Continuous separation simulations-052621

Report date	May 26, 2021 10:53:06 AM

Contents

1 Global Definitions

Date	May 26, 2021 10:44:47 AM

GLOBAL SETTINGS

Name	Continuous separation simulations-052621.mph
Path	C:\Users\jrt3552\Documents\BED\final final simulations\Continuous separation simulations-052621.mph
Version	COMSOL Multiphysics 5.5 (Build: 359)
Unit system	SI

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

1.1 PARAMETERS

PARAMETERS 1

Name	Expression	Value	Description
cheight	15[um]	1.5E−5 m	channel height
cwidth	200[um]	2E−4 m	channel width
cH3O0	10^ - pH0[M]	1E−4 mol/m³	initial concentration of protons
pH0	7	7	initial solution pH
cOH0	10^ - (14 - pH0)[M]	1E−4 mol/m³	initial concentration of hydroxide
cK0	5 [mM]	5 mol/m³	initial concentration of K
cBead0	30 [fM]	3E−11 mol/m³	initial concentration of microbead
cCl0	cK0	5 mol/m³	initial concentration of Cl

Name	Expression	Value	Description
dH3O	9.103e-9[m^2/s]	9.103E−9 m^2/s	diffusivity of proton
dOH	5.286e-9[m^2/s]	5.286E−9 m^2/s	diffusivity of hydroxide
dK	1.97e-9[m^2/s]	1.97E−9 m^2/s	diffusivity of microbeads
dBead	0.785e-9[m^2/s]	7.85E−10 m^2/s	diffusivity of bead
dCl	2.033e-9[m^2/s]	2.033E−9 m^2/s	diffusivity of Cl
issTOT	4.3[uA]	4.3E−6 A	total current passed through driving electrodes
jssTOT	issTOT/(cwidth*cheight)	1433.3 A/m^2	current density passed through channel
issBPE	2900 [nA]	2.9E−6 A	steady-state current through BPE
jssBPE	issBPE/(elength*ewidth)	1160 A/m^2	current density at BPE
fssBPE	jssBPE/F	0.012023 $mol/(m^2 \cdot s)$	flux at BPE
elength	50[um]	5E−5 m	length of BPE end
ewidth	50[um]	5E−5 m	width of BPE end
F	96485 [C/mol]	96485 C/mol	Faraday's constant
kfhydro	2e-5 [1/(s)]	2E−5 1/s	forward reaction rate constant for water hydrolysis
kbhydro	1.4e11[1/(M*s)]	1.4E8 $m^3/(s \cdot mol)$	backward reaction rate constant for

Name	Expression	Value	Description
			water hydrolysis
cH2O0	55.5 [M]	55500 mol/m³	concentration of water
T	293 [K]	293 K	Temperature

2 Component 1

Date	Jan 3, 2020 8:56:10 AM

SETTINGS

Description	Value
Unit system	Same as global system
Geometry shape order	Automatic
Avoid inverted elements by curving interior domain elements	Off

SPATIAL FRAME COORDINATES

First	Second	Third
x	y	z

MATERIAL FRAME COORDINATES

First	Second	Third
X	Y	Z

GEOMETRY FRAME COORDINATES

First	Second	Third
Xg	Yg	Zg

MESH FRAME COORDINATES

First	Second	Third
Xm	Ym	Zm

2.1 DEFINITIONS

2.1.1 Coordinate Systems

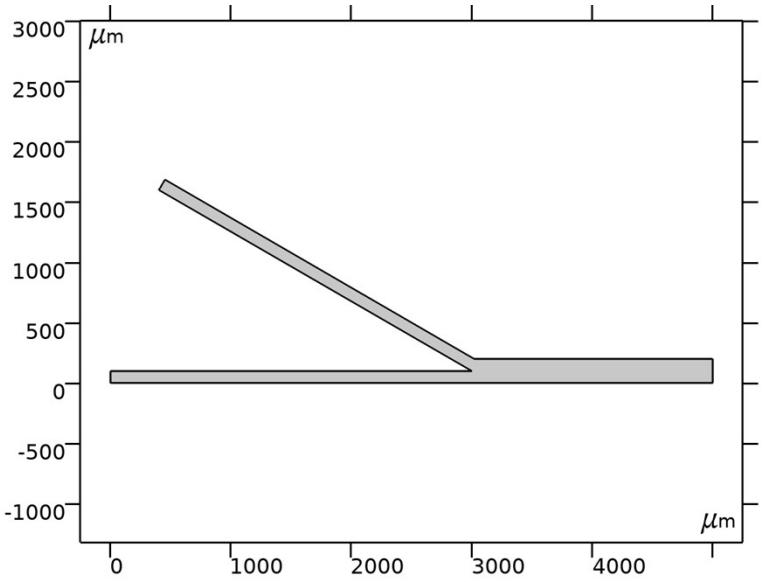
Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third
t1	n	to

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	µm
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	2
Number of domains	1
Number of boundaries	12
Number of vertices	12

2.2.1 Point 3 (pt3)

POINT

Description	Value
Point coordinate	{3200, 0}

2.2.2 Point 4 (pt4)

POINT

Description	Value
Point coordinate	{3250, 0}

2.2.3 Point 1 (pt1)

POINT

Description	Value
Point coordinate	{250, 0}

2.2.4 Point 2 (pt2)

POINT

Description	Value
Point coordinate	{300, 0}

2.2.5 0 0 (pol3)

OBJECT TYPE

Description	Value
Type	Solid

COORDINATES

Description	Value
Data source	Table

COORDINATES

x (µm)	y (µm)
0	0
0	100
3000	100
401.92	1600
451.92	1686.6
3020	200
5000	200
5000	0
0	0

2.2.6 Polygon 1 (pol1)

OBJECT TYPE

Description	Value
Type	Solid

COORDINATES

Description	Value
Data source	Table

COORDINATES

x (µm)	y (µm)
0	0
0	66.7
1000	66.7
133.974	566.7
167.324	624.464
1020	133.4
2960	133.4
2960	0
0	0

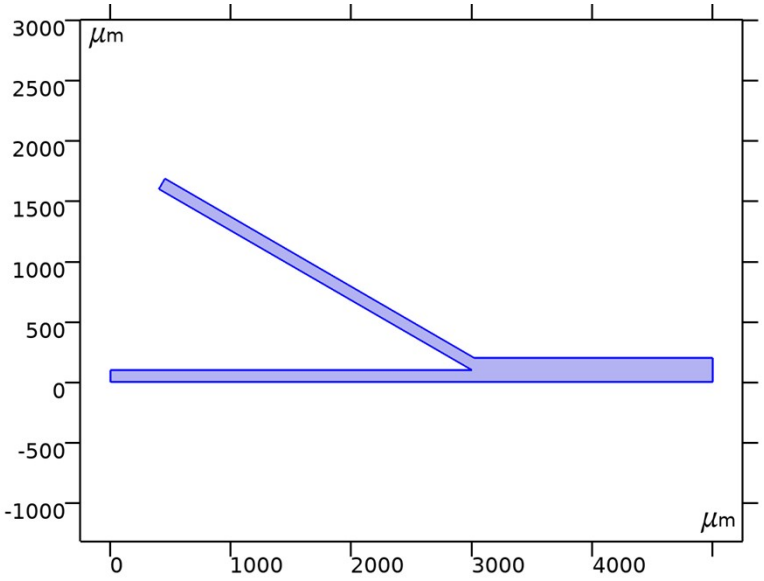
2.2.7 Form Union (fin)

SETTINGS

Description	Value
Repair tolerance	Automatic

2.3 MATERIALS

2.3.1 Water



Water

SELECTION

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

MATERIAL PARAMETERS

Name	Value	Unit
Dynamic viscosity	eta(T)	Pa·s
Density	rho(T)	kg/m³

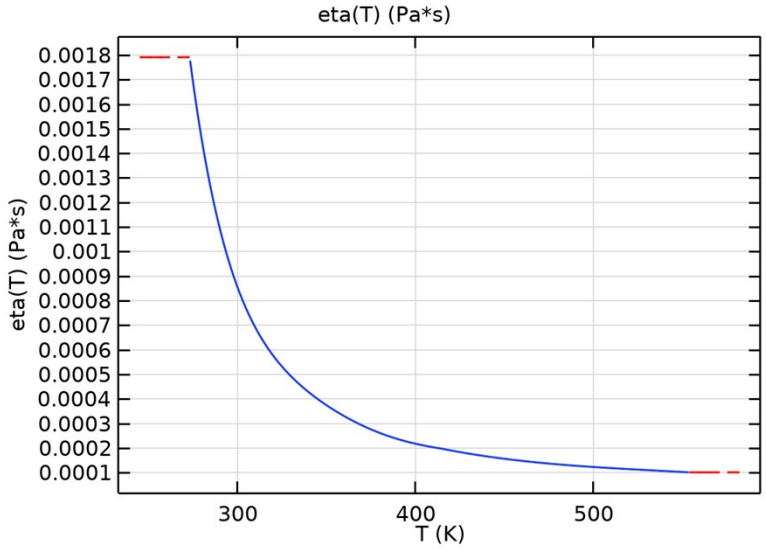
BASIC SETTINGS

Description	Value
Coefficient of thermal expansion	{{alpha_p(T), 0, 0}, {0, alpha_p(T), 0}, {0, 0, alpha_p(T)}}
Bulk viscosity	muB(T)
Dynamic viscosity	eta(T)
Ratio of specific heats	gamma_w(T)
Electrical conductivity	{{5.5e-6[S/m], 0, 0}, {0, 5.5e-6[S/m], 0}, {0, 0, 5.5e-6[S/m]}}
Heat capacity at constant pressure	Cp(T)
Density	rho(T)
Thermal conductivity	{{k(T), 0, 0}, {0, k(T), 0}, {0, 0, k(T)}}

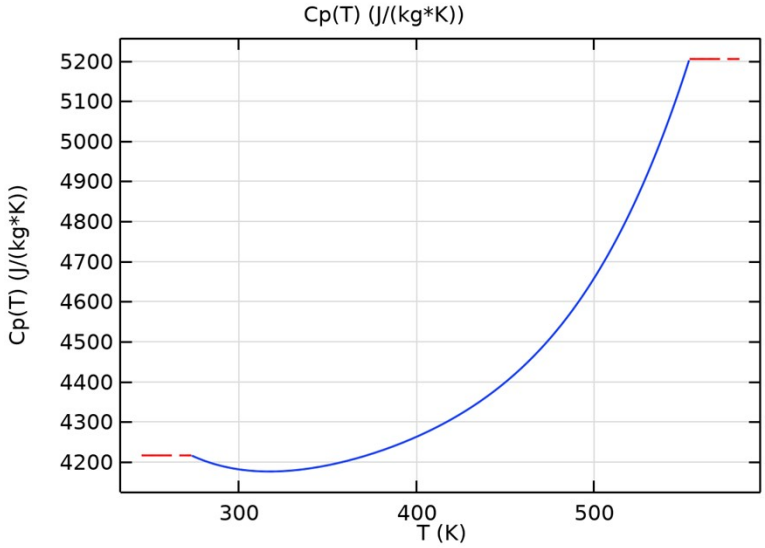
Description	Value
Speed of sound	cs(T)

FUNCTIONS

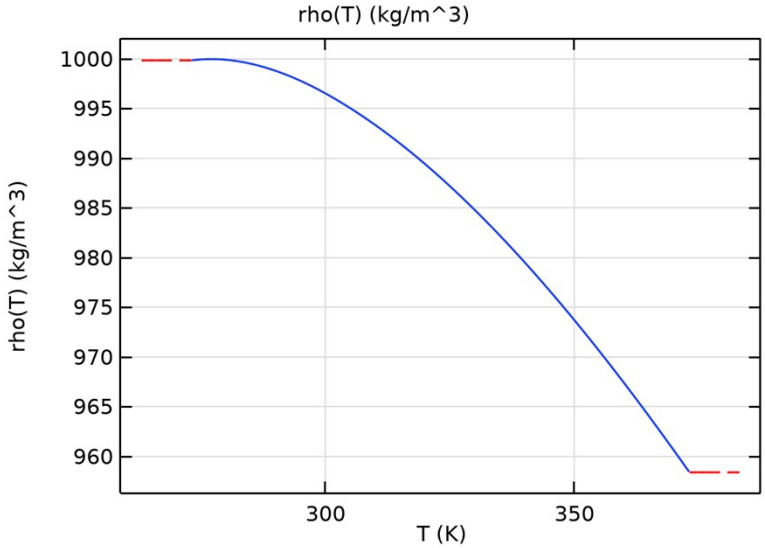
Function name	Type
eta	Piecewise
Cp	Piecewise
rho	Piecewise
k	Piecewise
cs	Interpolation
alpha_p	Analytic
gamma_w	Analytic
muB	Analytic



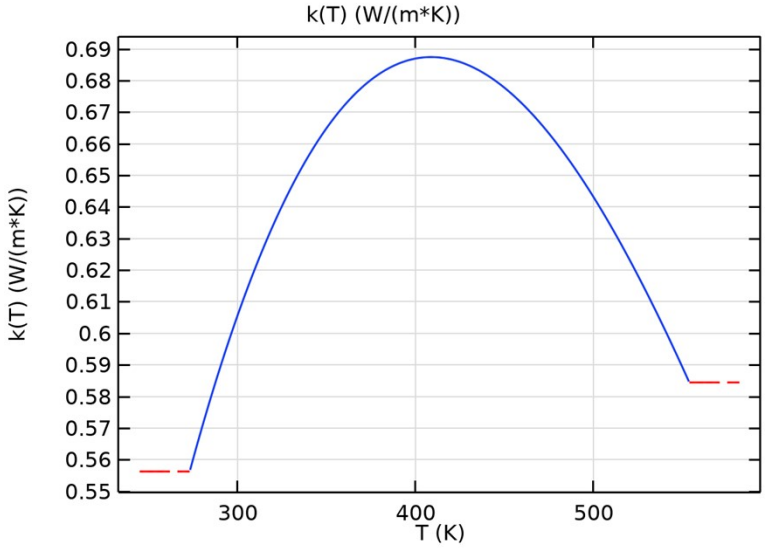
eta


Cp(T) (J/(kg*K))
5200
5100
5000
4900
4800
4700
4600
4500
4400
4300
4200
Cp(T) (J/(kg*K))
300
400
500
T (K)

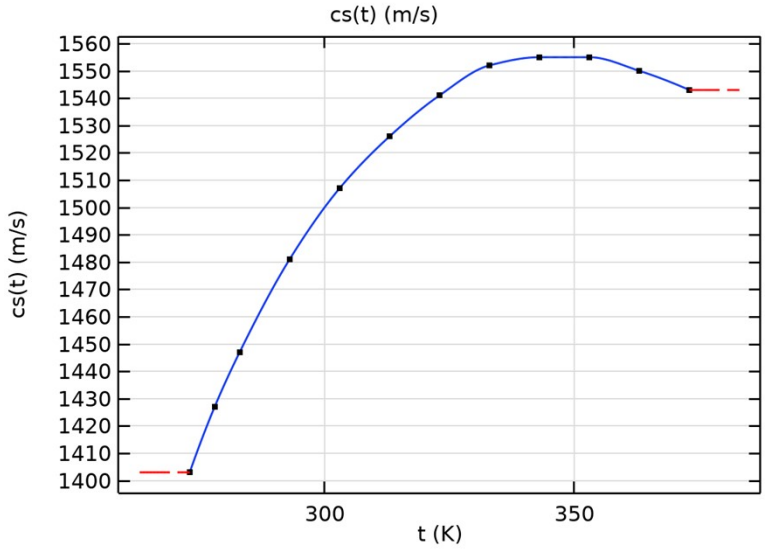
Cp


rho(T) (kg/m^3)
1000
995
990
985
980
975
970
965
960
rho(T) (kg/m^3)
300
350
T (K)

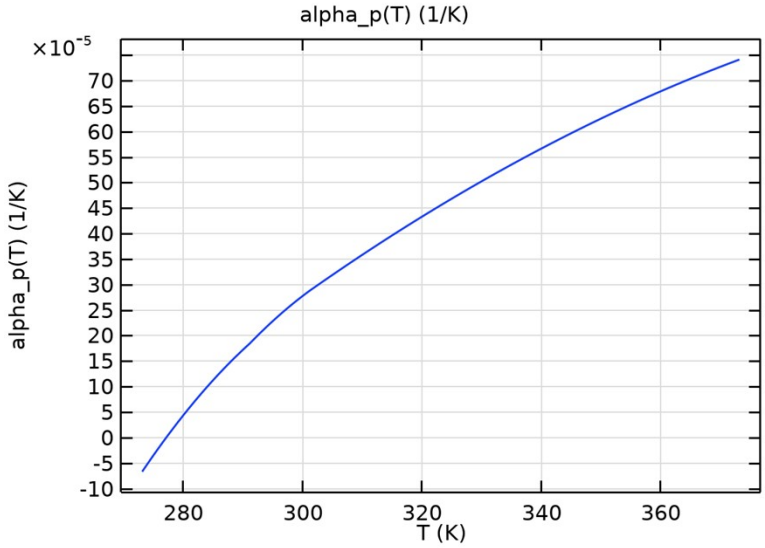
rho


k(T) (W/(m*K))
k(T) (W/(m*K))
0.69
0.68
0.67
0.66
0.65
0.64
0.63
0.62
0.61
0.6
0.59
0.58
0.57
0.56
0.55
300
400
500
T (K)

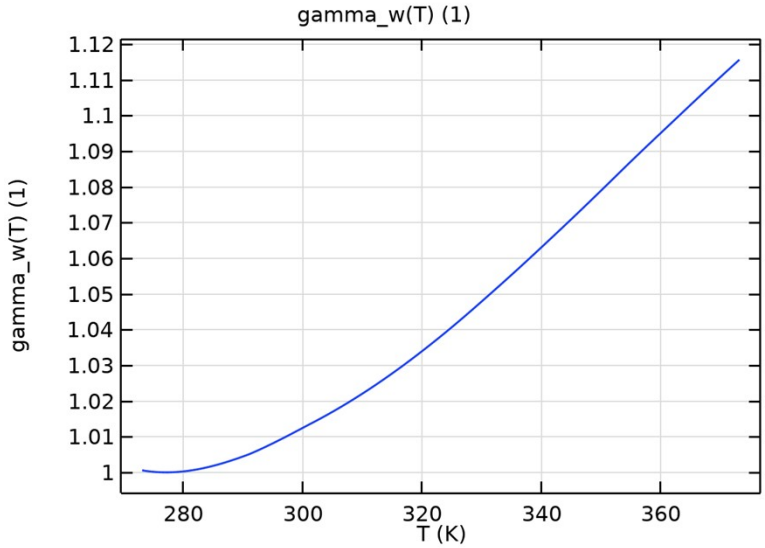
k


cs(t) (m/s)
cs(t) (m/s)
1560
1550
1540
1530
1520
1510
1500
1490
1480
1470
1460
1450
1440
1430
1420
1410
1400
300
350
t (K)

