESH 1

MESH STATISTICS

Description	Value
Minimum element quality	0.291
Average element quality	0.9639
Triangle	222187
Edge element	2869
Vertex element	8



Mesh 1

2.6.1 Size, default (size)

SETTINGS

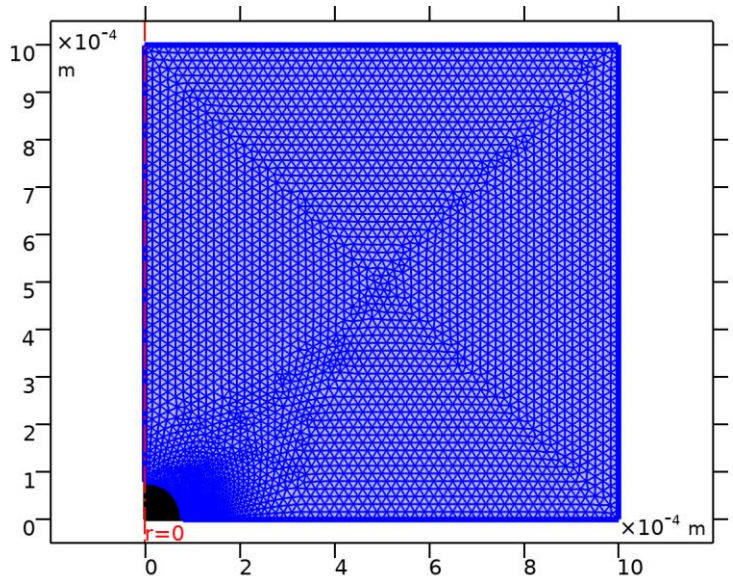
Description	Value
Maximum element size	2E-5

Description	Value
Minimum element size	1E-8
Curvature factor	0.3
Maximum element growth rate	1.16
Custom element size	Custom

2.6.2 Size, outer domain (size1)

SELECTION

Geometric entity level	Domain
Selection	Domain 2



Size, outer domain

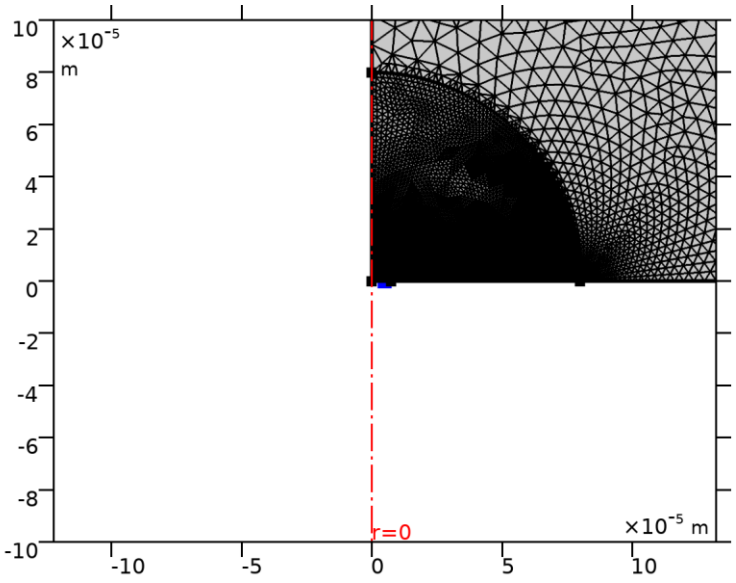
SETTINGS

Description	Value
Maximum element size	2E-5
Minimum element size	3.0E-7
Minimum element size	Off
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.08
Custom element size	Custom

