Serial fICP - COMSOL Model

Report date	Mar 14, 2020 8:10:19 PM

Contents

1 Global Definitions

Date	Mar 14, 2020 7:46:06 PM

GLOBAL SETTINGS

Name	2D - Nernst Planck with EN - trifurcated geometry of 2 BPE experiment with appropriate current densities - solved with 0.6 uA through BPE1 and 0.74 uA through BPE2 - final mesh.mph
Path	C:\Users\cdd2359\Desktop\Tris modeling\2003014\2D - Nernst Planck with EN - trifurcated geometry of 2 BPE experiment with appropriate current densities - solved with 0.6 uA through BPE1 and 0.74 uA through BPE2 - final mesh.mph
Version	COMSOL Multiphysics 5.4 (Build: 346)
Unit system	SI

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

1.1 PARAMETERS

PARAMETERS 1

Name	Expression	Value	Description
cheight	11.5[um]	1.15E−5 m	channel height
cwidth	200[um]	2E−4 m	channel width
cH3O0	10^ - pH0[M]	7.9433E−6 mol/m³	initial concentration of protons
pH0	8.1	8.1	initial solution pH
cOH0	10^ - (14 - pH0)[M]	0.0012589 mol/m³	initial concentration of hydroxide
cTrisH0	5.80 [mM]	5.8 mol/m³	initial concentration of TrisH
cTris0	4.20 [mM]	4.2 mol/m³	initial concentration of Tris
cCl0	cTrisH0	5.8 mol/m³	initial concentration

Name	Expression	Value	Description
			of Cl
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
dTrisH	0.785e-9[m^2/s]	7.85E−10 m^2/s	diffusivity of TrisH
dTris	0.785e-9[m^2/s]	7.85E−10 m^2/s	diffusivity of Tris
dCl	2.033e-9[m^2/s]	2.033E−9 m^2/s	diffusivity of Cl
issTOT	1.32[uA]	1.32E−6 A	total current passed through driving electrodes
jssTOT	issTOT/(cwidth*cheight)	573.91 A/m^2	current density passed through channel
issBPE	0.60[uA]	6E−7 A	steady-state current through BPE 1
jssBPE	issBPE/(elength*ewidth)	266.67 A/m^2	current density at BPE 1
fssBPE	jssBPE/F	0.0027638 $mol/(m^2 \cdot s)$	flux at BPE 1
issBPE2	0.74 [uA]	7.4E−7 A	steady-state current through BPE 2
jssBPE2	issBPE2/(elength*ewidth)	328.89 A/m^2	current density at BPE 2
fssBPE2	jssBPE2/F	0.0034087 $mol/(m^2 \cdot s)$	flux at BPE 2
elength	50[um]	5E−5 m	length of BPE end
ewidth	45[um]	4.5E−5 m	width of BPE

Name	Expression	Value	Description
			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	1.11e8[1/(M*s)]	1.11E5 m^3/(s·mol)	backward reaction rate constant for water hydrolysis
kfneut	2e-6[1/(s)]	2E−6 1/s	forward reaction rate constant for buffer neutralization
kbneut	1.11e7[1/(M*s)]	11100 m^3/(s·mol)	backward reaction rate constant for buffer neutralization
cH2O0	55.5 [M]	55500 mol/m^3	concentration of water
pKa	8.24	8.24	pKa of TrisHCl buffer at 293 K
Ka	10^ - pKa	5.7544E−9	Ka of TrisHCl buffer at 293 K
T	293 [K]	293 K	Temperature

1.2 VARIABLES

1.2.1 Variables 1

SELECTION

Geometric entity level	Entire model

Name	Expression	Unit	Description
jssBPEvarcat	2*jssBPE2*((x - 1200[um])/50[um])	A/m^2	

Name	Expression	Unit	Description
2			
jssBPEvaran2	2*jssBPE2*((-x + 300[um])/50[um])	A/m^2	
fssBPEvarcat2	jssBPEvarcat2/F	$mol/(m^2 \cdot s)$	
fssBPEvaran2	jssBPEvaran2/F	$mol/(m^2 \cdot s)$	
jssBPEvarcat1	2*jssBPE*((x - 2660[um])/50[um])	A/m^2	
jssBPEvaran1	2*jssBPE*((-x + 2010[um])/50[um])	A/m^2	
fssBPEvarcat1	jssBPEvarcat1/F	$mol/(m^2 \cdot s)$	
fssBPEvaran1	jssBPEvaran1/F	$mol/(m^2 \cdot s)$	

2 Component 1

Date	Jan 3, 2020 8:56:10 AM

SETTINGS

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

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

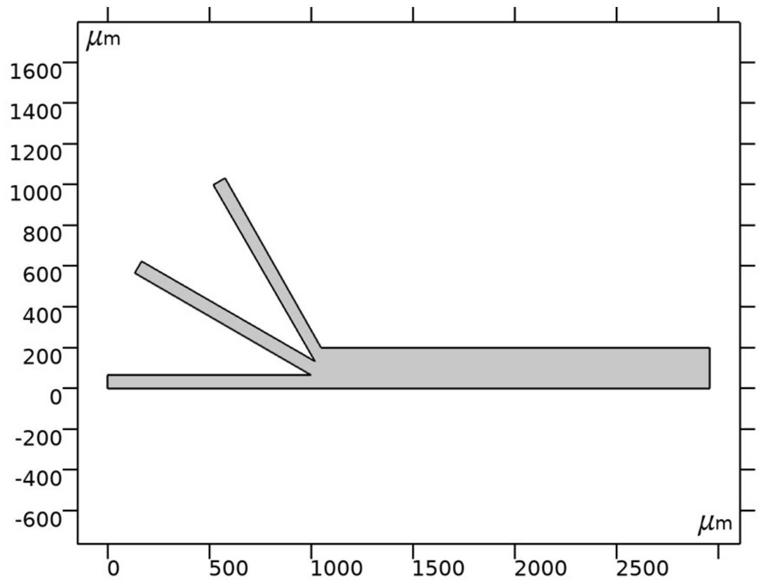
Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third

First	Secon d	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	19
Number of vertices	19

2.2.1 Point 1 (pt1)

POINT

Description	Value
Point coordinate	{250, 0}

2.2.2 Point 2 (pt2)

POINT

Description	Value
Point coordinate	{300, 0}

2.2.3 Point 3 (pt3)

POINT

Description	Value
Point coordinate	{1200, 0}

2.2.4 Point 4 (pt4)

POINT

Description	Value
Point coordinate	{1250, 0}

2.2.5 Point 5 (pt5)

POINT

Description	Value
Point coordinate	{1960, 199.99999999999997}

2.2.6 Point 6 (pt6)

POINT

Description	Value
Point coordinate	{2010, 199.99999999999997}

2.2.7 Point 7 (pt7)

POINT

Description	Value
Point coordinate	{2660, 199.99999999999997}

2.2.8 Point 8 (pt8)

POINT

Description	Value
Point coordinate	{2710,

Description	Value
	199.99999999999997}

2.2.9 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
520	999.426
577.764	1032.776
1050	200
2960	200
2960	0
0	0

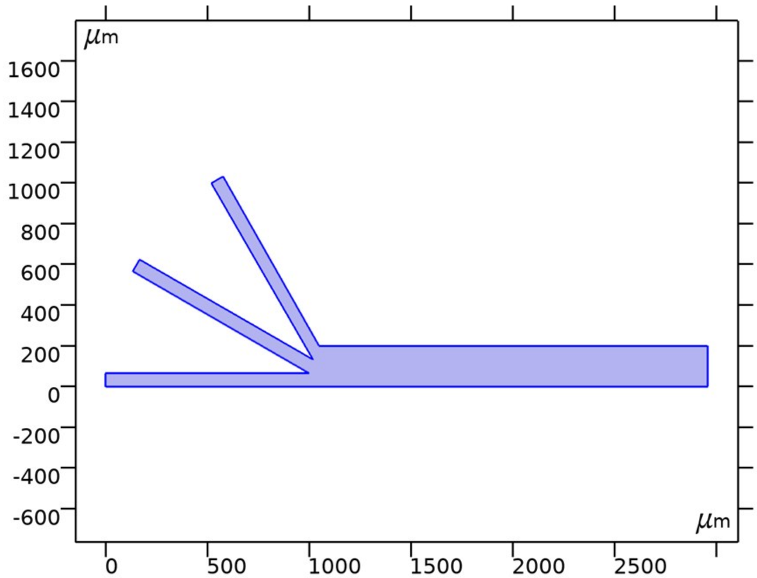
2.2.10 Form Union (fin)

SETTINGS

Description	Value
Repair tolerance	Automatic

2.3 MATERIALS

2.3.1 Water



Water

SELECTION

Geometric entity level	Domain
Selection	Domain 1

MATERIAL PARAMETERS

Name	Value	Unit
Dynamic viscosity	eta(T)	Pa·s
Density	rho(T)	kg/m^3

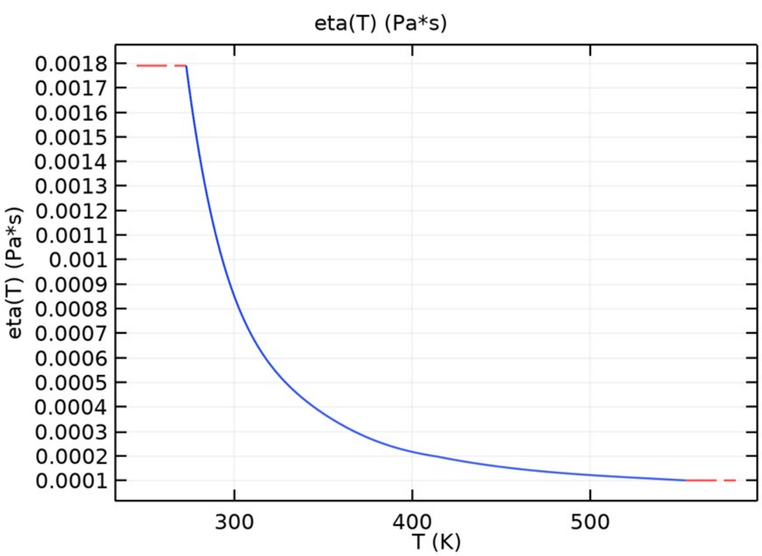
BASIC SETTINGS

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)