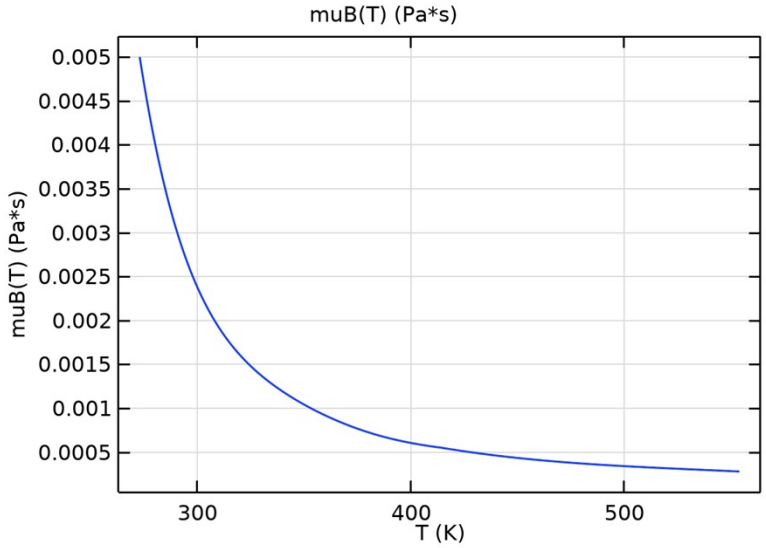
cs



alpha_p



gamma_w



muB

2.4 NERNST-PLANCK EQUATIONS

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

Nernst-Planck Equations

SELECTION

Geometric entity level	Domain

Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\nabla \cdot (\mathbf{J}_i + \mathbf{u}c_i) = R_i$$
$$\nabla \cdot \mathbf{i} = F\sum_i z_i R_i$$
$$\sum_i z_i c_i = 0$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$
$$\mathbf{i} = F\sum_i z_i(-D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V)$$

2.4.1 Interface settings

Discretization

SETTINGS

Description	Value
Concentration	Quadratic
Electric potential	Quadratic

2.4.2 Variables

Name	Expression	Unit	Description	Selection	Details
domflux.cH3Ox	npe.dflux_cH3Ox+npe.cflux_cH3Ox+npe.mflux_cH3Ox	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cH3Oy	npe.dflux_cH3Oy+npe.cflux_cH3Oy+npe.mflux_cH3Oy	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cOHx	npe.dflux_cOHx+npe.cflux_cOHx+npe.mflux_cOHx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cOHy	npe.dflux_cOHy+npe.cflux_cOHy+npe.mflux_cOHy	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cBeadx	npe.dflux_cBeadx+npe.cflux_cBeadx+npe.mflux_cBeadx	mol/(m²·s)	Domain flux, x component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
domflux.cBeady	npe.dflux_cBeady+npe.cflux_cBeady+npe.mflux_cBeady	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cKx	npe.dflux_cKx+npe.cflux_cKx+npe.mflux_cKx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cKy	npe.dflux_cKy+npe.cflux_cKy+npe.mflux_cKy	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cClx	npe.dflux_cClx+npe.cflux_cClx+npe.mflux_cClx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cCly	npe.dflux_cCly+npe.cflux_cCly+npe.mflux_cCly	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.Vx	npe.Jx	A/m²	Domain flux, x component	Domain 1	
domflux.Vy	npe.Jy	A/m²	Domain flux, y component	Domain 1	
npe.nx	dnx	1	Normal vector, x component	Boundaries 1–12	
npe.ny	dny	1	Normal vector, y component	Boundaries 1–12	
npe.nz	0	1	Normal vector, z component	Boundaries 1–12	
npe.nxmesh	dnxmesh	1	Normal vector (mesh), x component	Boundaries 1–12	
npe.nymesh	dnymesh	1	Normal vector (mesh), y component	Boundaries 1–12	
npe.nzmesh	0	1	Normal vector	Boundaries 1–12	

Name	Expression	Unit	Description	Selection	Details
			(mesh), z component		
npe.nxc	root.nxc/npe.ncLen	1	Normal vector, x component	Boundaries 1–12	
npe.nyc	root.nyc/npe.ncLen	1	Normal vector, y component	Boundaries 1–12	
npe.nzc	0	1	Normal vector, z component	Boundaries 1–12	
npe.ncLen	sqrt(root.nxc^2+root.nyc^2+eps)	1	Help variable	Boundaries 1–12	
npe.ndflux_cH3O	npe.dflux_cH3Ox*npe.nxc+npe.dflux_cH3Oy*npe.nyc+npe.dflux_cH3Oz*npe.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	
npe.ncflux_cH3O	npe.cflux_cH3Ox*npe.nxc+npe.cflux_cH3Oy*npe.nyc+npe.cflux_cH3Oz*npe.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–12	
npe.nmflux_cH3O	npe.mflux_cH3Ox*npe.nxc+npe.mflux_cH3Oy*npe.nyc+npe.mflux_cH3Oz*npe.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	
npe.ntflux_cH3O	npe.bndFlux_cH3O	mol/(m²·s)	Normal total flux	Boundaries 1–12	
npe.ndflux_cOH	npe.dflux_cOHx*npe.nxc+npe.dflux_cOHy*npe.nyc+npe.dflux_cOHz*npe.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	
npe.ncflux_cOH	npe.cflux_cOHx*npe.nxc+npe.cflux_cOHy*npe.nyc+npe.	mol/(m²·s)	Normal convective flux	Boundaries 1–12	

Name	Expression	Unit	Description	Selection	Details
	cflux_cOHz*npe.nzc				
npe.nmflux_cOH	npe.mflux_cOHx*npe.nxc+npe.mflux_cOHy*npe.nyc+npe.mflux_cOHz*npe.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	
npe.ntflux_cOH	npe.bndFlux_cOH	mol/(m²·s)	Normal total flux	Boundaries 1–12	
npe.ndflux_cBead	npe.dflux_cBeadx*npe.nxc+npe.dflux_cBeady*npe.nyc+npe.dflux_cBeadz*npe.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	
npe.ncflux_cBead	npe.cflux_cBeadx*npe.nxc+npe.cflux_cBeady*npe.nyc+npe.cflux_cBeadz*npe.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–12	
npe.nmflux_cBead	npe.mflux_cBeadx*npe.nxc+npe.mflux_cBeady*npe.nyc+npe.mflux_cBeadz*npe.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	
npe.ntflux_cBead	npe.bndFlux_cBead	mol/(m²·s)	Normal total flux	Boundaries 1–12	
npe.ndflux_cK	npe.dflux_cKx*npe.nxc+npe.dflux_cKy*npe.nyc+npe.dflux_cKz*npe.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	
npe.ncflux_cK	npe.cflux_cKx*npe.nxc+npe.cflux_cKy*npe.nyc+npe.cflux_cKz*npe.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–12	
npe.nmflux_cK	npe.mflux_cKx*npe.nxc+npe.mflux_cKy*np	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	

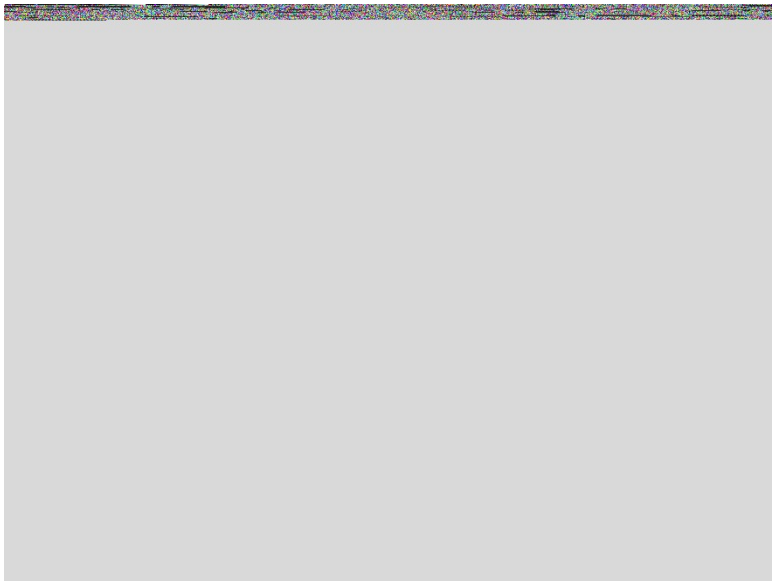
Name	Expression	Unit	Description	Selection	Details
	e.nyc+npe.mflux_cKz*npe.nzc				
npe.ntflux_cK	npe.bndFlux_cK	mol/(m²·s)	Normal total flux	Boundaries 1–12	
npe.ndflux_cCl	npe.dflux_cClx*npe.nxc+npe.dflux_cCly*npe.nyc+npe.dflux_cClz*npe.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	
npe.ncflux_cCl	npe.cflux_cClx*npe.nxc+npe.cflux_cCly*npe.nyc+npe.cflux_cClz*npe.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–12	
npe.nmflux_cCl	npe.mflux_cClx*npe.nxc+npe.mflux_cCly*npe.nyc+npe.mflux_cClz*npe.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	
npe.ntflux_cCl	(npe.cflux_cClx+npe.mflux_cClx)*npe.nxc+(npe.cflux_cCly+npe.mflux_cCly)*npe.nyc+(npe.cflux_cClz+npe.mflux_cClz)*npe.nzc+npe.ndflux_cCl	mol/(m²·s)	Normal total flux	Boundaries 1–12	
npe.bndFlux_cH3O	-dflux_spatial(cH3O)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
npe.bndFlux_cOH	-dflux_spatial(cOH)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
npe.bndFlux_cBead	-dflux_spatial(cBead)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
npe.bndFlux_	-	mol/(m	Boundary flux	Boundarie	

Name	Expression	Unit	Description	Selection	Details
cK	dflux_spatial(cK)	^{2}·s)		s 1–12	
npe.bndFlux_V	-dflux_spatial(npe.V)	A/m^2	Boundary flux	Boundaries 1–12	
npe.nJl	npe.bndFlux_V	A/m^2	Normal electrolyte current density	Boundaries 1–12	
npe.R_cH3O	0	mol/(m^3·s)	Total rate expression	Domain 1	+ operation
npe.cP_cH3O	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
npe.cP_cH3O	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
npe.KP_cH3O	0	m^3/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
npe.KP_cH3O	0	m^3/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
npe.R_cOH	0	mol/(m^3·s)	Total rate expression	Domain 1	+ operation
npe.cP_cOH	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
npe.cP_cOH	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
npe.KP_cOH	0	m^3/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
npe.KP_cOH	0	m^3/kg	Adsorption isotherm, first	Boundaries 1–12	+ operation

Name	Expression	Unit	Description	Selection	Details
			concentration derivative		
npe.R_cBead	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.cP_cBead	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
npe.cP_cBead	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
npe.KP_cBead	0	m³/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
npe.KP_cBead	0	m³/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
npe.R_cK	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.cP_cK	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
npe.cP_cK	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
npe.KP_cK	0	m³/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
npe.KP_cK	0	m³/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
npe.R_cCl	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.cP_cCl	0	mol/kg	Concentration species absorbed to	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			the solid		
npe.cP_cCl	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
npe.KP_cCl	0	m^3/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
npe.KP_cCl	0	m^3/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
npe.cbf_cH3O	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	
npe.cbf_cOH	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	
npe.cbf_cBead	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	
npe.cbf_cK	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	

2.4.3 Convection, Diffusion, and Migration 1



Convection, Diffusion, and Migration 1

SELECTION

Geometric entity level	Domain

Selection	Geometry geom1: Dimension 2: All domains

EQUATIONS

$$\nabla \cdot (\mathbf{J}_i + \mathbf{u}c_i) = R_i$$
$$\nabla \cdot \mathbf{i} = F\sum_i z_i R_i$$
$$\sum_i z_i c_i = 0$$
$$\mathbf{J}_i = -D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V$$
$$\mathbf{i} = F\sum_i z_i(-D_i \nabla c_i - z_i u_{m,i} F c_i \nabla V)$$

Convection

SETTINGS

Description	Value
Velocity field	Velocity field (spf)

Diffusion

SETTINGS

Description	Value
Material	Water (mat1)
Diffusion coefficient	User defined
Diffusion coefficient	{{dH3O, 0, 0}, {0, dH3O, 0}, {0, 0, dH3O}}
Diffusion coefficient	User defined
Diffusion coefficient	{{dOH, 0, 0}, {0, dOH, 0}, {0, 0, dOH}}
Diffusion coefficient	User defined
Diffusion coefficient	{{dBead, 0, 0}, {0, dBead, 0}, {0, 0, dBead}}
Diffusion coefficient	User defined
Diffusion coefficient	{{dK, 0, 0}, {0, dK, 0}, {0, 0, dK}}
Diffusion coefficient	User defined
Diffusion coefficient	{{dCl, 0, 0}, {0, dCl, 0}, {0, 0, dCl}}

Migration in electric field

SETTINGS

Description	Value
Mobility	Nernst - Einstein relation
Charge number	{1, -1, -1, 1, -1}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model input

SETTINGS

Description	Value
Temperature	User defined
Temperature	T

Variables

Name	Expression	Unit	Description	Selection	Details
cCl	npe.ctemp/(npe.z_cCl+eps)	mol/m³	Concentration	Domain 1	
npe.D_cH3Oxx	dH3O	m²/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cH3Oyx	0	m²/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cH3Ozx	0	m²/s	Diffusion coefficient, zx component	Domain 1	
npe.D_cH3Oxy	0	m²/s	Diffusion coefficient, xy component	Domain 1	
npe.D_cH3Oyy	dH3O	m²/s	Diffusion coefficient, yy component	Domain 1	
npe.D_cH3Ozy	0	m²/s	Diffusion coefficient, zy component	Domain 1	
npe.D_cH3Oxz	0	m²/s	Diffusion coefficient, xz component	Domain 1	
npe.D_cH3Oyz	0	m²/s	Diffusion coefficient, yz	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			component		
npe.D_cH3Ozz	dH3O	m^2/s	Diffusion coefficient, zz component	Domain 1	
npe.D_cOHxx	dOH	m^2/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cOHyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cOHzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	
npe.D_cOHxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	
npe.D_cOHyy	dOH	m^2/s	Diffusion coefficient, yy component	Domain 1	
npe.D_cOHzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	
npe.D_cOHxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	
npe.D_cOHyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	
npe.D_cOHzz	dOH	m^2/s	Diffusion coefficient, zz component	Domain 1	
npe.D_cBeadxx	dBead	m^2/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cBeadyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cBeadzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	
npe.D_cBeadxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.D_cBead yy	dBead	m^2/s	Diffusion coefficient, yy component	Domain 1	
npe.D_cBead zy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	
npe.D_cBead xz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	
npe.D_cBead yz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	
npe.D_cBead zz	dBead	m^2/s	Diffusion coefficient, zz component	Domain 1	
npe.D_cKxx	dK	m^2/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cKyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cKzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	
npe.D_cKxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	
npe.D_cKyy	dK	m^2/s	Diffusion coefficient, yy component	Domain 1	
npe.D_cKzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	
npe.D_cKxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	
npe.D_cKyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	
npe.D_cKzz	dK	m^2/s	Diffusion coefficient, zz component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.D_cClxx	dCl	m^2/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cClyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cClzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	
npe.D_cClxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	
npe.D_cClyy	dCl	m^2/s	Diffusion coefficient, yy component	Domain 1	
npe.D_cClzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	
npe.D_cClxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	
npe.D_cClyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	
npe.D_cClzz	dCl	m^2/s	Diffusion coefficient, zz component	Domain 1	
npe.um_cH3Oxx	npe.D_cH3Oxx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xx component	Domain 1	
npe.um_cH3Oyx	npe.D_cH3Oyx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yx component	Domain 1	
npe.um_cH3Ozx	npe.D_cH3Ozx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zx component	Domain 1	
npe.um_cH3Oxy	npe.D_cH3Oxy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xy component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.um_cH3Oyy	npe.D_cH3Oyy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yy component	Domain 1	
npe.um_cH3Ozy	npe.D_cH3Ozy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zy component	Domain 1	
npe.um_cH3Oxz	npe.D_cH3Oxz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xz component	Domain 1	
npe.um_cH3Oyz	npe.D_cH3Oyz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yz component	Domain 1	
npe.um_cH3Ozz	npe.D_cH3Ozz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zz component	Domain 1	
npe.z_cH3O	1	1	Charge number	Domain 1	
npe.um_cOHxx	npe.D_cOHxx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xx component	Domain 1	
npe.um_cOHyx	npe.D_cOHyx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yx component	Domain 1	
npe.um_cOHzx	npe.D_cOHzx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zx component	Domain 1	
npe.um_cOHxy	npe.D_cOHxy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xy component	Domain 1	
npe.um_cOHyy	npe.D_cOHyy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yy component	Domain 1	
npe.um_cOH	npe.D_cOHzy/(R_const*npe.c	s·mol/k	Mobility, zy	Domain 1	

Name	Expression	Unit	Description	Selection	Details
zy	dm1.minput_temperature)	g	component		
npe.um_cOHxz	npe.D_cOHxz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xz component	Domain 1	
npe.um_cOHyz	npe.D_cOHyz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yz component	Domain 1	
npe.um_cOHzz	npe.D_cOHzz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zz component	Domain 1	
npe.z_cOH	-1	1	Charge number	Domain 1	
npe.um_cBeadxx	npe.D_cBeadxx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xx component	Domain 1	
npe.um_cBeadyx	npe.D_cBeadyx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yx component	Domain 1	
npe.um_cBeadzx	npe.D_cBeadzx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zx component	Domain 1	
npe.um_cBeadxy	npe.D_cBeadxy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xy component	Domain 1	
npe.um_cBeadyy	npe.D_cBeadyy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yy component	Domain 1	
npe.um_cBeadzy	npe.D_cBeadzy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zy component	Domain 1	
npe.um_cBeadxz	npe.D_cBeadxz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xz component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.um_cBeadyz	npe.D_cBeadyz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yz component	Domain 1	
npe.um_cBeadzz	npe.D_cBeadzz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zz component	Domain 1	
npe.z_cBead	-1	1	Charge number	Domain 1	
npe.um_cKxx	npe.D_cKxx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xx component	Domain 1	
npe.um_cKyx	npe.D_cKyx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yx component	Domain 1	
npe.um_cKzx	npe.D_cKzx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zx component	Domain 1	
npe.um_cKxy	npe.D_cKxy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xy component	Domain 1	
npe.um_cKyy	npe.D_cKyy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yy component	Domain 1	
npe.um_cKzy	npe.D_cKzy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zy component	Domain 1	
npe.um_cKxz	npe.D_cKxz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xz component	Domain 1	
npe.um_cKyz	npe.D_cKyz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yz component	Domain 1	
npe.um_cKzz	npe.D_cKzz/(R_const*npe.cdm	s·mol/k	Mobility, zz	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	1.minput_temperature)	g	component		
npe.z_cK	1	1	Charge number	Domain 1	
npe.um_cClxx	npe.D_cClxx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xx component	Domain 1	
npe.um_cClyx	npe.D_cClyx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yx component	Domain 1	
npe.um_cClzx	npe.D_cClzx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zx component	Domain 1	
npe.um_cClxy	npe.D_cClxy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xy component	Domain 1	
npe.um_cClyy	npe.D_cClyy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yy component	Domain 1	
npe.um_cClzy	npe.D_cClzy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zy component	Domain 1	
npe.um_cClxz	npe.D_cClxz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xz component	Domain 1	
npe.um_cClyz	npe.D_cClyz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yz component	Domain 1	
npe.um_cClzz	npe.D_cClzz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zz component	Domain 1	
npe.z_cCl	-1	1	Charge number	Domain 1	
npe.Dav_cH3	0.5*(npe.D_cH	m^2/s	Average	Domain 1	