2.6.3 Size, UME edge point (size2)

SELECTION

Geometric entity level	Point
Selection	Point 4



Size, UME edge point

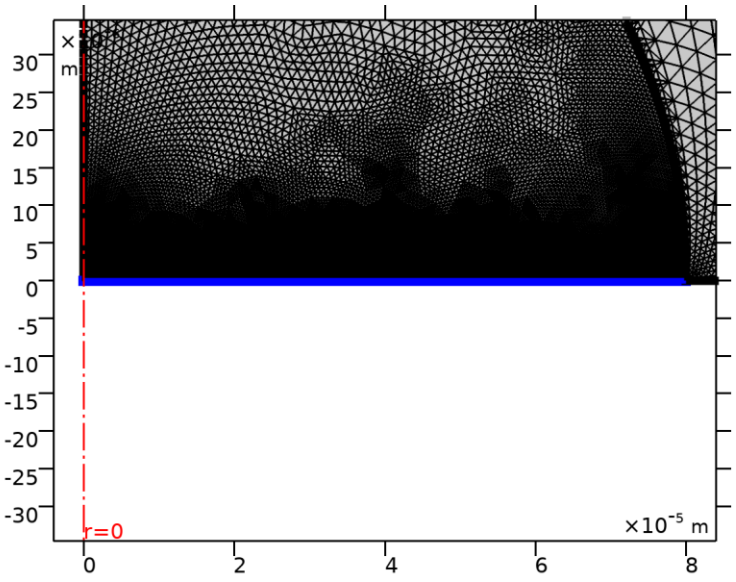
SETTINGS

Description	Value
Maximum element size	1E-9
Minimum element size	2E-10
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

2.6.4 Edge, UME and glass (edg1)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2, 5–6

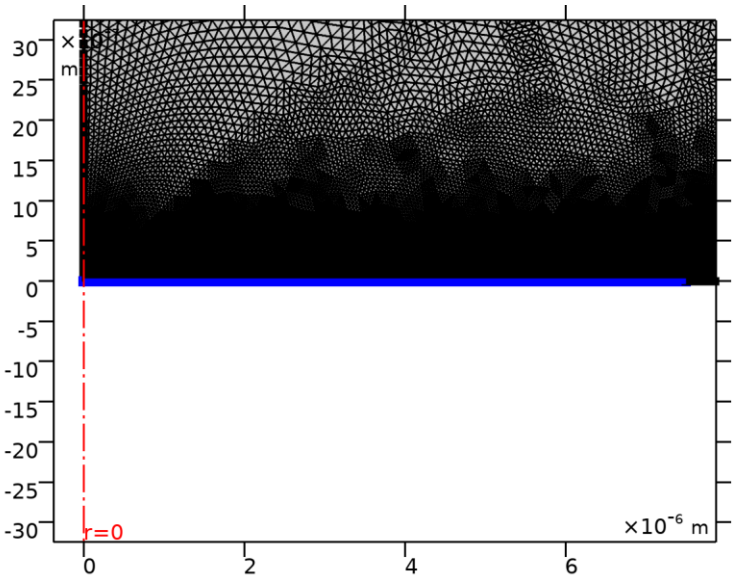


Edge, UME and glass

Size, near UME (size1)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2, 5



Size, near UME

SETTINGS

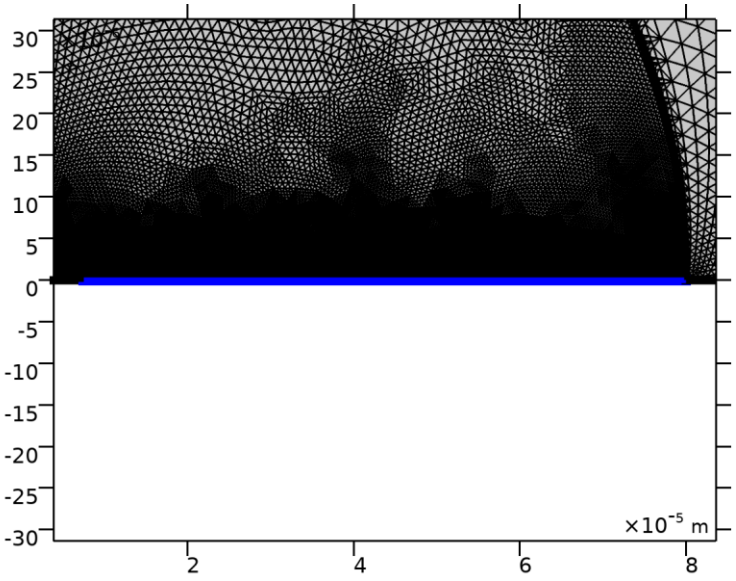
Description	Value
Maximum element size	2E-8