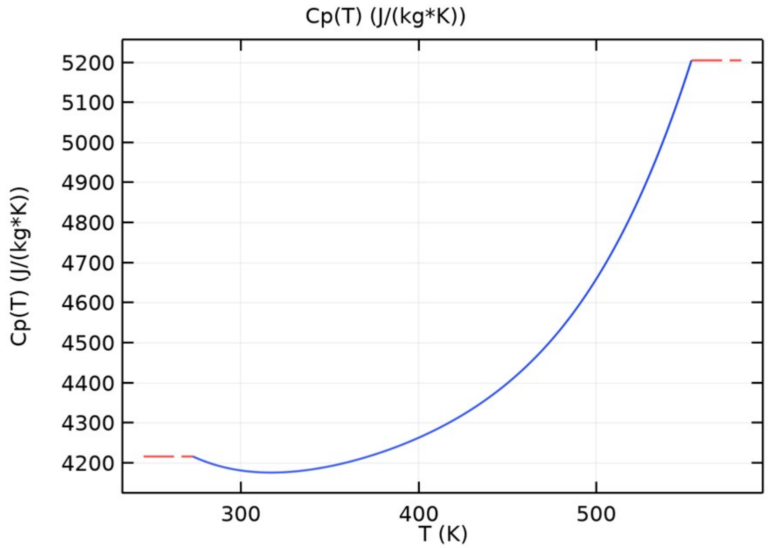
Description	Value
Thermal conductivity	{{k(T), 0, 0}, {0, k(T), 0}, {0, 0, k(T)}}
Speed of sound	cs(T)

FUNCTIONS

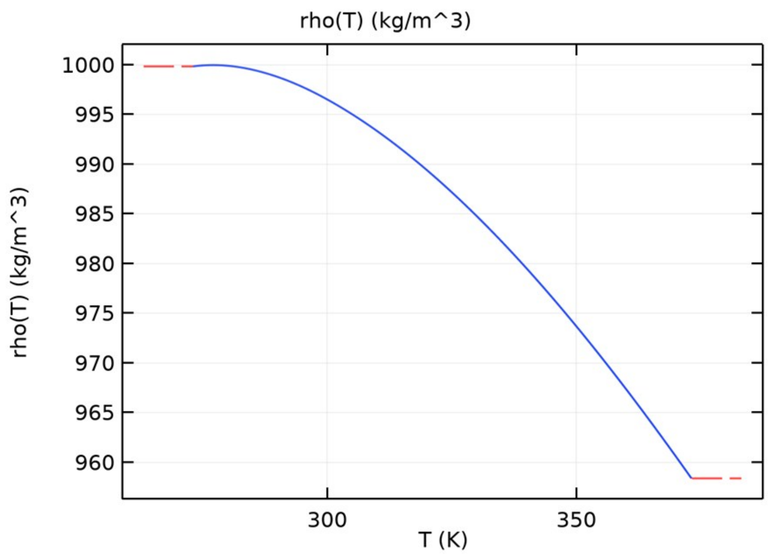
Function name	Type
eta	Piecewise
Cp	Piecewise
rho	Piecewise
k	Piecewise
cs	Interpolation
alpha_p	Analytic
gamma_w	Analytic
muB	Analytic



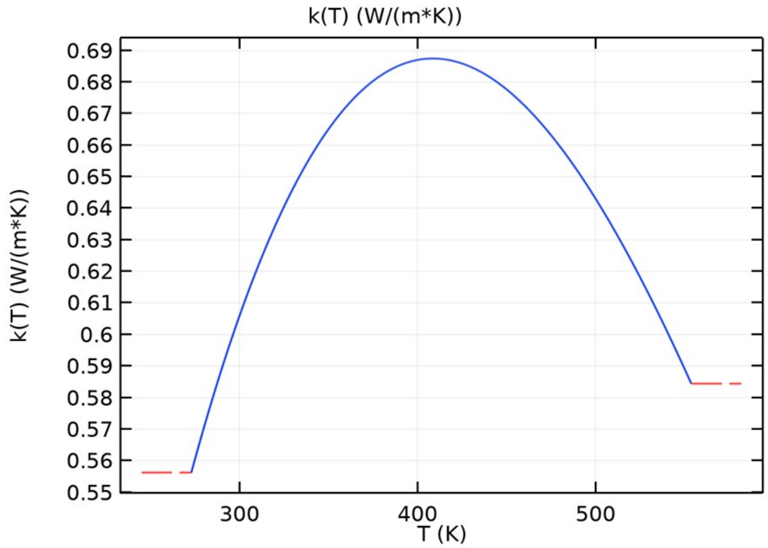
eta


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)

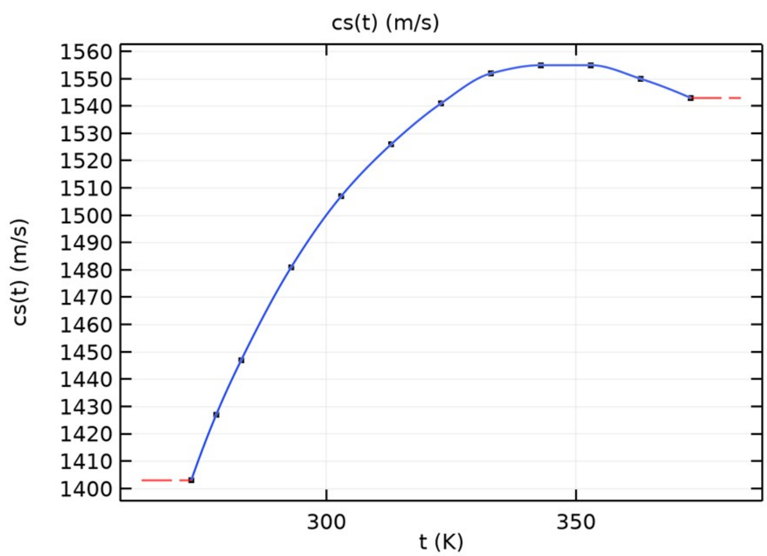
Cp


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

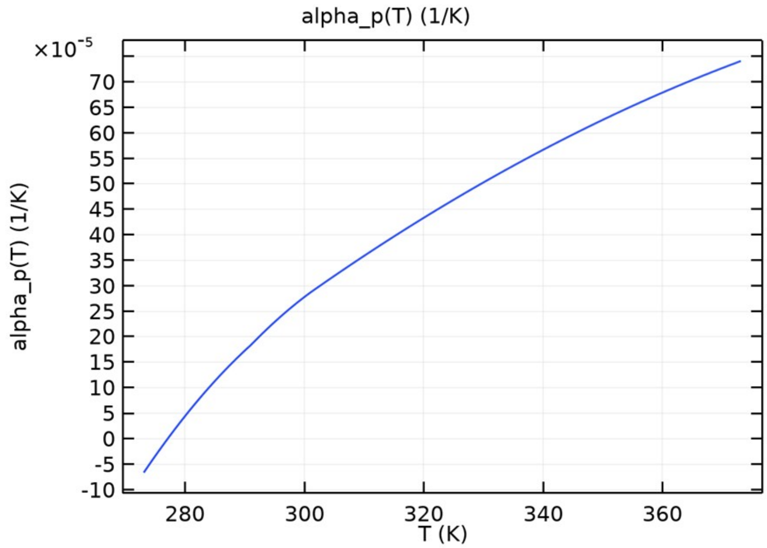
rho


k(T) (W/(m*K))
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
k(T) (W/(m*K))
300
400
500
T (K)