Name	Expression	Unit	Description	Selection	Details
O	3Oxx+npe.D_cH3Oyy)		diffusion coefficient		
npe.Dav_cOH	0.5*(npe.D_cOHxx+npe.D_cOHyy)	m^2/s	Average diffusion coefficient	Domain 1	
npe.Dav_cBead	0.5*(npe.D_cBeadxx+npe.D_cBeadyy)	m^2/s	Average diffusion coefficient	Domain 1	
npe.Dav_cK	0.5*(npe.D_cKxx+npe.D_cKyy)	m^2/s	Average diffusion coefficient	Domain 1	
npe.Dav_cCl	0.5*(npe.D_cClxx+npe.D_cClyy)	m^2/s	Average diffusion coefficient	Domain 1	
npe.tflux_cH3Ox	npe.dflux_cH3Ox+npe.cflux_cH3Ox+npe.mflux_cH3Ox	mol/(m^2·s)	Total flux, x component	Domain 1	+ operation
npe.tflux_cH3Oy	npe.dflux_cH3Oy+npe.cflux_cH3Oy+npe.mflux_cH3Oy	mol/(m^2·s)	Total flux, y component	Domain 1	+ operation
npe.tflux_cH3Oz	npe.dflux_cH3Oz+npe.cflux_cH3Oz+npe.mflux_cH3Oz	mol/(m^2·s)	Total flux, z component	Domain 1	+ operation
npe.dfluxMag_cH3O	sqrt(npe.dflux_cH3Ox^2+npe.dflux_cH3Oy^2+npe.dflux_cH3Oz^2)	mol/(m^2·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cH3O	sqrt(npe.tflux_cH3Ox^2+npe.tflux_cH3Oy^2+npe.tflux_cH3Oz^2)	mol/(m^2·s)	Total flux magnitude	Domain 1	
npe.mflux_cH3Ox	npe.z_cH3O*F_const*cH3O*(-npe.um_cH3Oxx*d(npe.V,x)-npe.um_cH3Oxy*d(npe.V,y))	mol/(m^2·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cH3Oy	npe.z_cH3O*F_const*cH3O*(-	mol/(m^2·s)	Electrophoretic flux, y	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	npe.um_cH3Oyx*d(npe.V,x)-npe.um_cH3Oyy*d(npe.V,y))		component		
npe.mflux_cH3Oz	npe.z_cH3O*F_const*cH3O*(-npe.um_cH3Ozx*d(npe.V,x)-npe.um_cH3Ozy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
npe.tflux_cOHx	npe.dflux_cOHx+npe.cflux_cOHx+npe.mflux_cOHx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
npe.tflux_cOHy	npe.dflux_cOHy+npe.cflux_cOHy+npe.mflux_cOHy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
npe.tflux_cOHz	npe.dflux_cOHz+npe.cflux_cOHz+npe.mflux_cOHz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
npe.dfluxMag_cOH	sqrt(npe.dflux_cOHx^2+npe.dflux_cOHy^2+npe.dflux_cOHz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cOH	sqrt(npe.tflux_cOHx^2+npe.tflux_cOHy^2+npe.tflux_cOHz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
npe.mflux_cOHx	npe.z_cOH*F_const*cOH*(-npe.um_cOHxx*d(npe.V,x)-npe.um_cOHxy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cOHy	npe.z_cOH*F_const*cOH*(-npe.um_cOHyx*d(npe.V,x)-npe.um_cOHyy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.mflux_cOHz	npe.z_cOH*F_const*cOH*(-npe.um_cOHzx*d(npe.V,x)-npe.um_cOHzy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
npe.tflux_cBeadx	npe.dflux_cBeadx+npe.cflux_cBeadx+npe.mflux_cBeadx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
npe.tflux_cBeady	npe.dflux_cBeady+npe.cflux_cBeady+npe.mflux_cBeady	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
npe.tflux_cBeadz	npe.dflux_cBeadz+npe.cflux_cBeadz+npe.mflux_cBeadz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
npe.dfluxMag_cBead	sqrt(npe.dflux_cBeadx^2+npe.dflux_cBeady^2+npe.dflux_cBeadz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cBead	sqrt(npe.tflux_cBeadx^2+npe.tflux_cBeady^2+npe.tflux_cBeadz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
npe.mflux_cBeadx	npe.z_cBead*F_const*cBead*(-npe.um_cBeadxx*d(npe.V,x)-npe.um_cBeadxy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cBeady	npe.z_cBead*F_const*cBead*(-npe.um_cBeadyx*d(npe.V,x)-npe.um_cBeadyy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
npe.mflux_cBeadz	npe.z_cBead*F_const*cBead*(-	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	npe.um_cBeadzx*d(npe.V,x)-npe.um_cBeadzy*d(npe.V,y))				
npe.tflux_cKx	npe.dflux_cKx+npe.cflux_cKx+npe.mflux_cKx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
npe.tflux_cKy	npe.dflux_cKy+npe.cflux_cKy+npe.mflux_cKy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
npe.tflux_cKz	npe.dflux_cKz+npe.cflux_cKz+npe.mflux_cKz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
npe.dfluxMag_cK	sqrt(npe.dflux_cKx^2+npe.dflux_cKy^2+npe.dflux_cKz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cK	sqrt(npe.tflux_cKx^2+npe.tflux_cKy^2+npe.tflux_cKz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
npe.mflux_cKx	npe.z_cK*F_const*cK*(-npe.um_cKxx*d(npe.V,x)-npe.um_cKxy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cKy	npe.z_cK*F_const*cK*(-npe.um_cKyx*d(npe.V,x)-npe.um_cKyy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
npe.mflux_cKz	npe.z_cK*F_const*cK*(-npe.um_cKzx*d(npe.V,x)-npe.um_cKzy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
npe.tflux_cClx	npe.dflux_cClx+npe.cflux_cClx+npe.mflux_cClx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
npe.tflux_cCly	npe.dflux_cCly+npe.cflux_cCly+npe.mflux_cCly	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
npe.tflux_cClz	npe.dflux_cClz+npe.cflux_cClz+npe.mflux_cClz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
npe.dfluxMag_cCl	sqrt(npe.dflux_cClx^2+npe.dflux_cCly^2+npe.dflux_cClz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cCl	sqrt(npe.tflux_cClx^2+npe.tflux_cCly^2+npe.tflux_cClz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
npe.mflux_cClx	npe.z_cCl*F_const*cCl*(-npe.um_cClxx*d(npe.V,x)-npe.um_cClxy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cCly	npe.z_cCl*F_const*cCl*(-npe.um_cClyx*d(npe.V,x)-npe.um_cClyy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
npe.mflux_cClz	npe.z_cCl*F_const*cCl*(-npe.um_cClzx*d(npe.V,x)-npe.um_cClzy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
npe.u	model.input.u1	m/s	Velocity field, x component	Domain 1	Meta
npe.v	model.input.u2	m/s	Velocity field, y component	Domain 1	Meta
npe.w	model.input.u3	m/s	Velocity field, z component	Domain 1	Meta
npe.cflux_cH3Ox	cH3O*npe.u	mol/(m²·s)	Convective flux, x component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.cflux_cH3Oy	cH3O*npe.v	mol/(m²·s)	Convective flux, y component	Domain 1	
npe.cflux_cH3Oz	cH3O*npe.w	mol/(m²·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cH3O	sqrt(npe.cflux_cH3Ox^2+npe.cflux_cH3Oy^2+npe.cflux_cH3Oz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
npe.cflux_cOHx	cOH*npe.u	mol/(m²·s)	Convective flux, x component	Domain 1	
npe.cflux_cOHy	cOH*npe.v	mol/(m²·s)	Convective flux, y component	Domain 1	
npe.cflux_cOHz	cOH*npe.w	mol/(m²·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cOH	sqrt(npe.cflux_cOHx^2+npe.cflux_cOHy^2+npe.cflux_cOHz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
npe.cflux_cBeadx	cBead*npe.u	mol/(m²·s)	Convective flux, x component	Domain 1	
npe.cflux_cBeady	cBead*npe.v	mol/(m²·s)	Convective flux, y component	Domain 1	
npe.cflux_cBeadz	cBead*npe.w	mol/(m²·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cBead	sqrt(npe.cflux_cBeadx^2+npe.cflux_cBeady^2+npe.cflux_cBeadz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
npe.cflux_cKx	cK*npe.u	mol/(m²·s)	Convective flux, x component	Domain 1	
npe.cflux_cKy	cK*npe.v	mol/(m	Convective	Domain 1	

Name	Expression	Unit	Description	Selection	Details
		^{2}·s)	flux, y component		
npe.cflux_cKz	cK*npe.w	mol/(m^2·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cK	sqrt(npe.cflux_cKx^2+npe.cflux_cKy^2+npe.cflux_cKz^2)	mol/(m^2·s)	Convective flux magnitude	Domain 1	
npe.cflux_cClx	cCl*npe.u	mol/(m^2·s)	Convective flux, x component	Domain 1	
npe.cflux_cCly	cCl*npe.v	mol/(m^2·s)	Convective flux, y component	Domain 1	
npe.cflux_cClz	cCl*npe.w	mol/(m^2·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cCl	sqrt(npe.cflux_cClx^2+npe.cflux_cCly^2+npe.cflux_cClz^2)	mol/(m^2·s)	Convective flux magnitude	Domain 1	
npe.dflux_cH3Ox	-npe.D_cH3Oxx*npe.grad_cH3Ox-npe.D_cH3Oxy*npe.grad_cH3Oy-npe.D_cH3Oxz*npe.grad_cH3Oz	mol/(m^2·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cH3Oy	-npe.D_cH3Oyx*npe.grad_cH3Ox-npe.D_cH3Oyy*npe.grad_cH3Oy-npe.D_cH3Oyz*npe.grad_cH3Oz	mol/(m^2·s)	Diffusive flux, y component	Domain 1	
npe.dflux_cH3Oz	-npe.D_cH3Ozx	mol/(m^2·s)	Diffusive flux, z component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	*npe.grad_cH3Ox-npe.D_cH3Ozy*npe.grad_cH3Oy-npe.D_cH3Ozz*npe.grad_cH3Oz				
npe.grad_cH3Ox	cH3Ox	mol/m^4	Concentration gradient, x component	Domain 1	
npe.grad_cH3Oy	cH3Oy	mol/m^4	Concentration gradient, y component	Domain 1	
npe.grad_cH3Oz	0	mol/m^4	Concentration gradient, z component	Domain 1	
npe.ctemp	-cH3O*npe.z_cH3O-cOH*npe.z_cOH-cBead*npe.z_cBead-cK*npe.z_cK	mol/m^3	Concentration	Domain 1	+ operation
npe.dflux_cOHx	-npe.D_cOHxx*npe.grad_cOHx-npe.D_cOHxy*npe.grad_cOHy-npe.D_cOHxz*npe.grad_cOHz	mol/(m^2·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cOHy	-npe.D_cOHyx*npe.grad_cOHx-npe.D_cOHyy*npe.grad_cOHy-npe.D_cOHyz*npe.grad_cOHz	mol/(m^2·s)	Diffusive flux, y component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.dflux_cOHz	-npe.D_cOHzx*npe.grad_cOHx-npe.D_cOHzy*npe.grad_cOHy-npe.D_cOHzz*npe.grad_cOHz	mol/(m²·s)	Diffusive flux, z component	Domain 1	
npe.grad_cOHx	cOHx	mol/m⁴	Concentration gradient, x component	Domain 1	
npe.grad_cOHy	cOHy	mol/m⁴	Concentration gradient, y component	Domain 1	
npe.grad_cOHz	0	mol/m⁴	Concentration gradient, z component	Domain 1	
npe.dflux_cBeadx	-npe.D_cBeadxx*npe.grad_cBeadx-npe.D_cBeadxy*npe.grad_cBeady-npe.D_cBeadxz*npe.grad_cBeadz	mol/(m²·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cBeady	-npe.D_cBeadyx*npe.grad_cBeadx-npe.D_cBeadyy*npe.grad_cBeady-npe.D_cBeadyz*npe.grad_cBeadz	mol/(m²·s)	Diffusive flux, y component	Domain 1	
npe.dflux_cBeadz	-npe.D_cBeadzx*npe.grad_cBeadx-npe.D_cBeadzy*npe.grad_cBe	mol/(m²·s)	Diffusive flux, z component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	ady-npe.D_cBeadzz*npe.grad_cBeadz				
npe.grad_cBeadx	cBeadx	mol/m^4	Concentration gradient, x component	Domain 1	
npe.grad_cBeady	cBeady	mol/m^4	Concentration gradient, y component	Domain 1	
npe.grad_cBeadz	0	mol/m^4	Concentration gradient, z component	Domain 1	
npe.dflux_cKx	-npe.D_cKxx*npe.grad_cKx-npe.D_cKxy*npe.grad_cKy-npe.D_cKxz*npe.grad_cKz	mol/(m^2·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cKy	-npe.D_cKyx*npe.grad_cKx-npe.D_cKyy*npe.grad_cKy-npe.D_cKyz*npe.grad_cKz	mol/(m^2·s)	Diffusive flux, y component	Domain 1	
npe.dflux_cKz	-npe.D_cKzx*npe.grad_cKx-npe.D_cKzy*npe.grad_cKy-npe.D_cKzz*npe.grad_cKz	mol/(m^2·s)	Diffusive flux, z component	Domain 1	
npe.grad_cKx	cKx	mol/m^4	Concentration gradient, x component	Domain 1	
npe.grad_cKy	cKy	mol/m^4	Concentration gradient, y component	Domain 1	
npe.grad_cKz	0	mol/m^4	Concentration gradient, z component	Domain 1	
npe.dflux_cCl	-	mol/(m	Diffusive flux,	Domain 1	

Name	Expression	Unit	Description	Selection	Details
x	npe.D_cClxx*npe.grad_cClx-npe.D_cClxy*npe.grad_cCly-npe.D_cClxz*npe.grad_cClz	^{2}·s)	x component		
npe.dflux_cCly	-npe.D_cClyx*npe.grad_cClx-npe.D_cClyy*npe.grad_cCly-npe.D_cClyz*npe.grad_cClz	mol/(m^2·s)	Diffusive flux, y component	Domain 1	
npe.dflux_cClz	-npe.D_cClzx*npe.grad_cClx-npe.D_cClzy*npe.grad_cCly-npe.D_cClzz*npe.grad_cClz	mol/(m^2·s)	Diffusive flux, z component	Domain 1	
npe.grad_cClx	d(cCl,x)	mol/m^4	Concentration gradient, x component	Domain 1	
npe.grad_cCly	d(cCl,y)	mol/m^4	Concentration gradient, y component	Domain 1	
npe.grad_cClz	0	mol/m^4	Concentration gradient, z component	Domain 1	
npe.kappa0xx	cH3O*npe.um_cH3Oxx*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHxx*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadxx*(npe.z_cBead*F_const)^2+cK*npe.um_cKxx*(npe.z_cK*F_const)^2+cCl*npe.um_cClxx*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, xx component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
npe.kappa0yx	cH3O*npe.um_cH3Oyx*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHyx*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadyx*(npe.z_cBead*F_const)^2+cK*npe.um_cKyx*(npe.z_cK*F_const)^2+cCl*npe.um_cClyx*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, yx component	Domain 1	+ operation
npe.kappa0zx	cH3O*npe.um_cH3Ozx*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHzx*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadzx*(npe.z_cBead*F_const)^2+cK*npe.um_cKzx*(npe.z_cK*F_const)^2+cCl*npe.um_cClzx*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, zx component	Domain 1	+ operation
npe.kappa0xy	cH3O*npe.um_cH3Oxy*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHxy*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadxy*(npe.z_cBead*F_const)^2+cK*npe.um_cKxy*(npe.z_cK*F_const)^2+cCl*npe.um_cClxy*(npe.z_cCl*F_c	S/m	Electrolyte conductivity, xy component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	onst)^2				
npe.kappa0yy	cH3O*npe.um_cH3Oyy*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHyy*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadyy*(npe.z_cBead*F_const)^2+cK*npe.um_cKyy*(npe.z_cK*F_const)^2+cCl*npe.um_cClyy*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, yy component	Domain 1	+ operation
npe.kappa0zy	cH3O*npe.um_cH3Ozy*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHzy*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadzy*(npe.z_cBead*F_const)^2+cK*npe.um_cKzy*(npe.z_cK*F_const)^2+cCl*npe.um_cClzy*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, zy component	Domain 1	+ operation
npe.kappa0xz	cH3O*npe.um_cH3Oxz*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHxz*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadxz*(npe.z_cBead*F_const)^2+cK*npe.um_cKxz*(npe.z_cK*F_const)^2+cCl*	S/m	Electrolyte conductivity, xz component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	npe.um_cClxz*(npe.z_cCl*F_const)^2				
npe.kappa0yz	cH3O*npe.um_cH3Oyz*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHyz*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadyz*(npe.z_cBead*F_const)^2+cK*npe.um_cKyz*(npe.z_cK*F_const)^2+cCl*npe.um_cClyz*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, yz component	Domain 1	+ operation
npe.kappa0zz	cH3O*npe.um_cH3Ozz*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHzz*(npe.z_cOH*F_const)^2+cBead*npe.um_cBeadzz*(npe.z_cBead*F_const)^2+cK*npe.um_cKzz*(npe.z_cK*F_const)^2+cCl*npe.um_cClzz*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, zz component	Domain 1	+ operation
npe.kappaxx	npe.kappa0xx	S/m	Electrolyte conductivity, xx component	Domain 1	
npe.kappayx	npe.kappa0yx	S/m	Electrolyte conductivity, yx component	Domain 1	
npe.kappazx	npe.kappa0zx	S/m	Electrolyte conductivity, zx	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			component		
npe.kappaxy	npe.kappa0xy	S/m	Electrolyte conductivity, xy component	Domain 1	
npe.kappayy	npe.kappa0yy	S/m	Electrolyte conductivity, yy component	Domain 1	
npe.kappazy	npe.kappa0zy	S/m	Electrolyte conductivity, zy component	Domain 1	
npe.kappaxz	npe.kappa0xz	S/m	Electrolyte conductivity, xz component	Domain 1	
npe.kappayz	npe.kappa0yz	S/m	Electrolyte conductivity, yz component	Domain 1	
npe.kappazz	npe.kappa0zz	S/m	Electrolyte conductivity, zz component	Domain 1	
npe.J0x	F_const*(npe.z_cH3O*(-npe.D_cH3Oxx*npe.grad_cH3Ox-npe.D_cH3Oxy*npe.grad_cH3Oy-npe.D_cH3Oxz*npe.grad_cH3Oz+npe.z_cH3O*F_const*cH3O*(-npe.um_cH3Oxx*Vx-npe.um_cH3Oxy*Vy))+npe.z_cOH*(-npe.D_cOHxx*npe.grad_cOH	A/m²	Current density, x component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	x- npe.D_cOHxy* npe.grad_cOH y- npe.D_cOHxz* npe.grad_cOH z+npe.z_cOH* F_const*cOH*(- npe.um_cOHxx *Vx- npe.um_cOHxy *Vy))+npe.z_cB ead*(- npe.D_cBeadxx *npe.grad_cBe adx- npe.D_cBeadxy *npe.grad_cBe ady- npe.D_cBeadxz *npe.grad_cBe adz+npe.z_cBe ad*F_const*cB ead*(- npe.um_cBead xx*Vx- npe.um_cBead xy*Vy))+npe.z_ cK*(- npe.D_cKxx*np e.grad_cKx- npe.D_cKxy*np e.grad_cKy- npe.D_cKxz*np e.grad_cKz+np e.z_cK*F_const *cK*(- npe.um_cKxx* Vx- npe.um_cKxy* Vy))+npe.z_cCl *(- npe.D_cClxx*n pe.grad_cClx- npe.D_cClxy*n pe.grad_cCly- npe.D_cClxz*n				