Description	Value
Minimum element size	1E-9
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

Size, glass further from UME (size2)

SELECTION

Geometric entity level	Boundary
Selection	Boundary 6



Size, glass further from UME

SETTINGS

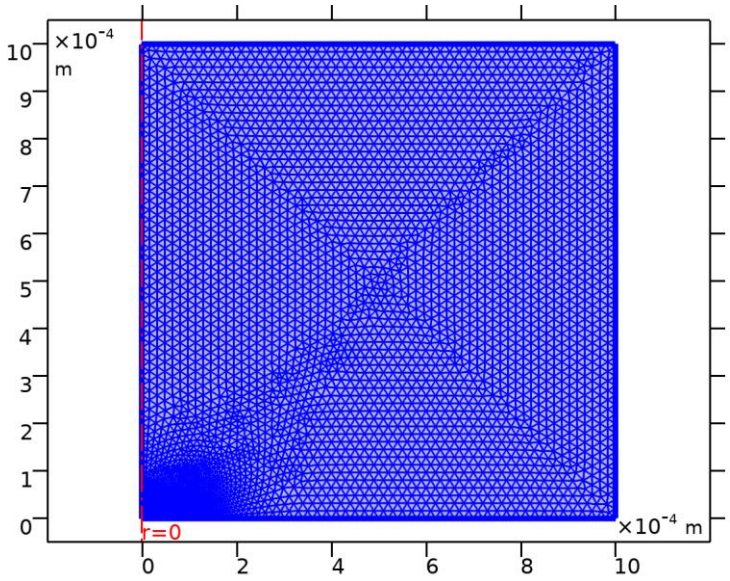
Description	Value
Maximum element size	0.5E-6
Minimum element size	3.0E-7
Minimum element size	Off
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off

Description	Value
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

2.6.5 Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Remaining

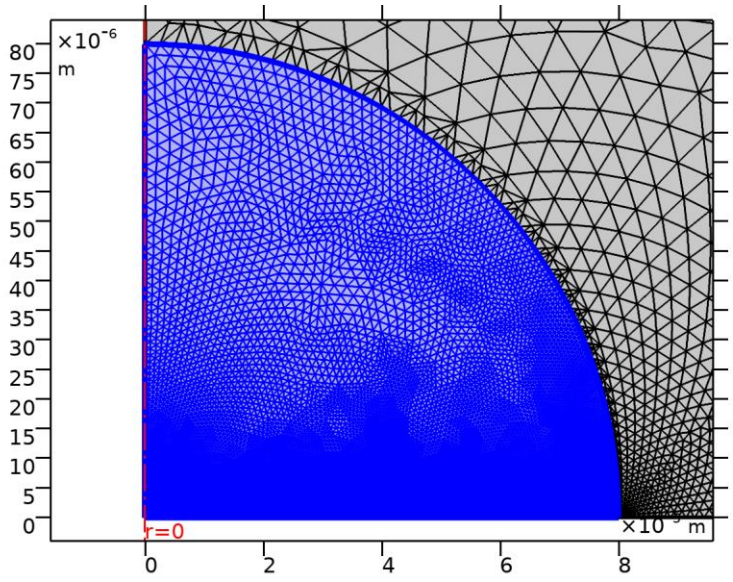


Free Triangular 1

2.6.6 Refine 1 (ref1)

SELECTION

Geometric entity level	Domain
Selection	Domain 1



Refine 1

SETTINGS

Description	Value
Number of refinements	2

3 Study 1

COMPUTATION INFORMATION

Computation time	10 min 1 s
CPU	Intel64 Family 6 Model 60 Stepping 3, 4 cores
Operating system	Windows 10

3.1 STATIONARY

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

MESH SELECTION

Geometry	Mesh
mesh1	mesh1

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Tertiary Current Distribution, Nernst-Planck (tcd)	physics
Creeping Flow (spf)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.2 SOLVER CONFIGURATIONS

3.2.1 Solution 1

Compile Equations: Stationary (st1)

STUDY AND STEP

Description	Value
Use study	Study 1
Use study step	Stationary