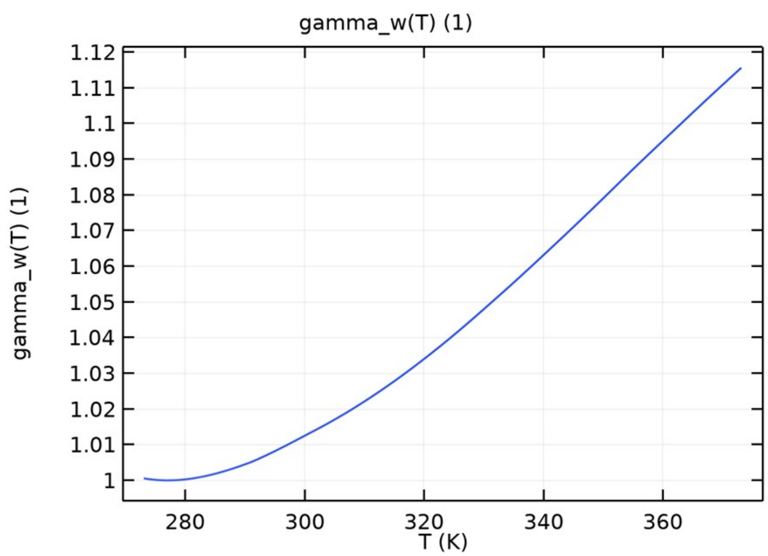
k


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

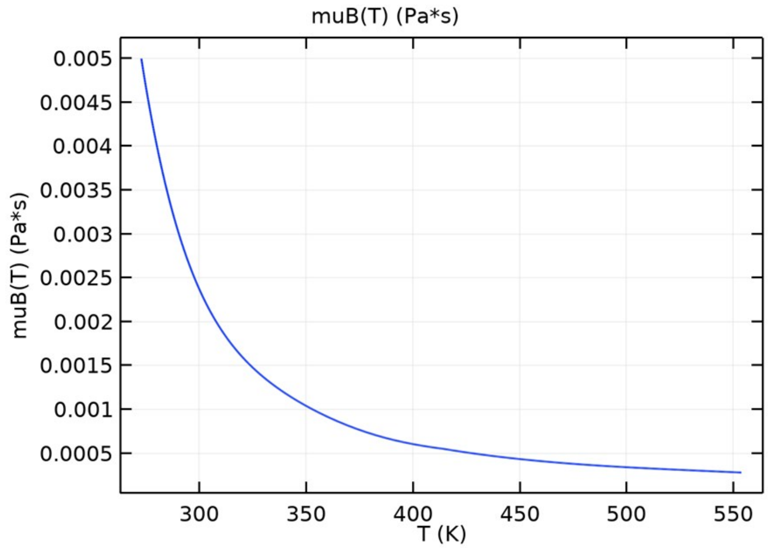
cs



alpha_p



gamma_w

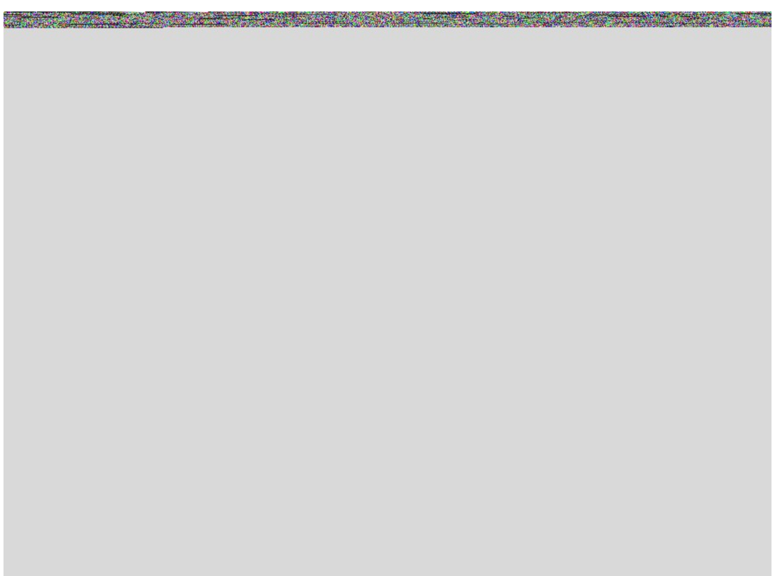


muB

2.4 NERNST-PLANCK EQUATIONS

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module



Nernst-Planck Equations

SELECTION

Geometric entity level	Domain

Selection	Domain 1

EQUATIONS

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

$$\nabla\cdot\mathbf{i}=F\sum_i z_iR_i$$

$$\sum_i z_ic_i=0$$

$$\mathbf{J}_i=-D_i\nabla c_i - z_iu_{m,i}Fc_i\nabla V$$

$$\mathbf{i}=F\sum_i z_i(-D_i\nabla c_i - z_iu_{m,i}Fc_i\nabla V)$$

2.4.1 Interface settings

Discretization

SETTINGS

Description	Value
Concentration	Quadratic
Electric potential	Quadratic

Consistent stabilization

SETTINGS

Description	Value
Streamline diffusion	On
Crosswind diffusion	Off
Equation residual	Approximate residual

Inconsistent stabilization

SETTINGS

Description	Value
Isotropic diffusion	Off

Advanced settings

SETTINGS

Description	Value
Convective term	Conservative form

2.4.2 Variables

Name	Expression	Unit	Description	Selection	Details
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.cTrisx	npe.dflux_cTrisx+npe.cflux_cTrisx+npe.mflux_cTrisx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cTrisy	npe.dflux_cTrisy+npe.cflux_cTrisy+npe.mflux_cTrisy	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cTrisHx	npe.dflux_cTrisHx+npe.cflux_cTrisHx+npe.mflux_cTrisHx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cTrisHy	npe.dflux_cTrisHy+npe.cflux_cTrisHy+npe.mflux_cTrisHy	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	

Name	Expression	Unit	Description	Selection	Details
domflux.Vy	npe.Jy	A/m²	Domain flux, y component	Domain 1	
npe.nx	dnx	1	Normal vector, x component	Boundaries 1–19	
npe.ny	dny	1	Normal vector, y component	Boundaries 1–19	
npe.nz	0	1	Normal vector, z component	Boundaries 1–19	
npe.nxmesh	dnxmesh	1	Normal vector (mesh), x component	Boundaries 1–19	
npe.nymesh	dnymesh	1	Normal vector (mesh), y component	Boundaries 1–19	
npe.nzmesh	0	1	Normal vector (mesh), z component	Boundaries 1–19	
npe.nxc	root.nxc/npe.ncLen	1	Normal vector, x component	Boundaries 1–19	
npe.nyc	root.nyc/npe.ncLen	1	Normal vector, y component	Boundaries 1–19	
npe.nzc	0	1	Normal vector, z component	Boundaries 1–19	
npe.ncLen	sqrt(root.nxc^2+root.nyc^2+eps)	1	Help variable	Boundaries 1–19	
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 1–19	
npe.ncflux_cH3O	npe.cflux_cH3Ox*npe.nxc+n	mol/(m²·s)	Normal convective	Boundaries 1–19	

Name	Expression	Unit	Description	Selection	Details
	pe.cflux_cH3Oy*npe.nyc+npe.cflux_cH3Oz*npe.nzc		flux		
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 1–19	
npe.ntflux_cH3O	npe.bndFlux_cH3O	mol/(m²·s)	Normal total flux	Boundaries 1–19	
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 1–19	
npe.ncflux_cOH	npe.cflux_cOHx*npe.nxc+npe.cflux_cOHy*npe.nyc+npe.cflux_cOHz*npe.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–19	
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 1–19	
npe.ntflux_cOH	npe.bndFlux_cOH	mol/(m²·s)	Normal total flux	Boundaries 1–19	
npe.ndflux_cTris	npe.dflux_cTrisx*npe.nxc+npe.dflux_cTrisy*npe.nyc+npe.dflux_cTrisz*npe.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–19	
npe.ncflux_cTris	npe.cflux_cTrisx*npe.nxc+npe.cflux_cTrisy*npe.nyc+npe.cflux_cTrisz*npe.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–19	

Name	Expression	Unit	Description	Selection	Details
npe.nmflux_cTris	npe.mflux_cTrisx*npe.nxc+npe.mflux_cTrisy*npe.nyc+npe.mflux_cTrisz*npe.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–19	
npe.ntflux_cTris	npe.bndFlux_cTris	mol/(m²·s)	Normal total flux	Boundaries 1–19	
npe.ndflux_cTrisH	npe.dflux_cTrisHx*npe.nxc+npe.dflux_cTrisHy*npe.nyc+npe.dflux_cTrisHz*npe.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–19	
npe.ncflux_cTrisH	npe.cflux_cTrisHx*npe.nxc+npe.cflux_cTrisHy*npe.nyc+npe.cflux_cTrisHz*npe.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–19	
npe.nmflux_cTrisH	npe.mflux_cTrisHx*npe.nxc+npe.mflux_cTrisHy*npe.nyc+npe.mflux_cTrisHz*npe.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–19	
npe.ntflux_cTrisH	npe.bndFlux_cTrisH	mol/(m²·s)	Normal total flux	Boundaries 1–19	
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 1–19	
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 1–19	
npe.nmflux_cCl	npe.mflux_cClx*npe.nxc+npe.mflux_cCly*npe.nyc+npe.	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–19	

Name	Expression	Unit	Description	Selection	Details
	mflux_cClz*npe.nzc				
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 1–19	
npe.bndFlux_cH3O	-dflux_spatial(cH3O)	mol/(m²·s)	Boundary flux	Boundaries 1–19	
npe.bndFlux_cOH	-dflux_spatial(cOH)	mol/(m²·s)	Boundary flux	Boundaries 1–19	
npe.bndFlux_cTris	-dflux_spatial(cTris)	mol/(m²·s)	Boundary flux	Boundaries 1–19	
npe.bndFlux_cTrisH	-dflux_spatial(cTrisH)	mol/(m²·s)	Boundary flux	Boundaries 1–19	
npe.bndFlux_V	-dflux_spatial(npe.V)	A/m²	Boundary flux	Boundaries 1–19	
npe.nJl	npe.bndFlux_V	A/m²	Normal electrolyte current density	Boundaries 1–19	
npe.R_cH3O	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cOH	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cTris	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cTrisH	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation
npe.R_cCl	0	mol/(m³·s)	Total rate expression	Domain 1	+ operation

2.4.3 Convection, Diffusion, and Migration 1

Convection, Diffusion, and Migration 1

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

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

$$\nabla\cdot\mathbf{i}=F\sum_i z_iR_i$$

$$\sum_i z_ic_i=0$$

$$\mathbf{J}_i=-D_i\nabla c_i-z_iu_{m,i}Fc_i\nabla V$$

$$\mathbf{i}=F\sum_i z_i(-D_i\nabla c_i-z_iu_{m,i}Fc_i\nabla V)$$

Convection

SETTINGS

Description	Value
Velocity field	Velocity field (spf)