Name	Expression	Unit	Description	Selection	Details
	pe.grad_cClz+npe.z_cCl*F_const*cCl*(-npe.um_cClxx*Vx-npe.um_cClxy*Vy)))				
npe.J0y	F_const*(npe.z_cH3O*(-npe.D_cH3Oyx*npe.grad_cH3Ox-npe.D_cH3Oyy*npe.grad_cH3Oy-npe.D_cH3Oyz*npe.grad_cH3Oz+npe.z_cH3O*F_const*cH3O*(-npe.um_cH3Oyx*Vx-npe.um_cH3Oyy*Vy))+npe.z_cOH*(-npe.D_cOHyx*npe.grad_cOHx-npe.D_cOHyy*npe.grad_cOHy-npe.D_cOHyz*npe.grad_cOHz+npe.z_cOH*F_const*cOH*(-npe.um_cOHyx*Vx-npe.um_cOHyy*Vy))+npe.z_cBead*(-npe.D_cBeadyx*npe.grad_cBeadx-npe.D_cBeadyy*npe.grad_cBeady-	A/m²	Current density, y component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	npe.D_cBeadyz*npe.grad_cBeadz+npe.z_cBead*F_const*cBead*(-npe.um_cBeadyx*Vx-npe.um_cBeadyy*Vy))+npe.z_cK*(-npe.D_cKyx*npe.grad_cKx-npe.D_cKyy*npe.grad_cKy-npe.D_cKyz*npe.grad_cKz+npe.z_cK*F_const*cK*(-npe.um_cKyx*Vx-npe.um_cKyy*Vy))+npe.z_cCl*(-npe.D_cClyx*npe.grad_cClx-npe.D_cClyy*npe.grad_cCly-npe.D_cClyz*npe.grad_cClz+npe.z_cCl*F_const*cCl*(-npe.um_cClyx*Vx-npe.um_cClyy*Vy)))				
npe.J0z	F_const*(npe.z_cH3O*(-npe.D_cH3Ozx*npe.grad_cH3Ox-npe.D_cH3Ozy*npe.grad_cH3Oy-npe.D_cH3Ozz*npe.grad_cH3Oz+npe.z_cH3O*F_const*cH3	A/m²	Current density, z component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	O*(-npe.um_cH3Ozx*Vx-npe.um_cH3Ozy*Vy))+npe.z_cOH*(-npe.D_cOHzx*npe.grad_cOHx-npe.D_cOHzy*npe.grad_cOHy-npe.D_cOHzz*npe.grad_cOHz+npe.z_cOH*F_const*cOH*(-npe.um_cOHzx*Vx-npe.um_cOHzy*Vy))+npe.z_cBead*(-npe.D_cBeadzx*npe.grad_cBeadx-npe.D_cBeadzy*npe.grad_cBeady-npe.D_cBeadzz*npe.grad_cBeadz+npe.z_cBead*F_const*cBead*(-npe.um_cBeadzx*Vx-npe.um_cBeadzy*Vy))+npe.z_cK*(-npe.D_cKzx*npe.grad_cKx-npe.D_cKzy*npe.grad_cKy-npe.D_cKzz*npe.grad_cKz+npe.z_cK*F_const*cK*(-npe.um_cKzx*Vx-				

Name	Expression	Unit	Description	Selection	Details
	npe.um_cKzy*Vy))+npe.z_cCl*(-npe.D_cClzx*npe.grad_cClx-npe.D_cClzy*npe.grad_cCly-npe.D_cClzz*npe.grad_cClz+npe.z_cCl*F_const*cCl*(-npe.um_cClzx*Vx-npe.um_cClzy*Vy)))				
npe.Jx	npe.J0x	A/m²	Current density, x component	Domain 1	
npe.Jy	npe.J0y	A/m²	Current density, y component	Domain 1	
npe.Jz	npe.J0z	A/m²	Current density, z component	Domain 1	
npe.V	V	V	Electric potential	Domain 1	
npe.gradVx	Vx	V/m	Potential gradient, x component	Domain 1	
npe.gradVy	Vy	V/m	Potential gradient, y component	Domain 1	
npe.gradVz	0	V/m	Potential gradient, z component	Domain 1	
npe.Res_cH3O	-npe.D_cH3Oxx*cH3Oxx-npe.D_cH3Oxy*cH3Oxy-npe.D_cH3Oyx*cH3Oyx-npe.D_cH3Oyy*cH3Oyy+d(cH3O*(npe.u-	mol/(m³·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	npe.z_cH3O*npe.um_cH3Oxx*F_const*d(npe.V,x)-npe.z_cH3O*npe.um_cH3Oxy*F_const*d(npe.V,y)),x)+d(cH3O*(npe.v-npe.z_cH3O*npe.um_cH3Oyx*F_const*d(npe.V,x)-npe.z_cH3O*npe.um_cH3Oyy*F_const*d(npe.V,y)),y)-npe.R_cH3O				
npe.Res_cOH	-npe.D_cOHxx*cOHxx-npe.D_cOHxy*cOHxy-npe.D_cOHyx*cOHyx-npe.D_cOHyy*cOHyy+d(cOH*(npe.u-npe.z_cOH*npe.um_cOHxx*F_const*d(npe.V,x)-npe.z_cOH*npe.um_cOHxy*F_const*d(npe.V,y)),x)+d(cOH*(npe.v-npe.z_cOH*npe.um_cOHyx*F_const*d(npe.V,x)-npe.z_cOH*npe.um_cOHyy*F_const*d(npe.V,y)),y)-npe.R_cOH	mol/(m³·s)	Equation residual	Domain 1	
npe.Res_cBea	-	mol/(m	Equation	Domain 1	

Name	Expression	Unit	Description	Selection	Details
d	npe.D_cBeadxx*cBeadxx-npe.D_cBeadxy*cBeadxy-npe.D_cBeadyx*cBeadyx-npe.D_cBeadyy*cBeadyy+d(cBead*(npe.u-npe.z_cBead*npe.um_cBeadxx*F_const*d(npe.V,x)-npe.z_cBead*npe.um_cBeadxy*F_const*d(npe.V,y)),x)+d(cBead*(npe.v-npe.z_cBead*npe.um_cBeadyx*F_const*d(npe.V,x)-npe.z_cBead*npe.um_cBeadyy*F_const*d(npe.V,y)),y)-npe.R_cBead	^{3}·s)	residual		
npe.Res_cK	-npe.D_cKxx*cKxx-npe.D_cKxy*cKxy-npe.D_cKyx*cKyx-npe.D_cKyy*cKyy+d(cK*(npe.u-npe.z_cK*npe.um_cKxx*F_const*d(npe.V,x)-npe.z_cK*npe.um_cKxy*F_const*d(npe.V,y)),x)+d(cK*(npe.v-npe.z_cK*npe.um_cKyx*F_const*d(npe.V,x)-	mol/(m^{3}·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	npe.z_cK*npe.um_cKyy*F_const*d(npe.V,y)),y)-npe.R_cK				

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
cH3O	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
cOH	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
cBead	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
cK	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
V	Lagrange (Quadratic)	V	Electric potential	Spatial	Domain 1

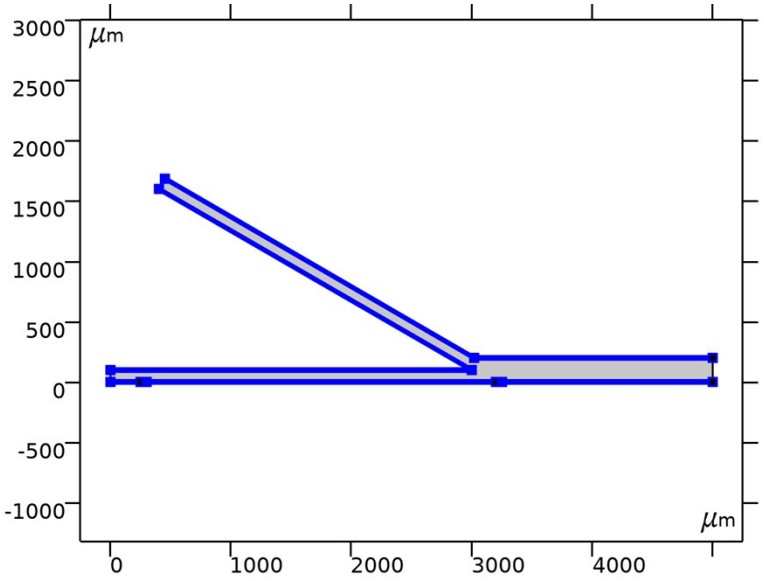
Weak expressions

Weak expression	Integration order	Integration frame	Selection
cH3O*(npe.u*test(cH3Ox)+npe.v*test(cH3Oy))*(isScalingSystemDomain==0)	4	Spatial	Domain 1
npe.cbf_cH3O*test(cH3O)	4	Spatial	Boundaries 1–12
cOH*(npe.u*test(cOHx)+npe.v*test(cOHy))*(isScalingSystemDomain==0)	4	Spatial	Domain 1
npe.cbf_cOH*test(cOH)	4	Spatial	Boundaries 1–12
cBead*(npe.u*test(cBeadx)+npe.v*test(cBeady))*(isScalingSystemDomain==0)	4	Spatial	Domain 1
npe.cbf_cBead*test(cBead)	4	Spatial	Boundaries 1–12
cK*(npe.u*test(cKx)+npe.v*test(cKy))*(isScaling	4	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
SystemDomain==0)			
npe.cbf_cK*test(cK)	4	Spatial	Boundaries 1–12
npe.z_cH3O*F_const*cH3O*((-npe.um_cH3Oxx*d(npe.V,x)-npe.um_cH3Oxy*d(npe.V,y))*test(cH3Ox)+(-npe.um_cH3Oyx*d(npe.V,x)-npe.um_cH3Oyy*d(npe.V,y))*test(cH3Oy))	4	Spatial	Domain 1
npe.z_cOH*F_const*cOH*((-npe.um_cOHxx*d(npe.V,x)-npe.um_cOHxy*d(npe.V,y))*test(cOHx)+(-npe.um_cOHyx*d(npe.V,x)-npe.um_cOHyy*d(npe.V,y))*test(cOHy))	4	Spatial	Domain 1
npe.z_cBead*F_const*cBead*((-npe.um_cBeadxx*d(npe.V,x)-npe.um_cBeadxy*d(npe.V,y))*test(cBeadx)+(-npe.um_cBeadyx*d(npe.V,x)-npe.um_cBeadyy*d(npe.V,y))*test(cBeady))	4	Spatial	Domain 1
npe.z_cK*F_const*cK*((-npe.um_cKxx*d(npe.V,x)-npe.um_cKxy*d(npe.V,y))*test(cKx)+(-npe.um_cKyx*d(npe.V,x)-npe.um_cKyy*d(npe.V,y))*test(cKy))	4	Spatial	Domain 1
npe.dflux_cH3Ox*test(cH3Ox)+npe.dflux_cH3O	4	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
y*test(cH3Oy)			
npe.dflux_cOHx*test(cOHx)+npe.dflux_cOHy*test(cOHy)	4	Spatial	Domain 1
npe.dflux_cBeadx*test(cBeadx)+npe.dflux_cBeady*test(cBeady)	4	Spatial	Domain 1
npe.dflux_cKx*test(cKx)+npe.dflux_cKy*test(cKy)	4	Spatial	Domain 1
npe.Jx*test(Vx)+npe.Jy*test(Vy)	4	Spatial	Domain 1
npe.streamline*(isScalingSystemDomain==0)	4	Spatial	Domain 1

2.4.4 No Flux 1



No Flux 1

SELECTION

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

EQUATIONS

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

Convection

SETTINGS

Description	Value
Include	Off

Variables

Name	Expression	Unit	Description	Selection
npe.cbf_cH3O	cH3O*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 2–3, 5, 7–9, 11
npe.cbf_cOH	cOH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 2–3, 5, 7–9, 11
npe.cbf_cBead	cBead*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 2–3, 5, 7–9, 11
npe.cbf_cK	cK*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 2–3, 5, 7–9, 11

2.4.5 Electric Insulation 1

Electric Insulation 1

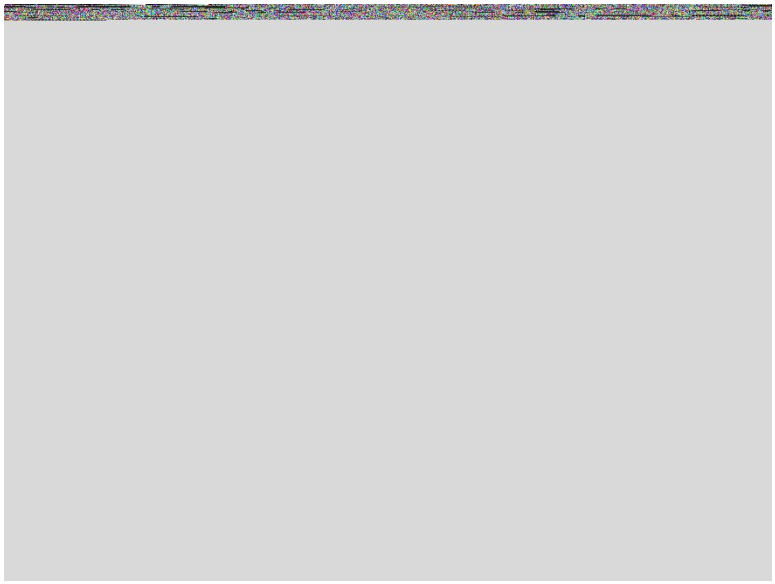
SELECTION

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

EQUATIONS

$$-\mathbf{n} \cdot \mathbf{i} = 0$$

2.4.6 Initial Values 1



Initial Values 1

SELECTION

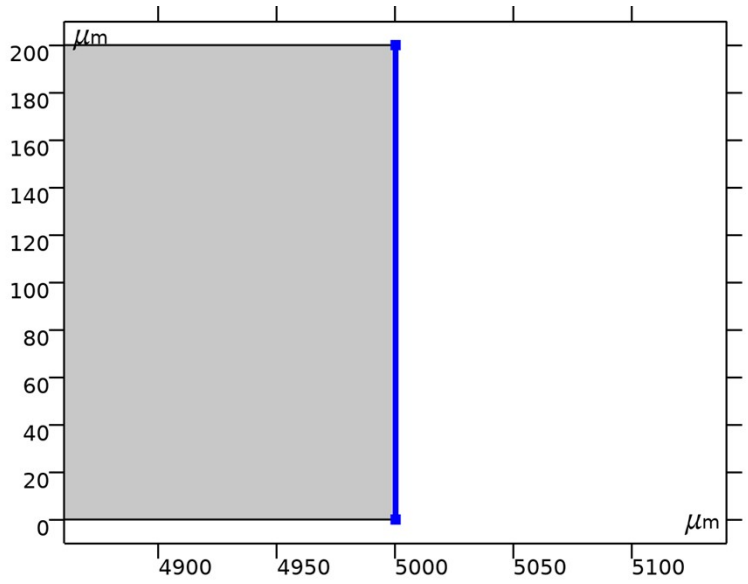
Geometric entity level	Domain
Selection	Geometry geom1: Dimension 2: All domains

Initial values

SETTINGS

Description	Value
Concentration	{cH3O0, cOH0, cBead0, cK0 + cBead0, 0}
Electric potential	0

2.4.7 Inflow 1



Inflow 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 12

EQUATIONS

$c_i = c_{0,i}$

Concentration

SETTINGS

Description	Value
Concentration	{cH3O0, cOH0, cBead0, cK0 + cBead0, 0}

Boundary condition type

SETTINGS

Description	Value
Boundary condition type	Concentration constraint

Variables

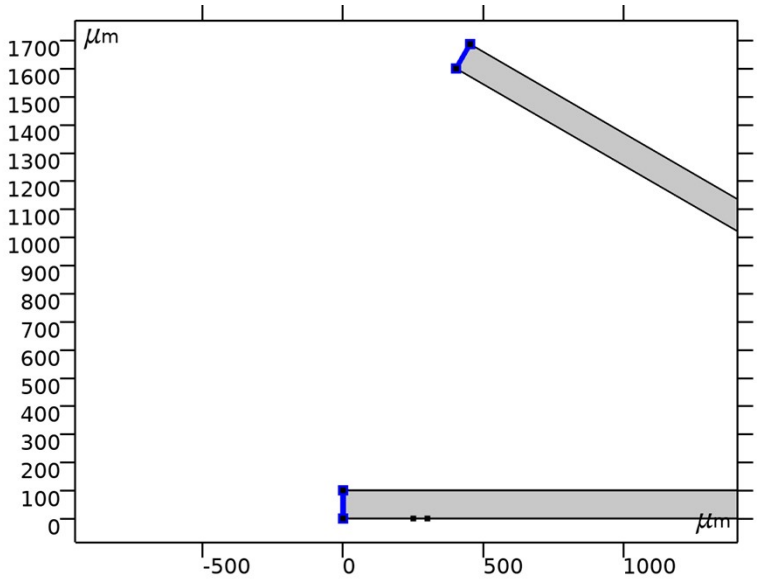
Name	Expression	Unit	Description	Selection	Details
npe.c0_	cH3O0	mol/m³	Concentration	Boundary	+ operati

Name	Expression	Unit	Description	Selection	Details
cH3O				12	on
npe.c0_cOH	cOH0	mol/m³	Concentration	Boundary 12	+ operation
npe.c0_cBead	cBead0	mol/m³	Concentration	Boundary 12	+ operation
npe.c0_cK	cK0+cBead0	mol/m³	Concentration	Boundary 12	+ operation

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-cH3O+npe.c0_cH3O	-test(cH3O)	Lagrange (Quadratic)	Boundary 12	Elemental
-cOH+npe.c0_cOH	-test(cOH)	Lagrange (Quadratic)	Boundary 12	Elemental
-cBead+npe.c0_cBead	-test(cBead)	Lagrange (Quadratic)	Boundary 12	Elemental
-cK+npe.c0_cK	-test(cK)	Lagrange (Quadratic)	Boundary 12	Elemental

2.4.8 Outflow 1



Outflow 1

SELECTION

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

EQUATIONS

$$\mathbf{n} \cdot D_i \nabla c_i = 0$$

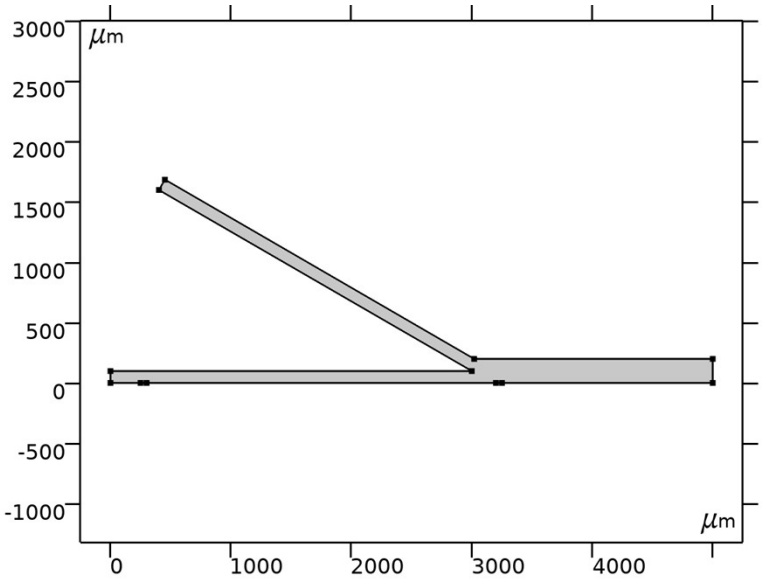
Weak expressions

Weak expression	Integration order	Integration frame	Selection
-(npe.nx*npe.u+npe.ny*npe.v+npe.nz*npe.w)*cH3O*test(cH3O)	4	Spatial	Boundaries 1, 6
-npe.z_cH3O*F_const*cH3O*(-npe.nx*(npe.um_cH3Oxx*mean(d(npe.V,x))+npe.um_cH3Oxy*mean(d(npe.V,y))+npe.um_cH3Oxz*mean(0))-npe.ny*(npe.um_cH3Oyx*mean(d(npe.V,x))+npe.um_cH3Oyy*mean(d(npe.V,y))+npe.um_cH3Oyz*mean(0))-npe.nz*(npe.um_cH3Ozx*mean(d(npe.V,x))+npe.um_cH3Ozy*mean(d(npe.V,y))+npe.um_cH3Ozz*mean(0)))*test(cH3O)	4	Spatial	Boundaries 1, 6
-(npe.nx*npe.u+npe.ny*npe.v+npe.nz*npe.w)*cOH*test(cOH)	4	Spatial	Boundaries 1, 6
-npe.z_cOH*F_const*cOH*(-npe.nx*(npe.um_cOHxx*mean(d(npe.V,x))+npe.um_cOHxy*mean(d(npe.V,y))+npe.um_cOHxz*mean(0))-npe.ny*(npe.um_cOHyx*mean(d(npe.V,x))+npe.	4	Spatial	Boundaries 1, 6

Weak expression	Integration order	Integration frame	Selection
um_cOHyy*mean(d(npe.V,y))+npe.um_cOHyz*mean(0))-npe.nz*(npe.um_cOHzx*mean(d(npe.V,x))+npe.um_cOHzy*mean(d(npe.V,y))+npe.um_cOHzz*mean(0)))*test(cOH)			
-(npe.nx*npe.u+npe.ny*npe.v+npe.nz*npe.w)*cBead*test(cBead)	4	Spatial	Boundaries 1, 6
-npe.z_cBead*F_const*cBead*(-npe.nx*(npe.um_cBeadxx*mean(d(npe.V,x))+npe.um_cBeadxy*mean(d(npe.V,y))+npe.um_cBeadxz*mean(0))-npe.ny*(npe.um_cBeadyx*mean(d(npe.V,x))+npe.um_cBeadyy*mean(d(npe.V,y))+npe.um_cBeadyz*mean(0))-npe.nz*(npe.um_cBeadzx*mean(d(npe.V,x))+npe.um_cBeadzy*mean(d(npe.V,y))+npe.um_cBeadzz*mean(0)))*test(cBead)	4	Spatial	Boundaries 1, 6
-(npe.nx*npe.u+npe.ny*npe.v+npe.nz*npe.w)*cK*test(cK)	4	Spatial	Boundaries 1, 6
-npe.z_cK*F_const*cK*(-npe.nx*(npe.um_cKxx*mean(d(npe.V,x))+npe.um_cKxy*mean(d(npe.V,y))+npe.um_cKxz*mean(0))-npe.ny*(npe.um_cKyx*mean(d(npe.V,x))+npe.um_cKyy*mean(d(npe.V,y))+npe.um_cKyz*mean(	4	Spatial	Boundaries 1, 6

Weak expression	Integration order	Integration frame	Selection
0))-npe.nz*(npe.um_cKzx*mean(d(npe.V,x))+npe.um_cKzy*mean(d(npe.V,y))+npe.um_cKzz*mean(0)))*test(cK)			

2.4.9 Electric Potential 1



Electric Potential 1

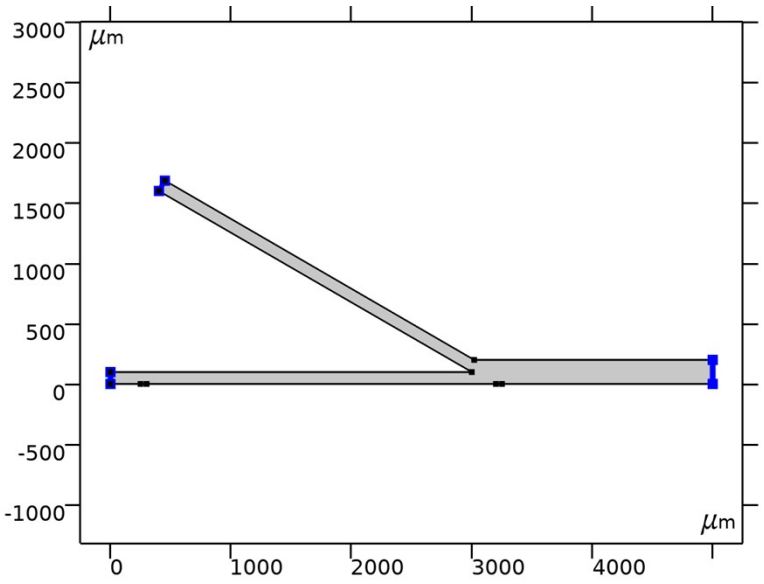
SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: No boundaries

EQUATIONS

$V = V_0$

2.4.10 Electric Potential 2



Electric Potential 2

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 1, 6, 12

EQUATIONS

$V = V_0$

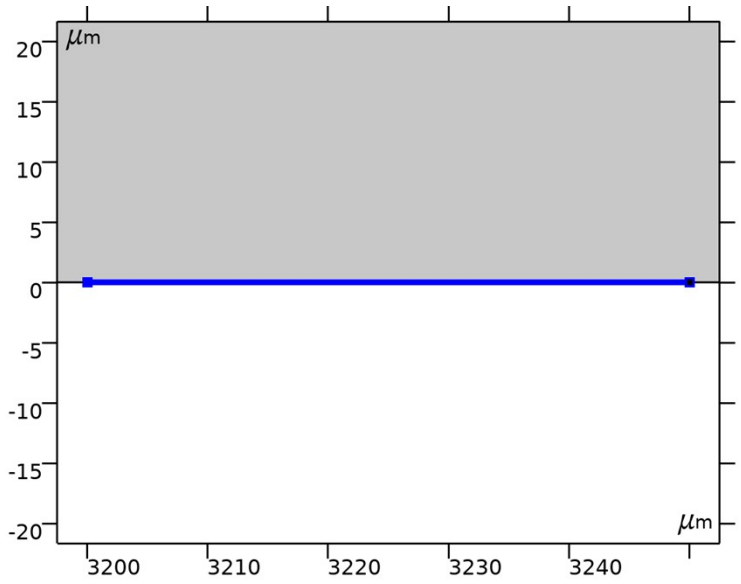
Variables

Name	Expression	Unit	Description	Selection
npe.V0	30	V	Electric potential	Boundaries 1, 6, 12

Constraints

Constraint	Constraint force	Shape function	Selection	Details
npe.V0-V	test(npe.V0-V)	Lagrange (Quadratic)	Boundaries 1, 6, 12	Elemental

2.4.11 Flux 1



Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 10

EQUATIONS

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

Convection

SETTINGS

Description	Value
Include	Off

Inward flux

SETTINGS

Description	Value
Species cH3O	Off
Species cOH	On
Species cBead	Off
Species cK	Off
Species cCl	Off

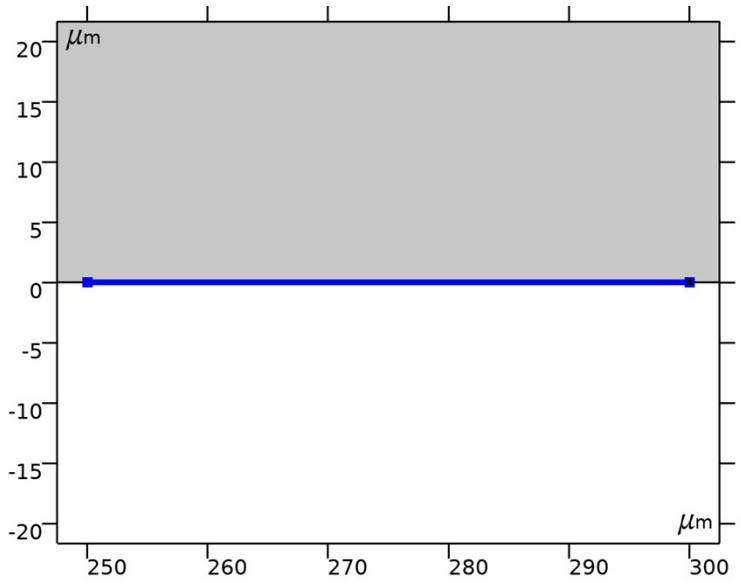
Variables

Name	Expression	Unit	Description	Selection
npe.cbf_cH3O	cH3O*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 10
npe.cbf_cOH	cOH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 10
npe.cbf_cBead	cBead*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 10
npe.cbf_cK	cK*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 10

Weak expressions

Weak expression	Integration order	Integration frame	Selection
0	4	Spatial	Boundary 10
fssBPE*test(cOH)	4	Spatial	Boundary 10
0	4	Spatial	Boundary 10
0	4	Spatial	Boundary 10

2.4.12 Flux 2



Flux 2

SELECTION

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

EQUATIONS

$$-\mathbf{n}\cdot\mathbf{j}_i = j_{0,i}$$

Convection

SETTINGS

Description	Value
Include	Off

Inward flux

SETTINGS

Description	Value
Species cH3O	On
Species cOH	Off
Species cBead	Off
Species cK	Off
Species cCl	Off

Description	Value
Inward flux	{fssBPE, 0, 0, 0, 0}

Variables

Name	Expression	Unit	Description	Selection
npe.cbf_cH3O	cH3O*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 4
npe.cbf_cOH	cOH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 4
npe.cbf_cBead	cBead*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 4
npe.cbf_cK	cK*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 4

Weak expressions

Weak expression	Integration order	Integration frame	Selection
fssBPE*test(cH3O)	4	Spatial	Boundary 4
0	4	Spatial	Boundary 4
0	4	Spatial	Boundary 4
0	4	Spatial	Boundary 4

2.4.13 Current Density 1

Current Density 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 10

EQUATIONS

$$-\mathbf{n}\cdot\mathbf{i}=i_{0}$$

Inward current density

SETTINGS

Description	Value
Inward current density	-jssBPE

Variables

Name	Expression	Unit	Description	Selection
npe.i0_cdens4	-jssBPE	A/m²	Inward current density	Boundary 10

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.i0_cdens4*test(V)	4	Spatial	Boundary 10

2.4.14 Current Density 2

Current Density 2

SELECTION

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

EQUATIONS

$$-\mathbf{n}\cdot\mathbf{i} = i_0$$

Inward current density

SETTINGS

Description	Value
Inward current density	jssBPE

Variables

Name	Expression	Unit	Description	Selection
npe.i0_cdens5	jssBPE	A/m²	Inward current density	Boundary 4

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.i0_cdens5*test(V)	4	Spatial	Boundary 4

2.4.15 Reactions 1

Reactions 1

SELECTION

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

EQUATIONS

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

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

Reaction rates

SETTINGS

Description	Value
Total rate expression	User defined
Total rate expression	kfhydro*cH2O0 - kbhydro*cH3O*cOH
Total rate expression	User defined
Total rate expression	kfhydro*cH2O0 - kbhydro*cH3O*cOH
Total rate expression	User defined
Total rate expression	0
Total rate expression	User defined
Total rate expression	0

Description	Value
Total rate expression	User defined
Total rate expression	0

Variables

Name	Expression	Unit	Description	Selection	Details
npe.R_cH3O	npe.reac1.R_cH3O	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cOH	npe.reac1.R_cOH	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cBead	npe.reac1.R_cBead	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cK	npe.reac1.R_cK	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cCl	npe.reac1.R_cCl	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.reac1.R_cH3O	model.input.R_cH3O	mol/(m³·s)	Total rate expression	Domain 1	Meta
npe.reac1.R_cOH	model.input.R_cOH	mol/(m³·s)	Total rate expression	Domain 1	Meta
npe.reac1.R_cBead	model.input.R_cBead	mol/(m³·s)	Total rate expression	Domain 1	Meta
npe.reac1.R_cK	model.input.R_cK	mol/(m³·s)	Total rate expression	Domain 1	Meta
npe.reac1.R_cCl	model.input.R_cCl	mol/(m³·s)	Total rate expression	Domain 1	Meta

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.reac1.R_cH3O*test(cH3O)	4	Spatial	Domain 1
F_const*npe.reac1.R_cH3O*npe.z_cH3O*test(V)	4	Spatial	Domain 1
npe.reac1.R_cOH*test(cOH)	4	Spatial	Domain 1
F_const*npe.reac1.R_cOH*npe.z_cOH*test(V)	4	Spatial	Domain 1
npe.reac1.R_cBead*test(cBead)	4	Spatial	Domain 1
F_const*npe.reac1.R_cBead*npe.z_cBead*test(V)	4	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
npe.reac1.R_cK*test(cK)	4	Spatial	Domain 1
F_const*npe.reac1.R_cK*npe.z_cK*test(V)	4	Spatial	Domain 1
F_const*npe.reac1.R_cCl*npe.z_cCl*test(V)	4	Spatial	Domain 1

2.5 LAMINAR FLOW

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

Laminar Flow

SELECTION

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

EQUATIONS

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

2.5.1 Interface settings

Discretization

SETTINGS

Description	Value
Discretization of fluids	P1 + P1

Physical model

SETTINGS

Description	Value
Neglect inertial term (Stokes flow)	Off
Compressibility	Incompressible flow
Enable porous media domains	Off
Reference temperature	User defined
Reference temperature	T
Reference pressure level	1[atm]

Turbulence

SETTINGS

Description	Value
Turbulence model type	None

2.5.2 Variables

Name	Expression	Unit	Description	Selection	Details
spf.Tref	model.input.Tref	K	Reference temperature	Global	Meta
spf.dz	1	m	Thickness	Domain 1	
spf.pref	1[atm]	Pa	Reference pressure level	Domain 1	
spf.pA	p+spf.pref	Pa	Absolute pressure	Domain 1	
spf.hasWF	0		Help variable	Boundaries 1–12	
spf.dt_CFL	1/max(spf.maxOp(sqrt(emetric_s	s	Time step, CFL=1	Global	

Name	Expression	Unit	Description	Selection	Details
	patial(u-d(x,TIME),v-d(y,TIME)))),eps)				
spf.usePseudoTimeStepping	0	1	Help variable	Global	+ operation
spf.localCFLvalue	1.3^min(niterCMP,9)+if(niterCMP>=25,9*1.3^min(-25+niterCMP,9),0)+if(niterCMP>=45,90*1.3^min(-45+niterCMP,9),0)		Local CFL number	Domain 1	
spf.locCFL	CFLCMP	1	Local CFL number	Domain 1	
spf.geometryLengthScale	4.216500000000001E-4	m	Geometry length scale	Domain 1	
spf.time_step_inv	max(sqrt(emetric_spatial(u,v)*2^gmg_level^2),spf.nu/spf.geometryLengthScale^2)	Hz	Inverse time step	Domain 1	
spf.tsti	nojac(spf.time_step_inv/spf.locCFL)	1/s	Help variable	Domain 1	
spf.nx	dnx	1	Normal vector, x component	Boundaries 1–12	
spf.ny	dny	1	Normal vector, y component	Boundaries 1–12	
spf.nz	0	1	Normal vector, z component	Boundaries 1–12	
spf.nxmesh	dnxmesh	1	Normal vector, x component	Boundaries 1–12	
spf.nymesh	dnymesh	1	Normal vector, y	Boundaries 1–12	

Name	Expression	Unit	Description	Selection	Details
			component		
spf.nzmesh	0	1	Normal vector, z component	Boundaries 1–12	

2.5.3 Fluid Properties 1

Fluid Properties 1

SELECTION

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

EQUATIONS

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

Fluid properties

SETTINGS

Description	Value
Density	From material
	Newtonian
Dynamic viscosity	From material

Model input

SETTINGS

Description	Value
Temperature	Common model input

USED PRODUCTS

COMSOL Multiphysics

PROPERTIES FROM MATERIAL

Property	Material	Property group
Density	Water	Basic
Dynamic viscosity	Water	Basic

Variables

Name	Expression	Unit	Description	Selection	Details
spf.mu	material.mu	Pa·s	Dynamic viscosity	Domain 1	Meta
spf.rho	subst(material.rho,spf.fp1.minput_temperature,spf.Trho,spf.fp1.minput_pressure,spf.prho)	kg/m³	Density	Domain 1	Meta
spf.Trho	spf.Tref	K	Temperature for density evaluation	Domain 1	
spf.prho	spf.pref	Pa	Pressure for the evaluation of density	Domain 1	
spf.rhoref	subst(material.rho,spf.fp1.minput_temperature,spf.Tref,spf.fp1.minput_pressure,spf.pref)	kg/m³	Reference density	Domain 1	Meta

Name	Expression	Unit	Description	Selection	Details
spf.mumat	material.mu	Pa·s	Dynamic viscosity	Domain 1	Meta
spf.srijxx	ux	1/s	Strain rate tensor, xx component	Domain 1	
spf.srijyx	0.5*(vx+uy)	1/s	Strain rate tensor, yx component	Domain 1	
spf.srijzx	0	1/s	Strain rate tensor, zx component	Domain 1	
spf.srijxy	0.5*(uy+vx)	1/s	Strain rate tensor, xy component	Domain 1	
spf.srijyy	vy	1/s	Strain rate tensor, yy component	Domain 1	
spf.srijzy	0	1/s	Strain rate tensor, zy component	Domain 1	
spf.srijxz	0	1/s	Strain rate tensor, xz component	Domain 1	
spf.srijyz	0	1/s	Strain rate tensor, yz component	Domain 1	
spf.srijzz	0	1/s	Strain rate tensor, zz component	Domain 1	
spf.rrijxx	0	1/s	Rotation rate tensor, xx component	Domain 1	
spf.rrijyx	0.5*(vx-uy)	1/s	Rotation rate tensor, yx component	Domain 1	
spf.rrijzx	0	1/s	Rotation rate tensor, zx component	Domain 1	
spf.rrijxy	0.5*(uy-vx)	1/s	Rotation rate tensor,	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			xy component		
spf.rrijyy	0	1/s	Rotation rate tensor, yy component	Domain 1	
spf.rrijzy	0	1/s	Rotation rate tensor, zy component	Domain 1	
spf.rrijxz	0	1/s	Rotation rate tensor, xz component	Domain 1	
spf.rrijyz	0	1/s	Rotation rate tensor, yz component	Domain 1	
spf.rrijzz	0	1/s	Rotation rate tensor, zz component	Domain 1	
spf.sr	sqrt(2*spf.srijxx^2+2*spf.srijxy^2+2*spf.srijxz^2+2*spf.srijyx^2+2*spf.srijyy^2+2*spf.srijyz^2+2*spf.srijzx^2+2*spf.srijzy^2+2*spf.srijzz^2+eps)	1/s	Shear rate	Domain 1	
spf.rr	sqrt(2*spf.rrijxx^2+2*spf.rrijxy^2+2*spf.rrijxz^2+2*spf.rrijyx^2+2*spf.rrijyy^2+2*spf.rrijyz^2+2*spf.rrijzx^2+2*spf.rrijzy^2+2*spf.rrijzz^2+e	1/s	Rotation rate	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	ps)				
spf.divu	ux+vy	1/s	Divergence of velocity field	Domain 1	
spf.Fx	0	N/m^3	Volume force, x component	Domain 1	+ operation
spf.Fy	0	N/m^3	Volume force, y component	Domain 1	+ operation
spf.Fz	0	N/m^3	Volume force, z component	Domain 1	+ operation
spf.U	sqrt(u^2+v^2)	m/s	Velocity magnitude	Domain 1	
spf.vorticityx	0	1/s	Vorticity field, x component	Domain 1	
spf.vorticityy	0	1/s	Vorticity field, y component	Domain 1	
spf.vorticityz	vx-uy	1/s	Vorticity field, z component	Domain 1	
spf.vort_magn	sqrt(spf.vorticityx^2+spf.vorticityy^2+spf.vorticityz^2)	1/s	Vorticity magnitude	Domain 1	
spf.cellRe	0.25*spf.rho*sqrt(emetric_spatial(u-d(x,TIME),v-d(y,TIME))/emetric2_spatial)/spf.mu	1	Cell Reynolds number	Domain 1	
spf.nu	spf.mu/spf.rho	m^2/s	Kinematic viscosity	Domain 1	
spf.betaT	0	1/Pa	Isothermal compressibility coefficient	Domain 1	
spf.Qm	0	$kg/(m^3 \cdot s)$	Source term	Domain 1	+ operati