Diffusion

SETTINGS

Description	Value

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	{{dTris, 0, 0}, {0, dTris, 0}, {0, 0, dTris}}
Diffusion coefficient	User defined
Diffusion coefficient	{{dTrisH, 0, 0}, {0, dTrisH, 0}, {0, 0, dTrisH}}
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, 0, 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	

Name	Expression	Unit	Description	Selection	Details
npe.cbf_cH3O	0	mol/(m²·s)	Convective boundary flux	Boundaries 1–19	
npe.cbf_cOH	0	mol/(m²·s)	Convective boundary flux	Boundaries 1–19	
npe.cbf_cTris	0	mol/(m²·s)	Convective boundary flux	Boundaries 1–19	
npe.cbf_cTrisH	0	mol/(m²·s)	Convective boundary flux	Boundaries 1–19	
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 component	Domain 1	
npe.D_cH3Ozz	dH3O	m²/s	Diffusion coefficient, zz component	Domain 1	
npe.D_cOHxx	dOH	m²/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cOHyx	0	m²/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cOHzx	0	m²/s	Diffusion	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			coefficient, zx component		
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_cTrisxx	dTris	m^2/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cTrisyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cTriszx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	
npe.D_cTrisxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	
npe.D_cTrisyy	dTris	m^2/s	Diffusion coefficient, yy component	Domain 1	
npe.D_cTriszy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	
npe.D_cTrisxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	
npe.D_cTrisyz	0	m^2/s	Diffusion coefficient, yz	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			component		
npe.D_cTriszz	dTris	m^2/s	Diffusion coefficient, zz component	Domain 1	
npe.D_cTrisHxx	dTrisH	m^2/s	Diffusion coefficient, xx component	Domain 1	
npe.D_cTrisHyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	
npe.D_cTrisHzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	
npe.D_cTrisHxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	
npe.D_cTrisHyy	dTrisH	m^2/s	Diffusion coefficient, yy component	Domain 1	
npe.D_cTrisHzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	
npe.D_cTrisHxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	
npe.D_cTrisHyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	
npe.D_cTrisHzz	dTrisH	m^2/s	Diffusion coefficient, zz component	Domain 1	
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	

Name	Expression	Unit	Description	Selection	Details
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.z_cH3O	1	1	Charge number	Domain 1	
npe.z_cOH	-1	1	Charge number	Domain 1	
npe.z_cTris	0	1	Charge number	Domain 1	
npe.z_cTrisH	1	1	Charge number	Domain 1	
npe.z_cCl	-1	1	Charge number	Domain 1	
npe.Dav_cH3O	0.5*(npe.D_cH3Oxx+npe.D_cH3Oyy)	m^2/s	Average diffusion coefficient	Domain 1	
npe.Dav_cOH	0.5*(npe.D_cOHxx+npe.D_cOHyy)	m^2/s	Average diffusion coefficient	Domain 1	
npe.Dav_cTris	0.5*(npe.D_cTrisxx+npe.D_cTrisyy)	m^2/s	Average diffusion coefficient	Domain 1	
npe.Dav_cTrisH	0.5*(npe.D_cTrisHxx+npe.D_cTrisHyy)	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_	$mol/(m^2 \cdot s)$	Total flux, x component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	cH3Ox+npe.mflux_cH3Ox				
npe.tflux_cH3Oy	npe.dflux_cH3Oy+npe.cflux_cH3Oy+npe.mflux_cH3Oy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
npe.tflux_cH3Oz	npe.dflux_cH3Oz+npe.cflux_cH3Oz+npe.mflux_cH3Oz	mol/(m²·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/(m²·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cH3O	sqrt(npe.tflux_cH3Ox^2+npe.tflux_cH3Oy^2+npe.tflux_cH3Oz^2)	mol/(m²·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/(m²·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cH3Oy	npe.z_cH3O*F_const*cH3O*(-npe.um_cH3Oyx*d(npe.V,x)-npe.um_cH3Oyy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
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

Name	Expression	Unit	Description	Selection	Details
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	
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_cTrisx	npe.dflux_cTrisx+npe.cflux_cTrisx+npe.mflux_cTrisx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
npe.tflux_cTrisy	npe.dflux_cTrisy+npe.cflux_cTrisy+npe.mflux_cTrisy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
npe.tflux_cTrisz	npe.dflux_cTrisz+npe.cflux_cTrisz+npe.mflux_cTrisz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
npe.dfluxMag_cTris	sqrt(npe.dflux_cTrisx^2+npe.dflux_cTrisy^2+npe.dflux_cTrisz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cTris	sqrt(npe.tflux_cTrisx^2+npe.tflux_cTrisy^2+npe.tflux_cTrisz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
npe.mflux_cTrisx	npe.z_cTris*F_const*cTris*(-npe.um_cTrisxx*d(npe.V,x)-npe.um_cTrisxy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cTrisy	npe.z_cTris*F_const*cTris*(-npe.um_cTrisyx*d(npe.V,x)-npe.um_cTrisyy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
npe.mflux_cTrisz	npe.z_cTris*F_const*cTris*(-npe.um_cTriszx*d(npe.V,x)-npe.um_cTriszy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
npe.tflux_cTrisHx	npe.dflux_cTrisHx+npe.cflux_cTrisHx+npe.mflux_cTrisHx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
npe.tflux_cTrisHy	npe.dflux_cTrisHy+npe.cflux_cTrisHy+npe.mflux_cTrisHy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
npe.tflux_cTrisHz	npe.dflux_cTrisHz+npe.cflux_cTrisHz+npe.mflux_cTrisHz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
npe.dfluxMag_cTrisH	sqrt(npe.dflux_cTrisHx^2+npe.dflux_cTrisHy^2+npe.dflux_cTrisHz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
npe.tfluxMag_cTrisH	sqrt(npe.tflux_cTrisHx^2+npe.tflux_cTrisHy^2+npe.tflux_cTrisHz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
npe.mflux_cTrisHx	npe.z_cTrisH*F_const*cTrisH*(-npe.um_cTrisHxx*d(npe.V,x)-npe.um_cTrisHxy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
npe.mflux_cTrisHy	npe.z_cTrisH*F_const*cTrisH*(-npe.um_cTrisHyx*d(npe.V,x)-npe.um_cTrisHyy*d(npe.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
npe.mflux_cTrisHz	npe.z_cTrisH*F_const*cTrisH*(-npe.um_cTrisHzx*d(npe.V,x)-npe.um_cTrisHzy*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
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.df	mol/(m²·s)	Diffusive flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	lux_cCly^2+npe.dflux_cClz^2)				
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	
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_c	mol/(m²·s)	Convective flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	H3Oz^2)				
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_cTrisx	cTris*npe.u	mol/(m²·s)	Convective flux, x component	Domain 1	
npe.cflux_cTrisy	cTris*npe.v	mol/(m²·s)	Convective flux, y component	Domain 1	
npe.cflux_cTrisz	cTris*npe.w	mol/(m²·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cTris	sqrt(npe.cflux_cTrisx^2+npe.cflux_cTrisy^2+npe.cflux_cTrisz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
npe.cflux_cTrisHx	cTrisH*npe.u	mol/(m²·s)	Convective flux, x component	Domain 1	
npe.cflux_cTrisHy	cTrisH*npe.v	mol/(m²·s)	Convective flux, y component	Domain 1	
npe.cflux_cTrisHz	cTrisH*npe.w	mol/(m²·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cTrisH	sqrt(npe.cflux_cTrisHx^2+npe.cflux_cTrisHy^2+npe.cflux_cTrisHz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.cflux_cClx	cCl*npe.u	mol/(m²·s)	Convective flux, x component	Domain 1	
npe.cflux_cCly	cCl*npe.v	mol/(m²·s)	Convective flux, y component	Domain 1	
npe.cflux_cClz	cCl*npe.w	mol/(m²·s)	Convective flux, z component	Domain 1	
npe.cfluxMag_cCl	sqrt(npe.cflux_cClx^2+npe.cflux_cCly^2+npe.cflux_cClz^2)	mol/(m²·s)	Convective flux magnitude	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	
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_cH3	npe.D_cH3Oyz/(R_const*npe.	s·mol/k	Mobility, yz	Domain 1	

Name	Expression	Unit	Description	Selection	Details
Oyz	cdm1.minput_temperature)	g	component		
npe.um_cH3Ozz	npe.D_cH3Ozz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zz component	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_cOHzy	npe.D_cOHzy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zy component	Domain 1	
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.um_cTrisxx	npe.D_cTrisxx/(R_const*npe.c	s·mol/kg	Mobility, xx component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	dm1.minput_temperature)				
npe.um_cTrisyx	npe.D_cTrisyx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yx component	Domain 1	
npe.um_cTriszx	npe.D_cTriszx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zx component	Domain 1	
npe.um_cTrisxy	npe.D_cTrisxy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xy component	Domain 1	
npe.um_cTrisyy	npe.D_cTrisyy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yy component	Domain 1	
npe.um_cTriszy	npe.D_cTriszy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zy component	Domain 1	
npe.um_cTrisxz	npe.D_cTrisxz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xz component	Domain 1	
npe.um_cTrisyz	npe.D_cTrisyz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yz component	Domain 1	
npe.um_cTriszz	npe.D_cTriszz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zz component	Domain 1	
npe.um_cTrisHxx	npe.D_cTrisHxx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xx component	Domain 1	
npe.um_cTrisHyx	npe.D_cTrisHyx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yx component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
npe.um_cTrisHzx	npe.D_cTrisHzx/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zx component	Domain 1	
npe.um_cTrisHxy	npe.D_cTrisHxy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xy component	Domain 1	
npe.um_cTrisHyy	npe.D_cTrisHyy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yy component	Domain 1	
npe.um_cTrisHzy	npe.D_cTrisHzy/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zy component	Domain 1	
npe.um_cTrisHxz	npe.D_cTrisHxz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, xz component	Domain 1	
npe.um_cTrisHyz	npe.D_cTrisHyz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, yz component	Domain 1	
npe.um_cTrisHzz	npe.D_cTrisHzz/(R_const*npe.cdm1.minput_temperature)	s·mol/kg	Mobility, zz component	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_cClz	npe.D_cClzx/(	s·mol/k	Mobility, zx	Domain 1	