Name	Expression	Unit	Description	Selection	Details
					on
spf.Fgtotx	0	N/m³	Gravity force, x component	Domain 1	+ operation
spf.Fgtoty	0	N/m³	Gravity force, y component	Domain 1	+ operation
spf.Fgtotz	0	N/m³	Gravity force, z component	Domain 1	+ operation
spf.mu_eff	spf.mu+spf.muT	Pa·s	Dynamic viscosity	Domain 1	
spf.muT	0	Pa·s	Turbulent dynamic viscosity	Domain 1	
spf.T_stressx	spf.K_stressx-p*spf.nxmesh	N/m²	Total stress, x component	Boundaries 1–12	+ operation
spf.T_stressy	spf.K_stressy-p*spf.nymesh	N/m²	Total stress, y component	Boundaries 1–12	+ operation
spf.T_stressz	spf.K_stressz-p*spf.nzmesh	N/m²	Total stress, z component	Boundaries 1–12	+ operation
spf.K_stressx	spf.mu_eff*(2*ux*spf.nxmesh+(uy+vx)*spf.nymesh)	N/m²	Viscous stress, x component	Boundaries 1–12	+ operation
spf.K_stressy	spf.mu_eff*((vx+uy)*spf.nxmesh+2*vy*spf.nymesh)	N/m²	Viscous stress, y component	Boundaries 1–12	+ operation
spf.K_stressz	0	N/m²	Viscous stress, z component	Boundaries 1–12	+ operation
spf.K_stress_tensorxx	2*spf.mu_eff*ux	N/m²	Viscous stress tensor, xx component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
spf.K_stress_tensoryx	spf.mu_eff*(vx+uy)	N/m²	Viscous stress tensor, yx component	Domain 1	+ operation
spf.K_stress_tensorzx	0	N/m²	Viscous stress tensor, zx component	Domain 1	+ operation
spf.K_stress_tensorxy	spf.mu_eff*(uy+vx)	N/m²	Viscous stress tensor, xy component	Domain 1	+ operation
spf.K_stress_tensoryy	2*spf.mu_eff*vy	N/m²	Viscous stress tensor, yy component	Domain 1	+ operation
spf.K_stress_tensorzy	0	N/m²	Viscous stress tensor, zy component	Domain 1	+ operation
spf.K_stress_tensorxz	0	N/m²	Viscous stress tensor, xz component	Domain 1	+ operation
spf.K_stress_tensoryz	0	N/m²	Viscous stress tensor, yz component	Domain 1	+ operation
spf.K_stress_tensorzz	0	N/m²	Viscous stress tensor, zz component	Domain 1	+ operation
spf.K_stress_tensor_testxx	2*spf.mu_eff*test(ux)	N/m²	Viscous stress tensor test, xx component	Domain 1	+ operation
spf.K_stress_tensor_testyx	spf.mu_eff*(test(vx)+test(uy))	N/m²	Viscous stress tensor test, yx component	Domain 1	+ operation
spf.K_stress_tensor_testz	0	N/m²	Viscous stress	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
x			tensor test, zx component		
spf.K_stress_tensor_testxy	spf.mu_eff*(test(uy)+test(vx))	N/m²	Viscous stress tensor test, xy component	Domain 1	+ operation
spf.K_stress_tensor_testyy	2*spf.mu_eff*test(vy)	N/m²	Viscous stress tensor test, yy component	Domain 1	+ operation
spf.K_stress_tensor_testzy	0	N/m²	Viscous stress tensor test, zy component	Domain 1	+ operation
spf.K_stress_tensor_testxz	0	N/m²	Viscous stress tensor test, xz component	Domain 1	+ operation
spf.K_stress_tensor_testyz	0	N/m²	Viscous stress tensor test, yz component	Domain 1	+ operation
spf.K_stress_tensor_testzz	0	N/m²	Viscous stress tensor test, zz component	Domain 1	+ operation
spf.upwind_helpx	u-d(x,TIME)	m/s	Upwind term, x component	Domain 1	+ operation
spf.upwind_helpy	v-d(y,TIME)	m/s	Upwind term, y component	Domain 1	+ operation
spf.upwind_helpz	0	m/s	Upwind term, z component	Domain 1	+ operation
spf.tau_vdxx	2*spf.mu*spf.srijxx	Pa	Viscous stress	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			tensor, xx component		
spf.tau_vdyx	2*spf.mu*spf.srijyx	Pa	Viscous stress tensor, yx component	Domain 1	+ operation
spf.tau_vdzx	2*spf.mu*spf.srijzx	Pa	Viscous stress tensor, zx component	Domain 1	+ operation
spf.tau_vdxy	2*spf.mu*spf.srijxy	Pa	Viscous stress tensor, xy component	Domain 1	+ operation
spf.tau_vdyy	2*spf.mu*spf.srijyy	Pa	Viscous stress tensor, yy component	Domain 1	+ operation
spf.tau_vdzy	2*spf.mu*spf.srijzy	Pa	Viscous stress tensor, zy component	Domain 1	+ operation
spf.tau_vdxz	2*spf.mu*spf.srijxz	Pa	Viscous stress tensor, xz component	Domain 1	+ operation
spf.tau_vdyz	2*spf.mu*spf.srijyz	Pa	Viscous stress tensor, yz component	Domain 1	+ operation
spf.tau_vdzz	2*spf.mu*spf.srijzz	Pa	Viscous stress tensor, zz component	Domain 1	+ operation
spf.Qvd	spf.tau_vdxx*ux+spf.tau_vdxy*uy+spf.tau_vdyx*vx+spf.tau_vdyy*vy	W/m^3	Viscous dissipation	Domain 1	+ operation
spf.epsilon_p	1	1	Porosity	Domain 1	
spf.Fst_tensorxx	0	N/m^2	Surface tension	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			force, xx component		
spf.Fst_tensoryx	0	N/m²	Surface tension force, yx component	Domain 1	+ operation
spf.Fst_tensorzx	0	N/m²	Surface tension force, zx component	Domain 1	+ operation
spf.Fst_tensorxy	0	N/m²	Surface tension force, xy component	Domain 1	+ operation
spf.Fst_tensoryy	0	N/m²	Surface tension force, yy component	Domain 1	+ operation
spf.Fst_tensorzy	0	N/m²	Surface tension force, zy component	Domain 1	+ operation
spf.Fst_tensorxz	0	N/m²	Surface tension force, xz component	Domain 1	+ operation
spf.Fst_tensoryz	0	N/m²	Surface tension force, yz component	Domain 1	+ operation
spf.Fst_tensorzz	0	N/m²	Surface tension force, zz component	Domain 1	+ operation
spf.continuityEquation	spf.rho*spf.divu	kg/(m³·s)	Continuity equation	Domain 1	
spf.contCoeff	spf.rho	kg/m³	Help variable	Domain 1	
spf.res_u	px+spf.rho*u*ux+spf.rho*v*uy-(d(2*ux,x)+d(uy+vx,y))*spf.mu-spf.Fx	N/m³	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
spf.res_v	spf.rho*u*vx+py+spf.rho*v*vy-(d(vx+uy,x)+d(2*vy,y))*spf.mu-spf.Fy	N/m³	Equation residual	Domain 1	
spf.res_p	spf.rho*spf.divu	kg/(m³·s)	Pressure equation residual	Domain 1	

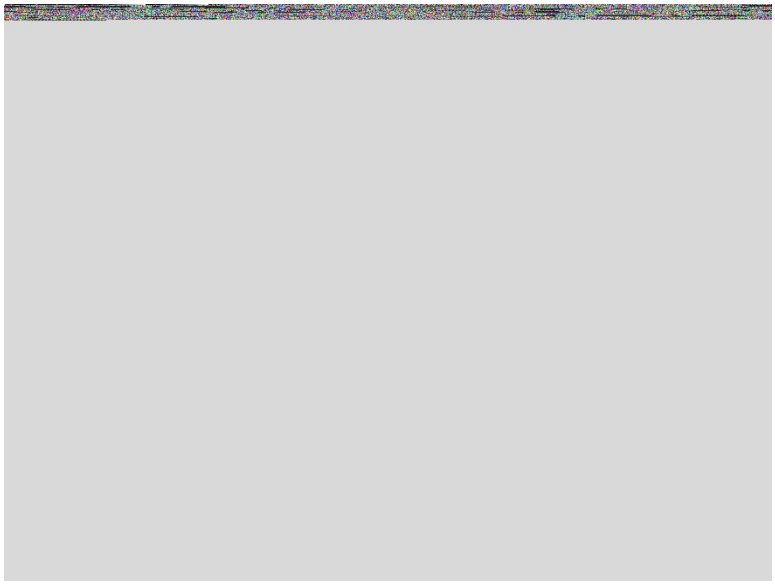
Shape functions

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

Weak expressions

Weak expression	Integration order	Integration frame	Selection
(p-spf.K_stress_tensorxx)*test(ux)-spf.K_stress_tensorxy*test(uy)-spf.K_stress_tensoryx*test(vx)+(p-spf.K_stress_tensoryy)*test(vy)	2	Spatial	Domain 1
spf.Fx*test(u)+spf.Fy*test(v)	2	Spatial	Domain 1
spf.rho*(-(d(u,x)*u+d(u,y)*v)*test(u)-(d(v,x)*u+d(v,y)*v)*test(v))	2	Spatial	Domain 1
-spf.continuityEquation*test(p)	2	Spatial	Domain 1
spf.streamlinens	2	Spatial	Domain 1
(spf.usePseudoTimeStepping>0)*spf.rho*spf.tsti*(-(u-nojac(u))*test(u)-(v-nojac(v))*test(v))	2	Spatial	Domain 1

2.5.4 Initial Values 1



Initial Values 1

SELECTION

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

Initial values

SETTINGS

Description	Value
Velocity field, x component	0
Velocity field, y component	0
Velocity field, z component	0
Pressure	0

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

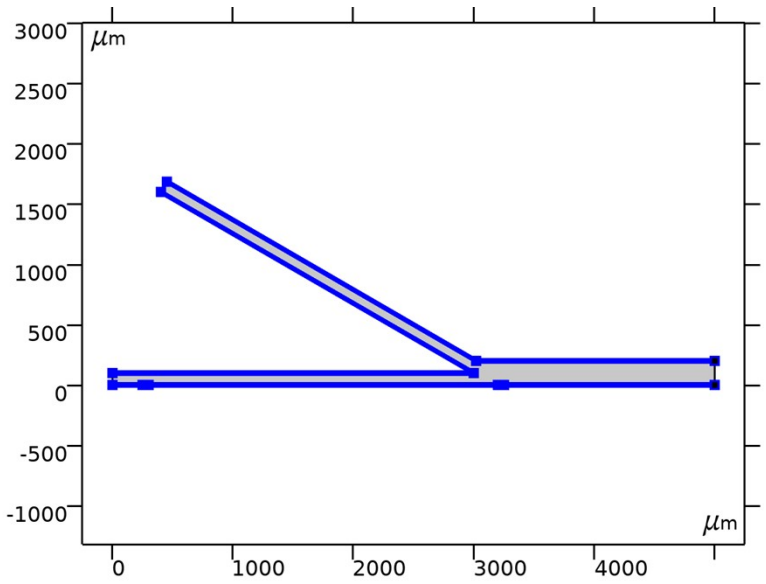
USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
spf.u_initx	0	m/s	Velocity field, x component	Domain 1
spf.u_inity	0	m/s	Velocity field, y component	Domain 1
spf.u_initz	0	m/s	Velocity field, z component	Domain 1
spf.p_init	0	Pa	Pressure	Domain 1

2.5.5 Wall 1



Wall 1

SELECTION

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

EQUATIONS

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

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

Boundary condition

SETTINGS

Description	Value
Wall condition	Electroosmotic velocity
Electric field	User defined
Electric field	{-npe.gradVx, -npe.gradVy, 0}

Description	Value
Electroosmotic mobility	Built - in expression
Zeta potential	-(0.080)[V]
Relative permittivity	80

Wall movement

SETTINGS

Description	Value
Translational velocity	Automatic from frame
Sliding wall	Off

Variables

Name	Expression	Unit	Description	Selection	Details
spf.KStressn_avx	spf.K_stress_tensorxx*spf.nxmesh+spf.K_stress_tensorxy*spf.nymesh+spf.K_stress_tensorxz*spf.nzmesh	N/m²	Average viscous stress, x component	Boundaries 2–5, 7–11	
spf.KStressn_avy	spf.K_stress_tensoryx*spf.nxmesh+spf.K_stress_tensoryy*spf.nymesh+spf.K_stress_tensoryz*spf.nzmesh	N/m²	Average viscous stress, y component	Boundaries 2–5, 7–11	
spf.KStressn_avz	spf.K_stress_tensorzx*spf.nxmesh+spf.K_stress_tensorzy*spf.nymesh+spf.K_stress_tensorzz*spf.nzmesh	N/m²	Average viscous stress, z component	Boundaries 2–5, 7–11	
spf.KStressTestn_avx	spf.K_stress_tensor_testxx*spf.nxmesh+spf.K_stress_tensor_testxy*spf.nymesh+spf.K_stress_tensor_testxz*spf.nzmesh	N/m²	Average viscous stress, x component	Boundaries 2–5, 7–11	
spf.KStressTe	spf.K_stress_tens	N/m²	Average	Boundarie	

Name	Expression	Unit	Description	Selection	Details
stn_avy	or_testyx*spf.nxmesh+spf.K_stress_tensor_testyy*spf.nymesh+spf.K_stress_tensor_testyz*spf.nzmesh		viscous stress, y component	s 2–5, 7–11	
spf.KStressTestn_avz	spf.K_stress_tensor_testzx*spf.nxmesh+spf.K_stress_tensor_testzy*spf.nymesh+spf.K_stress_tensor_testzz*spf.nzmesh	N/m^2	Average viscous stress, z component	Boundaries 2–5, 7–11	
spf.ujumpx	spf.u_herex-spf.u_therex	m/s	Velocity jump, x component	Boundaries 2–5, 7–11	
spf.ujumpy	spf.u_herey-spf.u_therey	m/s	Velocity jump, y component	Boundaries 2–5, 7–11	
spf.ujumpz	spf.u_herez-spf.u_therez	m/s	Velocity jump, z component	Boundaries 2–5, 7–11	
spf.meshVol	meshvol_spatial	m		Boundaries 2–5, 7–11	
spf.meshVolInt	down(meshvol_spatial)	m^2	Volume of interior mesh element	Boundaries 2–5, 7–11	
spf.c_here	24*nojac(down(spf.mu))*spf.meshVol/spf.meshVolInt	1	Intermediate variable	Boundaries 2–5, 7–11	
spf.sigma_dg_ns	4*spf.c_here	Pa·s/m		Boundaries 2–5, 7–11	
spf.rhoFace	down(spf.rho)	kg/m^3	Density face value	Boundaries 2–5, 7–11	
spf.umxTnFace	(spf.upwind_helpx*spf.nxmesh+spf.upwind_help	m/s	Relative velocity on face	Boundaries 2–5, 7–11	

Name	Expression	Unit	Description	Selection	Details
	y*spf.nymesh+spf.upwind_helpz*spf.nzmesh<0)*(spf.upwind_helpx*spf.nxmesh+spf.upwind_helpy*spf.nymesh+spf.upwind_helpz*spf.nzmesh)				
spf.upwind_ns	spf.rhoFace*spf.umxTnFace*(spf.ujumpx*test(spf.u_herex)+spf.ujumpy*test(spf.u_herey)+spf.ujumpz*test(spf.u_herez))	Pa	Upwind term	Boundaries 2–5, 7–11	
spf.zeta	(-0.08)[V]	V	Zeta potential	Boundaries 2–5, 7–11	
spf.epsilonr	80	1	Relative permittivity	Boundaries 2–5, 7–11	
spf.ubndx	spf.ueox+spf.utrx+spf.usx	m/s	Velocity at boundary, x component	Boundaries 2–5, 7–11	
spf.ubndy	spf.ueoy+spf.utry+spf.usy	m/s	Velocity at boundary, y component	Boundaries 2–5, 7–11	
spf.ubndz	spf.ueoz+spf.utrz+spf.usz	m/s	Velocity at boundary, z component	Boundaries 2–5, 7–11	
spf.usx	0	m/s	Velocity of sliding wall, x component	Boundaries 2–5, 7–11	
spf.usy	0	m/s	Velocity of sliding wall, y component	Boundaries 2–5, 7–11	
spf.usz	0	m/s	Velocity of sliding wall, z component	Boundaries 2–5, 7–11	

Name	Expression	Unit	Description	Selection	Details
spf.utrx	0	m/s	Velocity of moving wall, x component	Boundaries 2–5, 7–11	
spf.utry	0	m/s	Velocity of moving wall, y component	Boundaries 2–5, 7–11	
spf.utrz	0	m/s	Velocity of moving wall, z component	Boundaries 2–5, 7–11	
spf.uLeakagex	0	m/s	Leakage velocity, x component	Boundaries 2–5, 7–11	+ operation
spf.uLeakagey	0	m/s	Leakage velocity, y component	Boundaries 2–5, 7–11	+ operation
spf.uLeakagez	0	m/s	Leakage velocity, z component	Boundaries 2–5, 7–11	+ operation
spf.Ex	model.input.E1	V/m	Electric field, x component	Boundaries 2–5, 7–11	Meta
spf.Ey	model.input.E2	V/m	Electric field, y component	Boundaries 2–5, 7–11	Meta
spf.Ez	model.input.E3	V/m	Electric field, z component	Boundaries 2–5, 7–11	Meta
spf.mueo	-spf.zeta*epsilon0_const*spf.epsilonr/spf.mu	$m^2/(V·s)$	Electroosmotic mobility	Boundaries 2–5, 7–11	
spf.ueox	(spf.Ex-spf.nxmesh*(spf.nxmesh*spf.Ex+spf.nymesh*spf.Ey+spf.nzmesh*spf.Ez))*spf.mueo	m/s	Electroosmotic velocity, x component	Boundaries 2–5, 7–11	
spf.ueoy	(spf.Ey-spf.nymesh*(spf.nxmesh*spf.Ex+	m/s	Electroosmotic velocity, y	Boundaries 2–5, 7–	

Name	Expression	Unit	Description	Selection	Details
	spf.nymesh*spf.Ey+spf.nzmesh*spf.Ez))*spf.mueo		component	11	
spf.ueoz	(spf.Ez-spf.nzmesh*(spf.nxmesh*spf.Ex+spf.nymesh*spf.Ey+spf.nzmesh*spf.Ez))*spf.mueo	m/s	Electroosmotic velocity, z component	Boundaries 2–5, 7–11	
spf.u_herex	u	m/s	Intermediate variable, x component	Boundaries 2–5, 7–11	
spf.u_herey	v	m/s	Intermediate variable, y component	Boundaries 2–5, 7–11	
spf.u_herez	0	m/s	Intermediate variable, z component	Boundaries 2–5, 7–11	
spf.u_therex	spf.ubndx+spf.uLeakagex	m/s	Intermediate variable, x component	Boundaries 2–5, 7–11	
spf.u_therey	spf.ubndy+spf.uLeakagey	m/s	Intermediate variable, y component	Boundaries 2–5, 7–11	
spf.u_therez	spf.ubndz+spf.uLeakagez	m/s	Intermediate variable, z component	Boundaries 2–5, 7–11	
spf.contCoeffFace	down(spf.contCoeff)	kg/m^3	Help variable	Boundaries 2–5, 7–11	
spf.upwindCont	spf.contCoeffFace*(spf.ujumpx*spf.nxmesh+spf.ujumpy*spf.nymesh+spf.ujumpz*spf.nzmesh)*test(p)	$kg^2/(m^3 \cdot s^3)$	Upwind term for continuity equation	Boundaries 2–5, 7–11	
spf.pFace	p	Pa	Pressure face value	Boundaries 2–5, 7–11	
spf.consFlux	spf.pFace*(-test(spf.u_herex)	W/m^2	Conservative flux	Boundaries 2–5, 7–	+ operation

Name	Expression	Unit	Description	Selection	Details
	*spf.nxmesh-test(spf.u_herey) *spf.nymesh-test(spf.u_herez) *spf.nzmesh)			11	