Name	Expression	Unit	Description	Selection	Details
x	R_const*npe.cdm1.minput_temperature)	g	component		
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.dflux_cH3Ox	-npe.D_cH3Oxx*npe.grad_cH3Ox-npe.D_cH3Oxy*npe.grad_cH3Oy-npe.D_cH3Oxz*npe.grad_cH3Oz	mol/(m²·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	mol/(m²·s)	Diffusive flux, y component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	*npe.grad_cH3Oz				
npe.dflux_cH3Oz	-npe.D_cH3Ozx*npe.grad_cH3Ox-npe.D_cH3Ozy*npe.grad_cH3Oy-npe.D_cH3Ozz*npe.grad_cH3Oz	mol/(m²·s)	Diffusive flux, z component	Domain 1	
npe.grad_cH3Ox	cH3Ox	mol/m⁴	Concentration gradient, x component	Domain 1	
npe.grad_cH3Oy	cH3Oy	mol/m⁴	Concentration gradient, y component	Domain 1	
npe.grad_cH3Oz	0	mol/m⁴	Concentration gradient, z component	Domain 1	
npe.ctemp	-cH3O*npe.z_cH3O-cOH*npe.z_cOH-cTris*npe.z_cTris-cTrisH*npe.z_cTrisH	mol/m³	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/(m²·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cOHy	-npe.D_cOHyx*npe.grad_cOHx-npe.D_cOHyy*	mol/(m²·s)	Diffusive flux, y component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	npe.grad_cOHy-npe.D_cOHyz*npe.grad_cOHz				
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_cTrisx	-npe.D_cTrisxx*npe.grad_cTrisx-npe.D_cTrisxy*npe.grad_cTrisy-npe.D_cTrisxz*npe.grad_cTrisz	mol/(m²·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cTrisy	-npe.D_cTrisyx*npe.grad_cTrisx-npe.D_cTrisyy*npe.grad_cTrisy-npe.D_cTrisyz*npe.grad_cTrisz	mol/(m²·s)	Diffusive flux, y component	Domain 1	
npe.dflux_cTr	-	mol/(m	Diffusive flux,	Domain 1	

Name	Expression	Unit	Description	Selection	Details
isz	npe.D_cTriszx*npe.grad_cTrisx-npe.D_cTriszy*npe.grad_cTrisy-npe.D_cTriszz*npe.grad_cTrisz	²·s)	z component		
npe.grad_cTrisx	cTrisx	mol/m⁴	Concentration gradient, x component	Domain 1	
npe.grad_cTrisy	cTrisy	mol/m⁴	Concentration gradient, y component	Domain 1	
npe.grad_cTrisz	0	mol/m⁴	Concentration gradient, z component	Domain 1	
npe.dflux_cTrisHx	-npe.D_cTrisHxx*npe.grad_cTrisHx-npe.D_cTrisHxy*npe.grad_cTrisHy-npe.D_cTrisHxz*npe.grad_cTrisHz	mol/(m²·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cTrisHy	-npe.D_cTrisHyx*npe.grad_cTrisHx-npe.D_cTrisHyy*npe.grad_cTrisHy-npe.D_cTrisHyz*npe.grad_cTrisHz	mol/(m²·s)	Diffusive flux, y component	Domain 1	
npe.dflux_cTrisHz	-npe.D_cTrisHzx*npe.grad_cTrisHx-npe.D_cTrisHzy*npe.grad_cTrisHy-	mol/(m²·s)	Diffusive flux, z component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	npe.D_cTrisHzz*npe.grad_cTrisHz				
npe.grad_cTrisHx	cTrisHx	mol/m⁴	Concentration gradient, x component	Domain 1	
npe.grad_cTrisHy	cTrisHy	mol/m⁴	Concentration gradient, y component	Domain 1	
npe.grad_cTrisHz	0	mol/m⁴	Concentration gradient, z component	Domain 1	
npe.dflux_cClx	-npe.D_cClxx*npe.grad_cClx-npe.D_cClxy*npe.grad_cCly-npe.D_cClxz*npe.grad_cClz	mol/(m²·s)	Diffusive flux, x component	Domain 1	
npe.dflux_cCly	-npe.D_cClyx*npe.grad_cClx-npe.D_cClyy*npe.grad_cCly-npe.D_cClyz*npe.grad_cClz	mol/(m²·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/(m²·s)	Diffusive flux, z component	Domain 1	
npe.grad_cClx	d(cCl,x)	mol/m⁴	Concentration gradient, x component	Domain 1	
npe.grad_cCly	d(cCl,y)	mol/m⁴	Concentration gradient, y component	Domain 1	
npe.grad_cClz	0	mol/m⁴	Concentration gradient, z component	Domain 1	
npe.kappa0xx	cH3O*npe.um_cH3Oxx*(npe.	S/m	Electrolyte conductivity,	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	z_cH3O*F_const)^2+cOH*npe.um_cOHxx*(npe.z_cOH*F_const)^2+cTris*npe.um_cTrisxx*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHxx*(npe.z_cTrisH*F_const)^2+cCl*npe.um_cClxx*(npe.z_cCl*F_const)^2		xx component		
npe.kappa0yx	cH3O*npe.um_cH3Oyx*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHyx*(npe.z_cOH*F_const)^2+cTris*npe.um_cTrisyx*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHyx*(npe.z_cTrisH*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+cTris*npe.um_cTriszx*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHzx*(npe.z_cTrisH*F_const)^2+cCl*npe.um_cClzx*(np	S/m	Electrolyte conductivity, zx component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	e.z_cCl*F_const)^2				
npe.kappa0xy	cH3O*npe.um_cH3Oxy*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHxy*(npe.z_cOH*F_const)^2+cTris*npe.um_cTrisxy*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHxy*(npe.z_cTrisH*F_const)^2+cCl*npe.um_cClxy*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, xy component	Domain 1	+ operation
npe.kappa0yy	cH3O*npe.um_cH3Oyy*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHyy*(npe.z_cOH*F_const)^2+cTris*npe.um_cTrisyy*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHyy*(npe.z_cTrisH*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+cTris*npe.um_cTriszy*(npe.z_cTris*F_const)^2+c	S/m	Electrolyte conductivity, zy component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	TrisH*npe.um_cTrisHzy*(npe.z_cTrisH*F_const)^2+cCl*npe.um_cClzy*(npe.z_cCl*F_const)^2				
npe.kappa0xz	cH3O*npe.um_cH3Oxz*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHxz*(npe.z_cOH*F_const)^2+cTris*npe.um_cTrisxz*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHxz*(npe.z_cTrisH*F_const)^2+cCl*npe.um_cClxz*(npe.z_cCl*F_const)^2	S/m	Electrolyte conductivity, xz component	Domain 1	+ operation
npe.kappa0yz	cH3O*npe.um_cH3Oyz*(npe.z_cH3O*F_const)^2+cOH*npe.um_cOHyz*(npe.z_cOH*F_const)^2+cTris*npe.um_cTrisyz*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHyz*(npe.z_cTrisH*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*(	S/m	Electrolyte conductivity, zz component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	npe.z_cOH*F_const)^2+cTris*npe.um_cTriszz*(npe.z_cTris*F_const)^2+cTrisH*npe.um_cTrisHzz*(npe.z_cTrisH*F_const)^2+cCl*npe.um_cClzz*(npe.z_cCl*F_const)^2				
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 component	Domain 1	
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	

Name	Expression	Unit	Description	Selection	Details
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_cOHx-npe.D_cOHxy*npe.grad_cOHy-npe.D_cOHxz*npe.grad_cOHz+npe.z_cOH*F_const*cOH*(-npe.um_cOHxx*Vx-npe.um_cOHxy*Vy))+npe.z_cTris*(-npe.D_cTrisxx*npe.grad_cTrisx-npe.D_cTrisxy*npe.grad_cTrisy-npe.D_cTrisxz*npe.grad_cTrisz+npe.z_cTris*	A/m²	Current density, x component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	F_const*cTris*(-npe.um_cTrisxx*Vx-npe.um_cTrisxy*Vy))+npe.z_cTrisH*(-npe.D_cTrisHxx*npe.grad_cTrisHx-npe.D_cTrisHxy*npe.grad_cTrisHy-npe.D_cTrisHxz*npe.grad_cTrisHz+npe.z_cTrisH*F_const*cTrisH*(-npe.um_cTrisHxx*Vx-npe.um_cTrisHxy*Vy))+npe.z_cCl*(-npe.D_cClxx*npe.grad_cClx-npe.D_cClxy*npe.grad_cCly-npe.D_cClxz*npe.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*cH	A/m²	Current density, y component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	3O*(-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_cTris*(-npe.D_cTrisyx*npe.grad_cTrisx-npe.D_cTrisyy*npe.grad_cTrisy-npe.D_cTrisyz*npe.grad_cTrisz+npe.z_cTris*F_const*cTris*(-npe.um_cTrisyx*Vx-npe.um_cTrisyy*Vy))+npe.z_cTrisH*(-npe.D_cTrisHyx*npe.grad_cTrisHx-npe.D_cTrisHyy*npe.grad_cTrisHy-npe.D_cTrisHyz*npe.grad_cTrisHz+npe.z_cTrisH*F_const*				

Name	Expression	Unit	Description	Selection	Details
	cTrisH*(-npe.um_cTrisHyx*Vx-npe.um_cTrisHyy*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*cH3O*(-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*(-	A/m^2	Current density, z component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	npe.um_cOHzx*Vx-npe.um_cOHzy*Vy))+npe.z_cTris*(-npe.D_cTriszx*npe.grad_cTrisx-npe.D_cTriszy*npe.grad_cTrisy-npe.D_cTriszz*npe.grad_cTrisz+npe.z_cTris*F_const*cTris*(-npe.um_cTriszx*Vx-npe.um_cTriszy*Vy))+npe.z_cTrisH*(-npe.D_cTrisHzx*npe.grad_cTrisHx-npe.D_cTrisHzy*npe.grad_cTrisHy-npe.D_cTrisHzz*npe.grad_cTrisHz+npe.z_cTrisH*F_const*cTrisH*(-npe.um_cTrisHzx*Vx-npe.um_cTrisHzy*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*				

Name	Expression	Unit	Description	Selection	Details
	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-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*n	mol/(m³·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	pe.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_cTris	-npe.D_cTrisxx*cTrisxx-npe.D_cTrisxy*cTrisxy-npe.D_cTrisyx*cTrisyx-npe.D_cTrisyy*cTrisyy+d(cTris*(npe.u-npe.z_cTris*npe.um_cTrisxx*F_const*d(npe.V,x)-npe.z_cTris*np	mol/(m³·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	e.um_cTrisxy*F_const*d(npe.V,y)),x)+d(cTris*(npe.v-npe.z_cTris*npe.um_cTrisyx*F_const*d(npe.V,x)-npe.z_cTris*npe.um_cTrisyy*F_const*d(npe.V,y)),y)-npe.R_cTris				
npe.Res_cTrisH	-npe.D_cTrisHxx*cTrisHxx-npe.D_cTrisHxy*cTrisHxy-npe.D_cTrisHyx*cTrisHyx-npe.D_cTrisHyy*cTrisHyy+d(cTrisH*(npe.u-npe.z_cTrisH*npe.um_cTrisHxx*F_const*d(npe.V,x)-npe.z_cTrisH*npe.um_cTrisHxy*F_const*d(npe.V,y)),x)+d(cTrisH*(npe.v-npe.z_cTrisH*npe.um_cTrisHyx*F_const*d(npe.V,x)-npe.z_cTrisH*npe.um_cTrisHyy*F_const*d(npe.V,y)),y)-npe.R_cTrisH	mol/(m³·s)	Equation residual	Domain 1	

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
cH3O	Lagrange	mol/m³	Concentration	Spatial	Domain 1

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

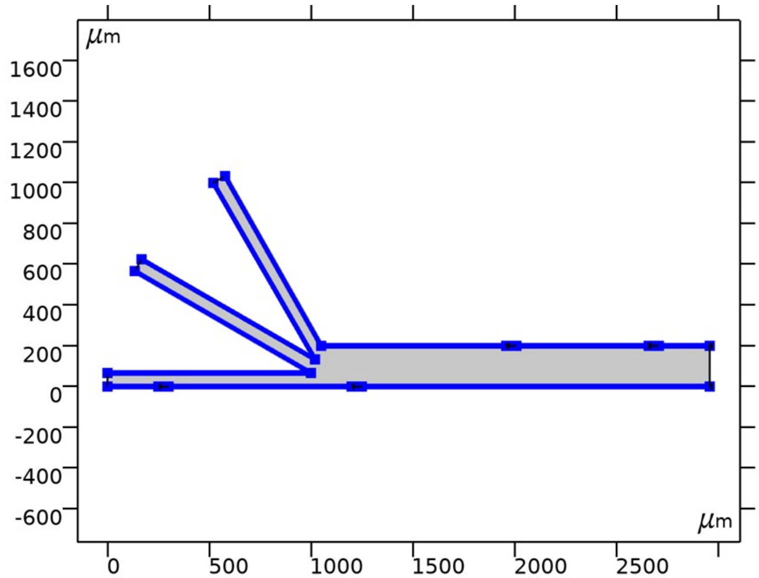
Weak expressions

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 1–19
cOH*(npe.u*test(cOHx)+npe.v*test(cOHy))*(isScalingSystemDomain==0)	4	Spatial	Domain 1
npe.cbf_cOH*test(cOH)	4	Spatial	Boundaries 1–19
cTris*(npe.u*test(cTrisx)+npe.v*test(cTrisy))*(isScalingSystemDomain==0)	4	Spatial	Domain 1
npe.cbf_cTris*test(cTris)	4	Spatial	Boundaries 1–19
cTrisH*(npe.u*test(cTrisHx)+npe.v*test(cTrisHy))*(isScalingSystemDomain==0)	4	Spatial	Domain 1
npe.cbf_cTrisH*test(cTrisH)	4	Spatial	Boundaries 1–19
npe.z_cH3O*F_const*cH3O*((-npe.um_cH3Oxx*d(npe.V,x)-npe.um_cH3Oxy*d(npe.	4	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
V,y))*test(cH3Ox)+(-npe.um_cH3Oyx*d(npe.V,x)-npe.um_cH3Oyy*d(npe.V,y))*test(cH3Oy))			
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_cTris*F_const*cTris*((-npe.um_cTrisxx*d(npe.V,x)-npe.um_cTrisxy*d(npe.V,y))*test(cTrisx)+(-npe.um_cTrisyx*d(npe.V,x)-npe.um_cTrisyy*d(npe.V,y))*test(cTrisy))	4	Spatial	Domain 1
npe.z_cTrisH*F_const*cTrisH*((-npe.um_cTrisHxx*d(npe.V,x)-npe.um_cTrisHxy*d(npe.V,y))*test(cTrisHx)+(-npe.um_cTrisHyx*d(npe.V,x)-npe.um_cTrisHyy*d(npe.V,y))*test(cTrisHy))	4	Spatial	Domain 1
npe.dflux_cH3Ox*test(cH3Ox)+npe.dflux_cH3Oy*test(cH3Oy)	4	Spatial	Domain 1
npe.dflux_cOHx*test(cOHx)+npe.dflux_cOHy*test(cOHy)	4	Spatial	Domain 1
npe.dflux_cTrisx*test(cTrisx)+npe.dflux_cTrisy*test(cTrisy)	4	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
npe.dflux_cTrisHx*test(cTrisHx)+npe.dflux_cTrisHy*test(cTrisHy)	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	Boundaries 2–3, 5–6, 8, 10–12, 14, 16, 18

EQUATIONS

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

Convection

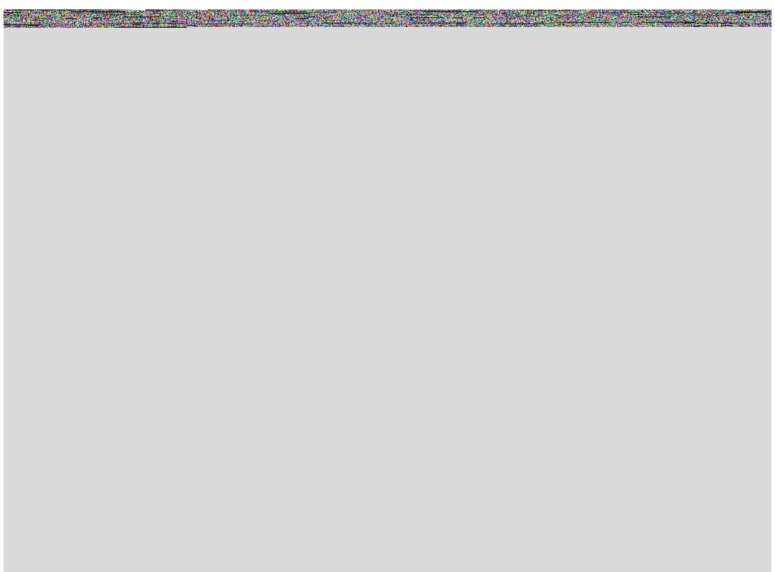
SETTINGS

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, 5–6, 8, 10–12, 14, 16, 18
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, 5–6, 8, 10–12, 14, 16, 18
npe.cbf_cTris	cTris*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 2–3, 5–6, 8, 10–12, 14, 16, 18
npe.cbf_cTrisH	cTrisH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundaries 2–3, 5–6, 8, 10–12, 14, 16, 18

2.4.5 Electric Insulation 1



Electric Insulation 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2–3, 5–6, 8, 10–12, 14, 16, 18

EQUATIONS

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

2.4.6 Initial Values 1

Initial Values 1

SELECTION

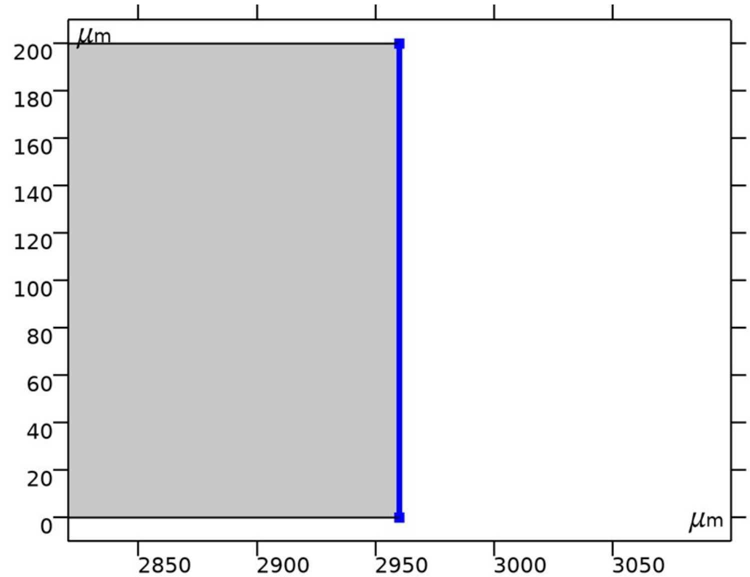
Geometric entity level	Domain
Selection	Domain 1