Weak expressions

Weak expression	Integration order	Integration frame	Selection
spf.KStressn_avx*test(spf.u_herex)+spf.KStressn_avy*test(spf.u_herey)+spf.KStressn_avz*test(spf.u_herez)+spf.KStressTestn_avx*spf.ujumpx+spf.KStressTestn_avy*spf.ujumpy+spf.KStressTestn_avz*spf.ujumpz-spf.sigma_dg_ns*spf.ujumpx*test(spf.u_herex)-spf.sigma_dg_ns*spf.ujumpy*test(spf.u_herey)-spf.sigma_dg_ns*spf.ujumpz*test(spf.u_herez)+spf.upwind_ns+spf.upwindCont+spf.consFlux	2	Spatial	Boundaries 2–5, 7–11

2.5.6 Inlet 1

Inlet 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 12

EQUATIONS

$$\mathbf{n}^T[-p\mathbf{I}+\mathbf{K}]\mathbf{n} = -\hat{p}_0$$
$$\hat{p}_0 \geq p_0\,,\ \mathbf{u}:\mathbf{t} = 0$$

Boundary condition

SETTINGS

Description	Value
Boundary condition	Pressure

Pressure conditions

SETTINGS

Description	Value
Pressure	0
Suppress backflow	On
Flow direction	Normal flow

USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
spf.KStressn_avx	spf.K_stress_tensorxx*spf.nxmesh+spf.K_stress_tensorxy*spf.nymesh+spf.K_stress_tensorxz*spf.nzmesh	N/m²	Average viscous stress, x component	Boundary 12
spf.KStressn_avy	spf.K_stress_tensoryx*spf.nxmesh+spf.K_stress_tensoryy*spf.nymesh+spf.K_stress_tensoryz*spf.nzmesh	N/m²	Average viscous stress, y component	Boundary 12
spf.KStressn_avz	spf.K_stress_tensorzx*spf.nxmesh+s	N/m²	Average viscous	Boundary 12

Name	Expression	Unit	Description	Selection
	pf.K_stress_tensorzy*spf.nymesh+spf.K_stress_tensorzz*spf.nzmesh		stress, z component	
spf.KStressTestn_avx	spf.K_stress_tensor_testxx*spf.nxmesh+spf.K_stress_tensor_testxy*spf.nymesh+spf.K_stress_tensor_testxz*spf.nzmesh	N/m²	Average viscous stress, x component	Boundary 12
spf.KStressTestn_avy	spf.K_stress_tensor_testyx*spf.nxmesh+spf.K_stress_tensor_testyy*spf.nymesh+spf.K_stress_tensor_testyz*spf.nzmesh	N/m²	Average viscous stress, y component	Boundary 12
spf.KStressTestn_avz	spf.K_stress_tensor_testzx*spf.nxmesh+spf.K_stress_tensor_testzy*spf.nymesh+spf.K_stress_tensor_testzz*spf.nzmesh	N/m²	Average viscous stress, z component	Boundary 12
spf.ujumpx	spf.ut_herex-spf.ut_therex	m/s	Velocity jump, x component	Boundary 12
spf.ujumpy	spf.ut_herey-spf.ut_therey	m/s	Velocity jump, y component	Boundary 12
spf.ujumpz	spf.ut_herez-spf.ut_therez	m/s	Velocity jump, z component	Boundary 12
spf.meshVol	meshvol_spatial	m		Boundary 12
spf.meshVolInt	down(meshvol_spatial)	m²	Volume of interior mesh element	Boundary 12
spf.c_here	96/spf.epsilon_p	Pa·s/m	Intermediate variable	Boundary 12
spf.sigma_dg_ns	4*spf.ct_here	Pa·s/m		Boundary 12

Name	Expression	Unit	Description	Selection
spf.rhoFace	down(spf.rho)	kg/m³	Density face value	Boundary 12
spf.umxTnFace	spf.upwind_helpx*spf.nxmesh+spf.upwind_helpy*spf.nymesh+spf.upwind_helpz*spf.nzmesh	m/s	Relative velocity on face	Boundary 12
spf.upwind_ns	spf.backflowPenaltyConv*spf.uNormal	W/m²	Upwind term	Boundary 12
spf.p0	0	Pa	Pressure	Boundary 12
spf.f0	spf.p0+spf.uNormal*(spf.backflowPenaltyDiff+spf.backflowPenaltyConv)*(spf.uNormal>0)	N/m²	Normal stress	Boundary 12
spf.un_here	u*nojac(spf.nxmesh)+v*nojac(spf.nymesh)	m/s	Intermediate variable	Boundary 12
spf.ut_herex	u-spf.un_here*nojac(spf.nxmesh)	m/s	Intermediate variable, x component	Boundary 12
spf.ut_herey	v-spf.un_here*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundary 12
spf.ut_herez	-spf.un_here*nojac(spf.nzmesh)	m/s	Intermediate variable, z component	Boundary 12
spf.un_there	0	m/s	Intermediate variable	Boundary 12
spf.ut_therex	-spf.un_there*nojac(spf.nxmesh)	m/s	Intermediate variable, x component	Boundary 12
spf.ut_therey	-spf.un_there*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundary 12
spf.ut_therez	-spf.un_there*nojac(spf.nzmesh)	m/s	Intermediate variable, z component	Boundary 12
spf.ct_here	24*nojac(down((spf.mu+spf.muT)/s	Pa·s/m	Intermediate variable	Boundary 12

Name	Expression	Unit	Description	Selection
	pf.epsilon_p))*spf.meshVol/spf.meshVolInt			
spf.inl1.Te0xx	0		Viscoelastic stress tensor, xx component	Boundary 12
spf.inl1.Te0xy	0		Viscoelastic stress tensor, xy component	Boundary 12
spf.inl1.Te0xz	0		Viscoelastic stress tensor, xz component	Boundary 12
spf.inl1.Te0yy	0		Viscoelastic stress tensor, yy component	Boundary 12
spf.inl1.Te0yz	0		Viscoelastic stress tensor, yz component	Boundary 12
spf.inl1.Te0zz	0		Viscoelastic stress tensor, zz component	Boundary 12
spf.uNormal	u*nojac(spf.nxmesh)+v*nojac(spf.nymesh)	m/s	Normal velocity	Boundary 12
spf.backflowPenaltyDiff	spf.c_here*min((down(spf.mu)+spf.muT)*spf.meshVol/spf.meshVolInt,down(spf.rho)*abs(spf.uNormal)/down(spf.epsilon_p))	$kg^2/(m^4 \cdot s^2)$	Backflow penalty parameter, diffusive contribution	Boundary 12
spf.backflowPenaltyConv	spf.rhoFace*spf.umxTnFace/spf.epsilon_p^2	$kg/(m^2 \cdot s)$	Backflow penalty parameter, convective contribution	Boundary 12

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-spf.f0*(test(u)*spf.nxmesh+test(v)*spf.nymesh)	2	Spatial	Boundary 12
spf.KStressn_avx*test(spf.ut_herex)+spf.KStressn_avy*test(spf.ut_herey)+spf.KStressn_avz*test(spf.ut_herez)+spf.KStressTestn_avx*spf.ujumpx+spf.KStressTestn_avy*spf.ujumpy+spf.KStressTestn_avz*spf.ujumpz-spf.sigma_dg_ns*spf.ujumpx*test(spf.ut_herex)-spf.sigma_dg_ns*spf.ujumpy*test(spf.ut_herey)-spf.sigma_dg_ns*spf.ujumpz*test(spf.ut_herez)	2	Spatial	Boundary 12

2.5.7 Outlet 1

Outlet 1

SELECTION

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

EQUATIONS

$$\mathbf{n}^{T}[-p\mathbf{I}+\mathbf{K}]\mathbf{n}=-p_0$$
$$\mathbf{u}\cdot\mathbf{t}=0$$

Boundary condition

SETTINGS

Description	Value
Boundary condition	Pressure

Pressure conditions

SETTINGS

Description	Value
Pressure	0
Normal flow	On
Suppress backflow	Off

USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
spf.KStressn_avx	spf.K_stress_tensorxx*spf.nxmesh+spf.K_stress_tensorxy*spf.nymesh+spf.K_stress_tensorxz*spf.nzmesh	N/m²	Average viscous stress, x component	Boundaries 1, 6
spf.KStressn_avy	spf.K_stress_tensoryx*spf.nxmesh+spf.K_stress_tensoryy*spf.nymesh+spf.K_stress_tensoryz*spf.nzmesh	N/m²	Average viscous stress, y component	Boundaries 1, 6
spf.KStressn_avz	spf.K_stress_tensorzx*spf.nxmesh+spf.K_stress_tensorzy*spf.nymesh+spf.K_stress_tensorzz*spf.nzmesh	N/m²	Average viscous stress, z component	Boundaries 1, 6
spf.KStressTestn_avx	spf.K_stress_tensor_testxx*spf.nxmesh+spf.K_stress_tensor_testxy*spf.nymesh+spf.K_stress_tensor_testxz*spf.nz	N/m²	Average viscous stress, x component	Boundaries 1, 6

Name	Expression	Unit	Description	Selection
	mesh			
spf.KStressTestn_avy	spf.K_stress_tensor_testyx*spf.nxmesh+spf.K_stress_tensor_testyy*spf.nymesh+spf.K_stress_tensor_testyz*spf.nzmesh	N/m²	Average viscous stress, y component	Boundaries 1, 6
spf.KStressTestn_avz	spf.K_stress_tensor_testzx*spf.nxmesh+spf.K_stress_tensor_testzy*spf.nymesh+spf.K_stress_tensor_testzz*spf.nzmesh	N/m²	Average viscous stress, z component	Boundaries 1, 6
spf.ujumpx	spf.ut_herex-spf.ut_therex	m/s	Velocity jump, x component	Boundaries 1, 6
spf.ujumpy	spf.ut_herey-spf.ut_therey	m/s	Velocity jump, y component	Boundaries 1, 6
spf.ujumpz	spf.ut_herez-spf.ut_therez	m/s	Velocity jump, z component	Boundaries 1, 6
spf.meshVol	meshvol_spatial	m		Boundaries 1, 6
spf.meshVolInt	down(meshvol_spatial)	m²	Volume of interior mesh element	Boundaries 1, 6
spf.sigma_dg_ns	4*spf.ct_here	Pa·s/m		Boundaries 1, 6
spf.p0	0	Pa	Pressure	Boundaries 1, 6
spf.f0	spf.p0	N/m²	Normal stress	Boundaries 1, 6
spf.un_here	u*nojac(spf.nxmesh)+v*nojac(spf.nymesh)	m/s	Intermediate variable	Boundaries 1, 6
spf.ut_herex	u-spf.un_here*nojac(spf.nxmesh)	m/s	Intermediate variable, x component	Boundaries 1, 6
spf.ut_herey	v-spf.un_here*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundaries 1, 6
spf.ut_herez	-	m/s	Intermediat	Boundarie

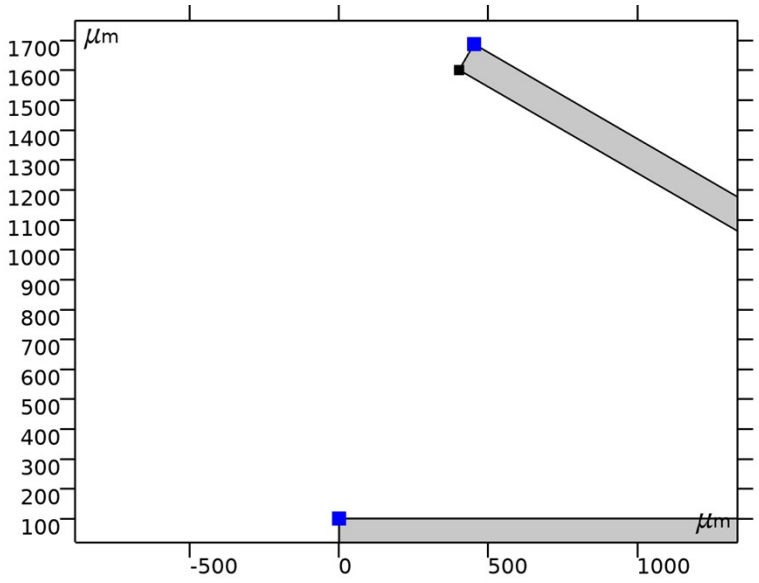
Name	Expression	Unit	Description	Selection
	spf.un_here*nojac(spf.nzmesh)		e variable, z component	s 1, 6
spf.un_there	0	m/s	Intermediate variable	Boundaries 1, 6
spf.ut_therex	-spf.un_there*nojac(spf.nxmesh)	m/s	Intermediate variable, x component	Boundaries 1, 6
spf.ut_therey	-spf.un_there*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundaries 1, 6
spf.ut_therez	-spf.un_there*nojac(spf.nzmesh)	m/s	Intermediate variable, z component	Boundaries 1, 6
spf.ct_here	24*nojac(down((spf.mu+spf.muT)/spf.epsilon_p))*spf.meshVol/spf.meshVolInt	Pa·s/m	Intermediate variable	Boundaries 1, 6
spf.out1.Uav	0	m/s	Average velocity	Global
spf.out1.Uavfdf	0	m/s	Average velocity	Global
spf.out1.Mflow	spf.out1.intFlow(spf.rho*(spf.nx*u+spf.ny*v))	kg/s	Mass flow	Global

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-spf.f0*(test(u)*spf.nxmesh+test(v)*spf.nymesh)	2	Spatial	Boundaries 1, 6
spf.KStressn_avx*test(spf.ut_herex)+spf.KStressn_avy*test(spf.ut_herey)+spf.KStressn_avz*test(spf.ut_herez)+spf.KStressTestn_avx*spf.ujumpx+spf.KStressTestn_avy*spf.ujumpy+spf.KStressTestn_avz*spf.ujumpz-spf.sigma_dg_ns*spf.ujumpx*test(spf.ut_herex)-spf.sigma_dg_ns*spf.ujumpy*test(spf.ut_herey)-spf.sigma_dg_ns*spf.uju	2	Spatial	Boundaries 1, 6

Weak expression	Integration order	Integration frame	Selection
mpz*test(spf.ut_herez)			

2.5.8 Pressure Point Constraint 1



Pressure Point Constraint 1

SELECTION

Geometric entity level	Point
Selection	Geometry geom1: Dimension 0: Points 2, 6

EQUATIONS

$$p = p_0$$

Pressure constraint

SETTINGS

Description	Value
Pressure	0

USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection

Name	Expression	Unit	Description	Selection
spf.p0	0	Pa	Pressure	Points 2, 6

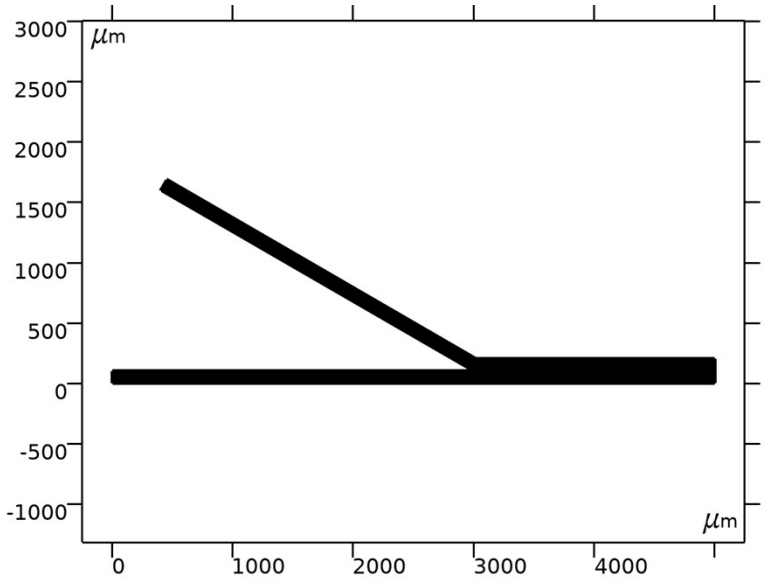
Constraints

Constraint	Constraint force	Shape function	Selection	Details
-p+spf.p0	test(-p)	Lagrange (Linear)	Points 2, 6	Elemental

2.6 MESH 1

MESH STATISTICS

Description	Value
Minimum element quality	0.6544
Average element quality	0.97
Triangle	34139
Quad	620
Edge element	1777
Vertex element	12



Mesh 1

2.6.1 Size (size)

SETTINGS

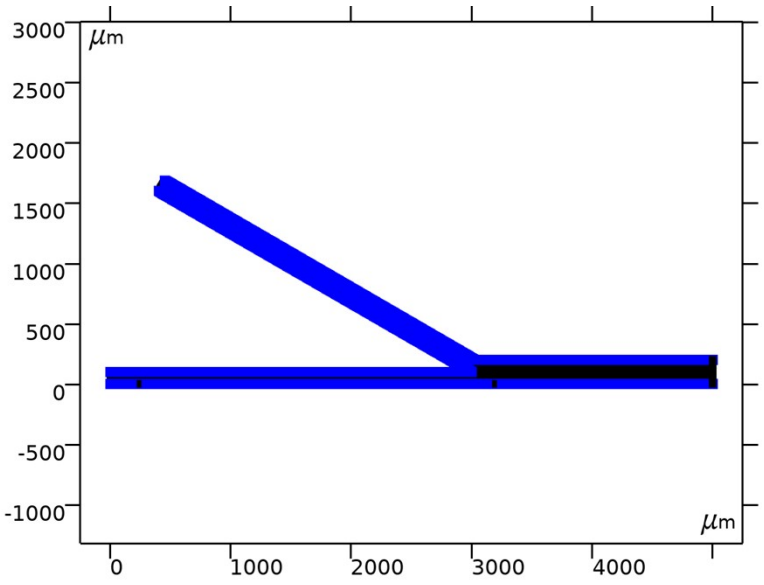
Description	Value

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	11.3
Minimum element size	0.0337
Curvature factor	0.2
Maximum element growth rate	1.05
Predefined size	Extremely fine

2.6.2 Size 1 (size1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 2–3, 5, 7–9, 11



Size 1

SETTINGS

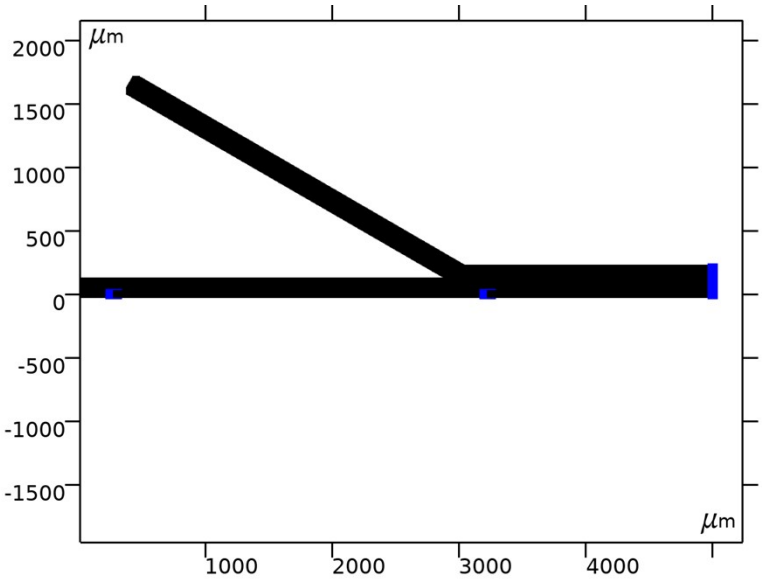
Description	Value
Calibrate for	Fluid dynamics
Maximum element size	11.3
Minimum element size	0.0337
Curvature factor	0.2
Maximum element growth rate	1.05