Initial values

SETTINGS

Description	Value
Concentration	{cH3O0, cOH0, cTris0, cTrisH0, 0}
Electric potential	0

2.4.7 Inflow 1



Inflow 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 19

EQUATIONS

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

Concentration

SETTINGS

Description	Value
Concentration	{cH3O0, cOH0, cTris0, cTrisH0, 0}

Boundary condition type

SETTINGS

Description	Value
Boundary condition type	Concentration constraint

Constraint settings

SETTINGS

Description	Value

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

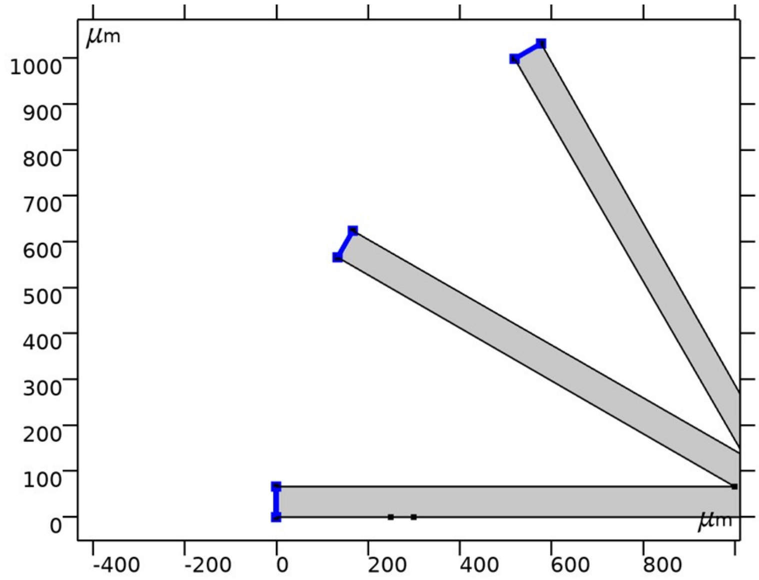
Variables

Name	Expression	Unit	Description	Selection	Details
npe.c0_cH3O	cH3O0	mol/m³	Concentration	Boundary 19	+ operation
npe.c0_cOH	cOH0	mol/m³	Concentration	Boundary 19	+ operation
npe.c0_cTris	cTris0	mol/m³	Concentration	Boundary 19	+ operation
npe.c0_cTrisH	cTrisH0	mol/m³	Concentration	Boundary 19	+ operation

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-cH3O+npe.c0_cH3O	-test(cH3O)	Lagrange (Quadratic)	Boundary 19	Elemental
-cOH+npe.c0_cOH	-test(cOH)	Lagrange (Quadratic)	Boundary 19	Elemental
-cTris+npe.c0_cTris	-test(cTris)	Lagrange (Quadratic)	Boundary 19	Elemental
-cTrisH+npe.c0_cTrisH	-test(cTrisH)	Lagrange (Quadratic)	Boundary 19	Elemental

2.4.8 Outflow 1



Outflow 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1, 4, 9

EQUATIONS

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

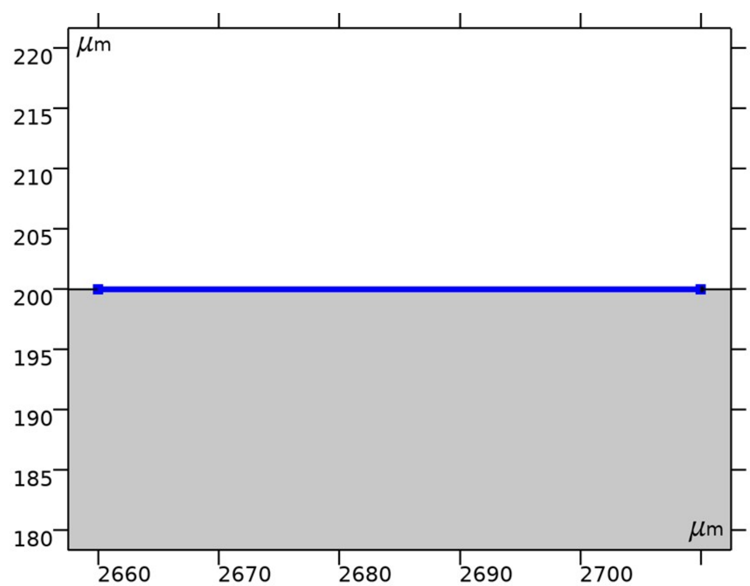
Weak expressions

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, 4, 9
-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*me	4	Spatial	Boundaries 1, 4, 9

Weak expression	Integration order	Integration frame	Selection
an(d(npe.V,x))+npe.um_cH3Ozy*mean(d(npe.V,y))+npe.um_cH3Ozz*mean(0)))*test(cH3O)			
-(npe.nx*npe.u+npe.ny*npe.v+npe.nz*npe.w)*cOH*test(cOH)	4	Spatial	Boundaries 1, 4, 9
-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.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)	4	Spatial	Boundaries 1, 4, 9
-(npe.nx*npe.u+npe.ny*npe.v+npe.nz*npe.w)*cTris*test(cTris)	4	Spatial	Boundaries 1, 4, 9
-npe.z_cTris*F_const*cTris*(-npe.nx*(npe.um_cTrisxx*mean(d(npe.V,x))+npe.um_cTrisxy*mean(d(npe.V,y))+npe.um_cTrisxz*mean(0))-npe.ny*(npe.um_cTrisyx*mean(d(npe.V,x))+npe.um_cTrisyy*mean(d(npe.V,y))+npe.um_cTrisyz*mean(0))-npe.nz*(npe.um_cTriszx*mean(d(npe.V,x))+npe.um_cTriszy*mean(d(npe.V,y))+npe.um_cTriszz*mean(0)))*test(cTris)	4	Spatial	Boundaries 1, 4, 9
-(npe.nx*npe.u+npe.ny*npe.v+npe.nz*npe.w)*cTrisH*test(cTrisH)	4	Spatial	Boundaries 1, 4, 9
-npe.z_cTrisH*F_const*cTrisH*	4	Spatial	Boundaries 1, 4, 9

Weak expression	Integration order	Integration frame	Selection
(-npe.nx*(npe.um_cTrisHxx*mean(d(npe.V,x))+npe.um_cTrisHxy*mean(d(npe.V,y))+npe.um_cTrisHxz*mean(0))-npe.ny*(npe.um_cTrisHyx*mean(d(npe.V,x))+npe.um_cTrisHyy*mean(d(npe.V,y))+npe.um_cTrisHyz*mean(0))-npe.nz*(npe.um_cTrisHzx*mean(d(npe.V,x))+npe.um_cTrisHzy*mean(d(npe.V,y))+npe.um_cTrisHzz*mean(0)))*test(cTrisH)			

2.4.9 Flux 1



Flux 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 17

EQUATIONS

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

Inward flux

SETTINGS

Description	Value
Species cH3O	Off
Species cOH	On
Species cTris	Off
Species cTrisH	Off
Species cCl	Off

Convection

SETTINGS

Description	Value
Include	Off

Variables

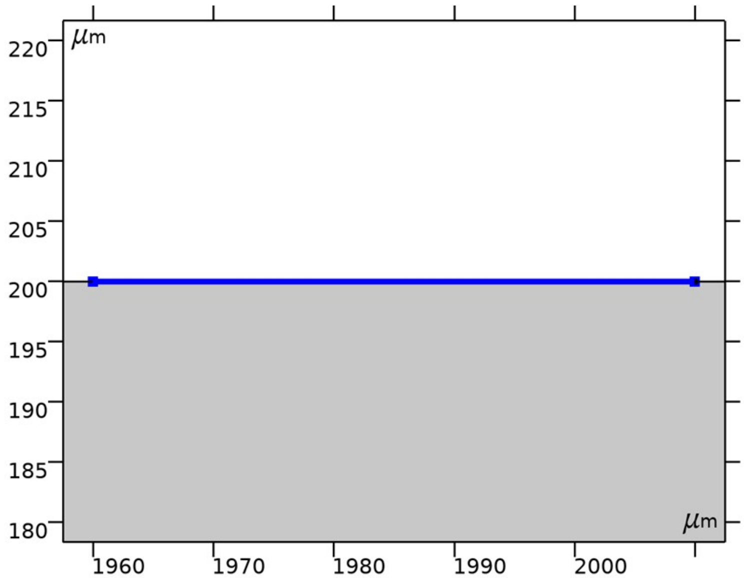
Name	Expression	Unit	Description	Selection
npe.cbf_cH3O	cH3O*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 17
npe.cbf_cOH	cOH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 17
npe.cbf_cTris	cTris*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 17
npe.cbf_cTrisH	cTrisH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 17

Weak expressions

Weak expression	Integration order	Integration frame	Selection
0	4	Spatial	Boundary 17
fssBPEvarcat1*test(cOH)	4	Spatial	Boundary 17
0	4	Spatial	Boundary 17
0	4	Spatial	Boundary