Description	Value
Predefined size	Extremely fine

2.6.3 Size 2 (size2)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 4, 10, 12



Size 2

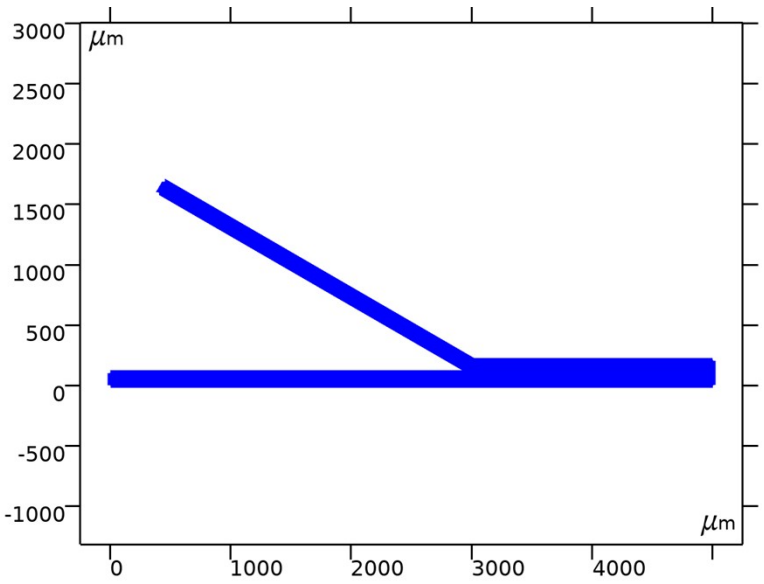
SETTINGS

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	1.5
Minimum element size	0.0207
Curvature factor	0.2
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.05
Maximum element growth rate	Off
Predefined size	Extremely fine
Custom element size	Custom

2.6.4 Corner Refinement 1 (cr1)

SELECTION

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



Corner Refinement 1

2.6.5 Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Remaining

Free Triangular 1

2.6.6 Boundary Layers 1 (bl1)

SELECTION

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

Boundary Layers 1

SETTINGS

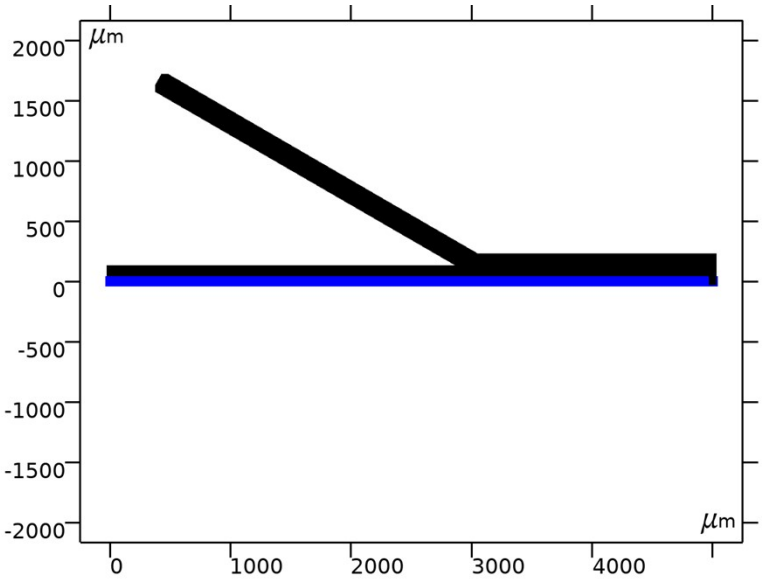
Description	Value

Description	Value
Handling of sharp corners	Trimming

Boundary Layer Properties 1 (blp1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 2, 4–5, 10–11



Boundary Layer Properties 1

SETTINGS

Description	Value
Number of boundary layers	1
Thickness adjustment factor	10

3 Study 1

COMPUTATION INFORMATION

Computation time	1 min 2 s
CPU	Intel64 Family 6 Model 44 Stepping 2, 12 cores
Operating system	Windows 7

3.1 STATIONARY

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Nernst-Planck Equations (npe)	physics
Laminar 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	
Use study step	

LOG

```
<---- Compile Equations: Stationary in Study 1/Solution 1 (sol1) ----------
--
Started at May 26, 2021 10:46:57 AM.
Geometry shape order: Linear
Running on Intel64 Family 6 Model 44 Stepping 2, GenuineIntel.
Using 1 socket with 12 cores in total on CNS-R-WEL870984.
Available memory: 110.59 GB.
Time: 3 s.
Physical memory: 1.96 GB
Virtual memory: 2.12 GB
Ended at May 26, 2021 10:47:01 AM.
----- Compile Equations: Stationary in Study 1/Solution 1 (sol1) ----------
->
```

Dependent Variables 1 (v1)

INITIAL VALUES OF VARIABLES SOLVED FOR

Description	Value
Method	Solution
Solution	

LOG

```
<---- Dependent Variables 1 in Study 1/Solution 1 (sol1) ----------
--
Started at May 26, 2021 10:47:02 AM.
Initial values of variables solved for: Solution 1 (sol1).
Solution time: 0 s.
Physical memory: 1.93 GB
Virtual memory: 2.09 GB
Ended at May 26, 2021 10:47:02 AM.
----- Dependent Variables 1 in Study 1/Solution 1 (sol1) ----------
->
```

Concentration (comp1.cBead) (comp1_cBead)

GENERAL

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

Concentration (comp1.cH3O) (comp1_cH3O)

GENERAL

Description	Value
Field components	comp1.cH3O
Internal variables	{comp1.uflux.cH3O, comp1.dflux.cH3O}

Concentration (comp1.cK) (comp1_cK)

GENERAL

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

Concentration (comp1.cOH) (comp1_cOH)

GENERAL

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

Pressure (comp1.p) (comp1_p)

GENERAL

Description	Value
Field components	comp1.p

Velocity field (comp1.u) (comp1_u)

GENERAL

Description	Value
Field components	{comp1.u, comp1.v}
Internal variables	comp1.spf.isFluidHasBeenSolved

Electric potential (comp1.V) (comp1_V)

GENERAL

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

Stationary Solver 1 (s1)

GENERAL

Description	Value
Defined by study step	

LOG

```
<---- Stationary Solver 1 in Study 1/Solution 1 (sol1) ----------------------
--
Started at May 26, 2021 10:47:02 AM.
Nonlinear solver
Number of degrees of freedom solved for: 418417 (plus 17831 internal DOFs).
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (comp1.cBead): 8.6e+06
Concentration (comp1.cH3O): 95
Concentration (comp1.cK): 3.1e+03
Concentration (comp1.cOH): 1.5e+02
Pressure (comp1.p): 1e+02
Velocity field (comp1.u): 2.7e+02
Electric potential (comp1.V): 30
Orthonormal null-space function used.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     0.00011     5.1e+03   0.0100000     0.00012    2    1    2  3.8e-
13  5.1e-16
   2      0.0001     4.6e+03   0.1000000     0.00011    3    2    4  1.3e-
12  5.1e-16
   3     4.4e-05     5.4e+02   1.0000000     0.00048    5    3    6  1.6e-
11  4.4e-16
Solution time: 57 s.
Physical memory: 5.31 GB
Virtual memory: 6.03 GB
Ended at May 26, 2021 10:47:59 AM.
----- Stationary Solver 1 in Study 1/Solution 1 (sol1) ----------------------
->
```

Advanced (aDef)

ASSEMBLY SETTINGS

Description	Value
Reuse sparsity pattern	On

Fully Coupled 1 (fc1)

GENERAL

Description	Value
Linear solver	

METHOD AND TERMINATION

Description	Value
Initial damping factor	0.01
Minimum damping factor	1.0E-6
Maximum number of iterations	100

Direct 1 (d1)

GENERAL

Description	Value
Solver	PARDISO
Pivoting perturbation	1.0E-13

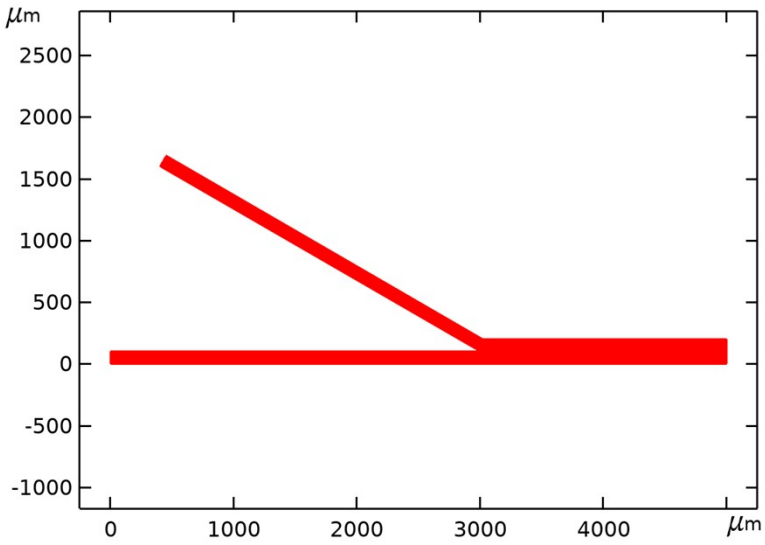
4 Results

4.1 DATA SETS

4.1.1 Study 1/Solution 1

SOLUTION

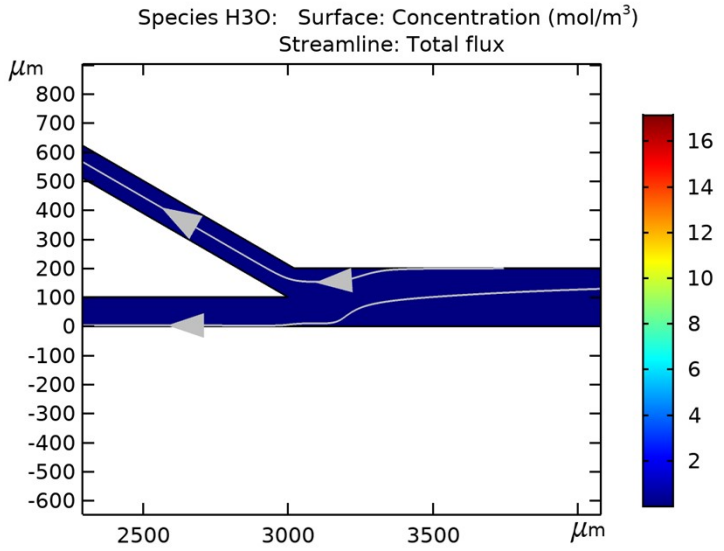
Description	Value
Solution	
Component	Save Point Geometry 1



Dataset: Study 1/Solution 1

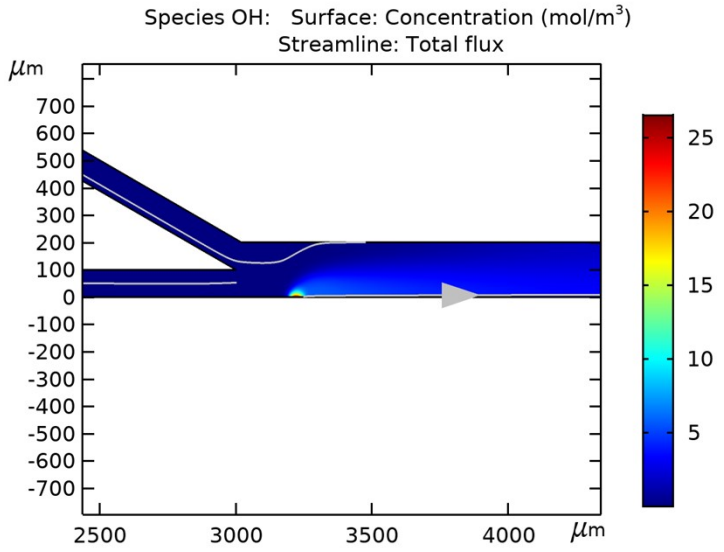
4.2 PLOT GROUPS

4.2.1 Concentration, H3O (npe)



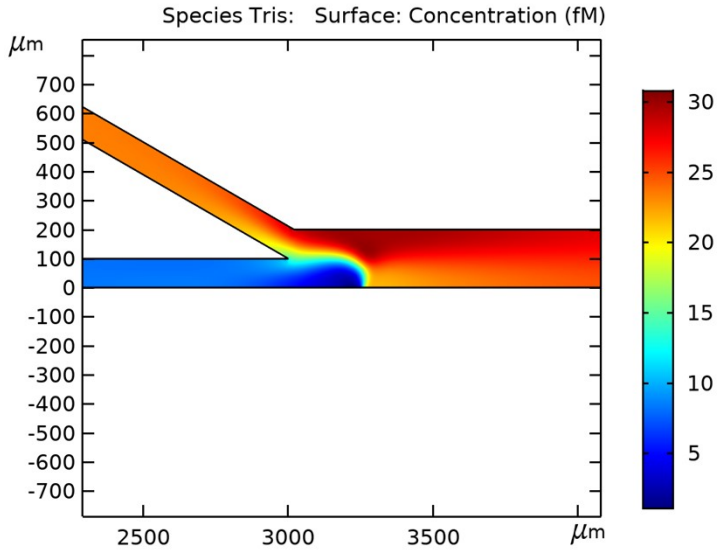
Species H3O: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.2 Concentration, OH (npe)



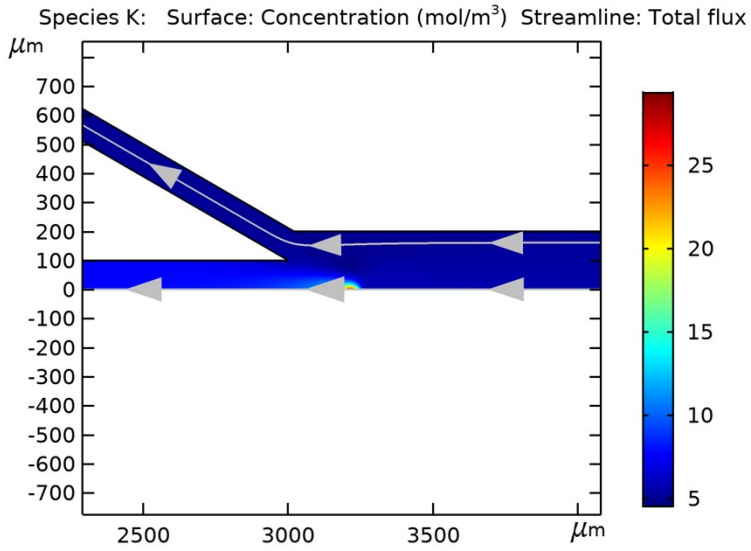
Species OH: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.3 Concentration, bead (npe)



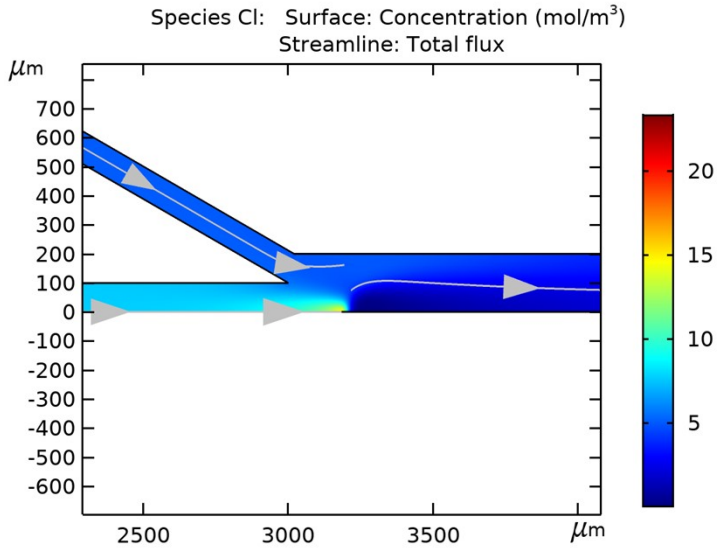
Species Tris: Surface: Concentration (fM)

4.2.4 Concentration, K (npe)



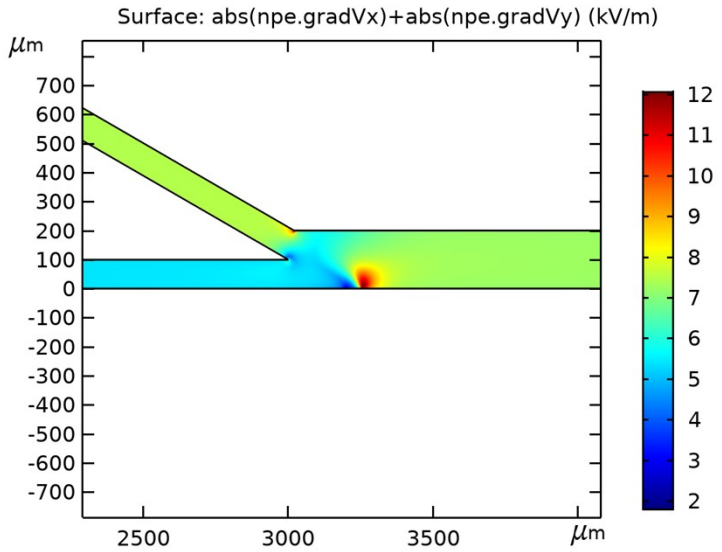
Species K: Surface: Concentration (mol/m^3) Streamline: Total flux

4.2.5 Concentration, Cl (npe)



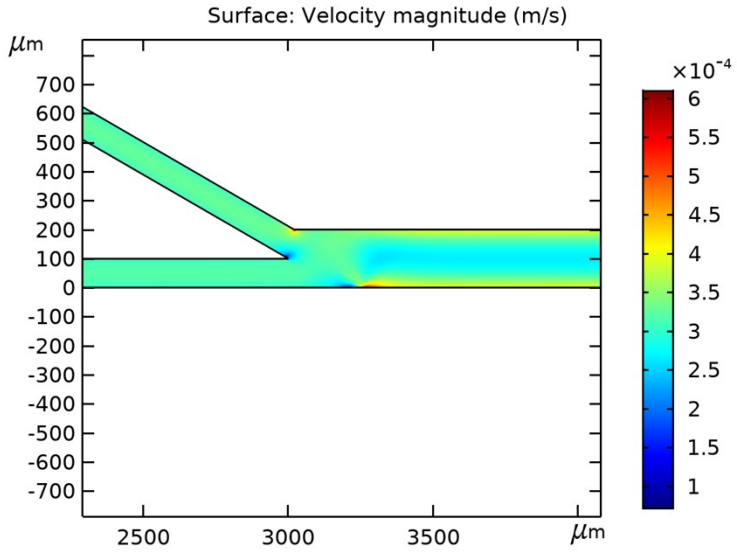
Species Cl: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.6 Electric field (npe)



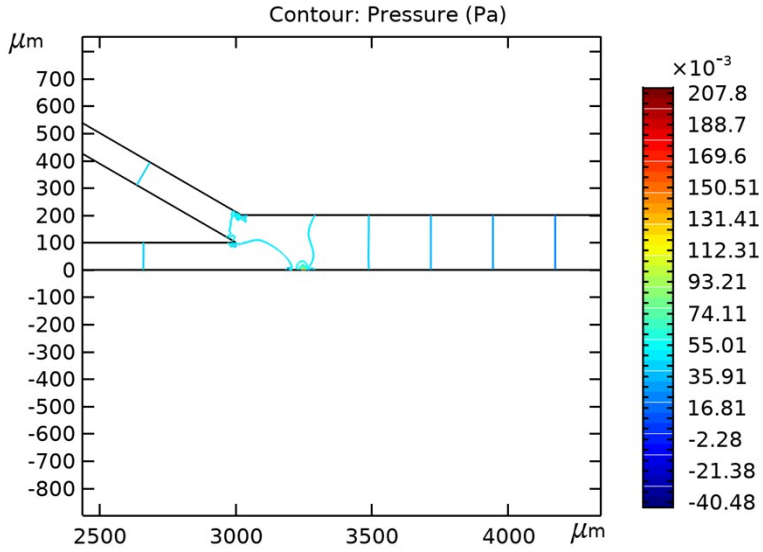
Surface: abs(npe.gradVx)+abs(npe.gradVy) (kV/m)

4.2.7 Velocity (spf)



Surface: Velocity magnitude (m/s)

4.2.8 Pressure (spf)



Contour: Pressure (Pa)