Weak expression	Integration order	Integration frame	Selection
			17

2.4.10 Flux 2



Flux 2

SELECTION

Geometric entity level	Boundary
Selection	Boundary 15

EQUATIONS

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

Inward flux

SETTINGS

Description	Value
Species cH3O	On
Species cOH	Off
Species cTris	Off
Species cTrisH	Off
Species cCl	Off
Inward flux	{fssBPEvaran1, 0, 0, 0, 0}

Convection

SETTINGS

Description	Value
Include	Off

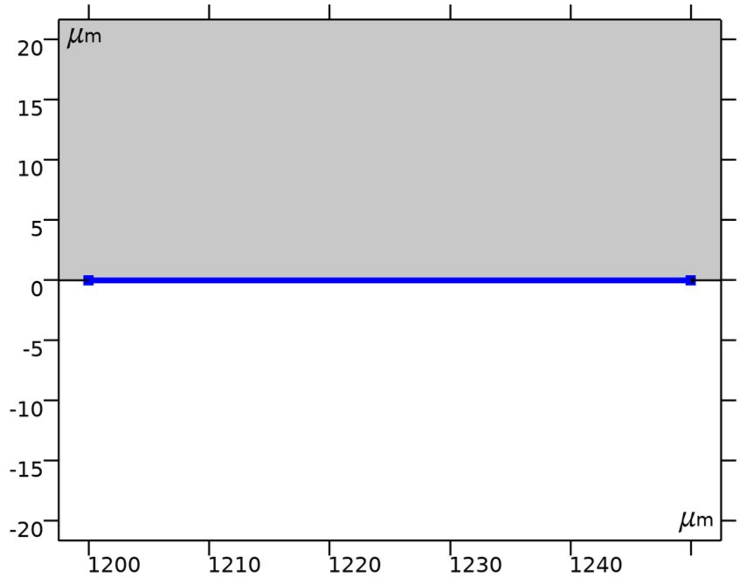
Variables

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	Boundary 15
npe.cbf_cOH	cOH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 15
npe.cbf_cTris	cTris*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 15
npe.cbf_cTrisH	cTrisH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	mol/(m²·s)	Convective boundary flux	Boundary 15

Weak expressions

Weak expression	Integration order	Integration frame	Selection
fssBPEvaran1*test(cH3O)	4	Spatial	Boundary 15
0	4	Spatial	Boundary 15
0	4	Spatial	Boundary 15
0	4	Spatial	Boundary 15

2.4.11 Flux 3



Flux 3

SELECTION

Geometric entity level	Boundary
Selection	Boundary 13

EQUATIONS

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

Inward flux

SETTINGS

Description	**Value**
Species cH3O	Off
Species cOH	On
Species cTris	Off
Species cTrisH	Off
Species cCl	Off

Convection

SETTINGS

Description	**Value**
Include	Off

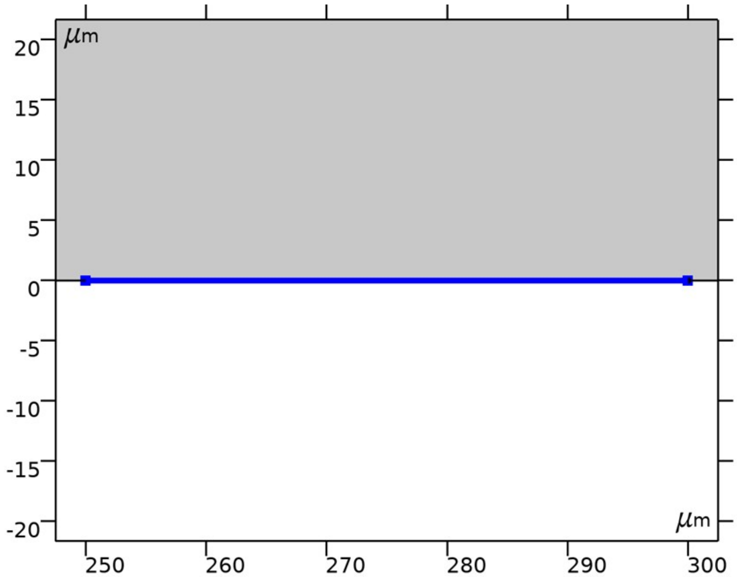
Variables

Name	Expression	Unit	Description	Selection
npe.cbf_cH3O	cH3O*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 13
npe.cbf_cOH	cOH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 13
npe.cbf_cTris	cTris*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 13
npe.cbf_cTrisH	cTrisH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 13

Weak expressions

Weak expression	Integration order	Integration frame	Selection
0	4	Spatial	Boundary 13
fssBPEvarcat2*test(cOH)	4	Spatial	Boundary 13
0	4	Spatial	Boundary 13
0	4	Spatial	Boundary 13

2.4.12 Flux 4



Flux 4

SELECTION

Geometric entity level	Boundary
Selection	Boundary 7

EQUATIONS

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

Inward flux

SETTINGS

Description	**Value**
Species cH3O	On
Species cOH	Off
Species cTris	Off
Species cTrisH	Off
Species cCl	Off
Inward flux	{fssBPEvaran2, 0, 0, 0, 0}

Convection

SETTINGS

Description	**Value**
Include	Off

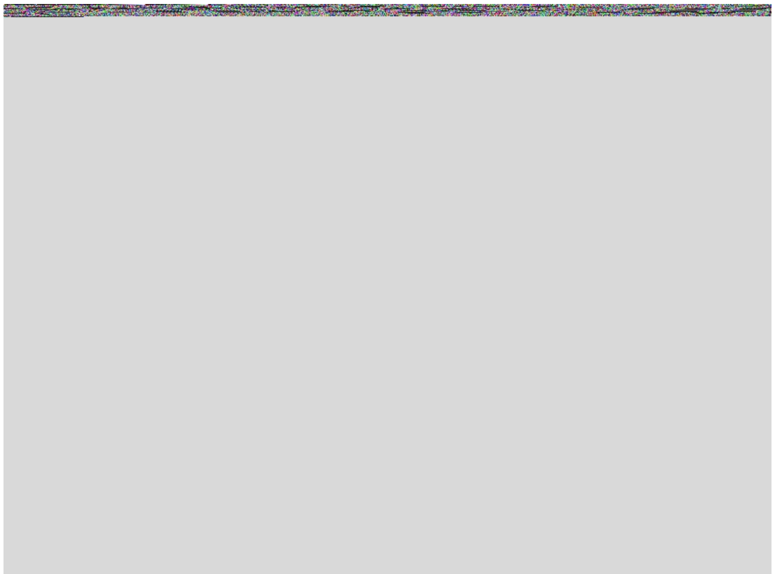
Variables

Name	Expression	Unit	Description	Selection
npe.cbf_cH3O	cH3O*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 7
npe.cbf_cOH	cOH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 7
npe.cbf_cTris	cTris*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 7
npe.cbf_cTrisH	cTrisH*(-npe.u*npe.nxmesh-npe.v*npe.nymesh-npe.w*npe.nzmesh)	$mol/(m^2 \cdot s)$	Convective boundary flux	Boundary 7

Weak expressions

Weak expression	Integration order	Integration frame	Selection
fssBPEvaran2*test(cH3O)	4	Spatial	Boundary 7
0	4	Spatial	Boundary 7
0	4	Spatial	Boundary 7
0	4	Spatial	Boundary 7

2.4.13 Current Density 1



Current Density 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 19

EQUATIONS

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

Inward current density

SETTINGS

Description	Value
Inward current density	jssTOT

Variables

Name	Expression	Unit	Description	Selection
npe.i0_cdens1	jssTOT	A/m^2	Inward current density	Boundary 19

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.i0_cdens1*test(V)	4	Spatial	Boundary 19

2.4.14 Current Density 2

Current Density 2

SELECTION

Geometric entity level	Boundary
Selection	Boundary 17

EQUATIONS

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

Inward current density

SETTINGS

Description	Value
Inward current density	-jssBPEvarcat1

Variables

Name	Expression	Unit	Description	Selection
npe.i0_cdens2	-jssBPEvarcat1	A/m²	Inward current density	Boundary 17

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.i0_cdens2*test(V)	4	Spatial	Boundary 17

2.4.15 Current Density 3

Current Density 3

SELECTION

Geometric entity level	Boundary
Selection	Boundary 15

EQUATIONS

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

Inward current density

SETTINGS

Description	Value
Inward current density	jssBPEvaran 1

Variables

Name	Expression	Unit	Description	Selection
npe.i0_cdens3	jssBPEvaran 1	A/m^2	Inward current density	Boundary 15

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.i0_cdens3*test(V)	4	Spatial	Boundary 15

2.4.16 Current Density 4

Current Density 4

SELECTION

Geometric entity level	Boundary
Selection	Boundary 13

EQUATIONS

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

Inward current density

SETTINGS

Description	Value
Inward current density	-jssBPEvarcat2

Variables

Name	Expression	Unit	Description	Selection
npe.i0_cdens4	-jssBPEvarcat2	A/m²	Inward current density	Boundary 13

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.i0_cdens4*test(V)	4	Spatial	Boundary 13

2.4.17 Current Density 5

Current Density 5

SELECTION

Geometric entity level	Boundary
Selection	Boundary 7

EQUATIONS

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

Inward current density

SETTINGS

Description	Value
Inward current density	jssBPEvaran 2

Variables

Name	Expression	Unit	Description	Selection
npe.i0_cdens5	jssBPEvaran 2	A/m^2	Inward current density	Boundary 7

Weak expressions

Weak expression	Integration order	Integration frame	Selection
npe.i0_cdens5*test(V)	4	Spatial	Boundary 7

2.4.18 Electric Potential 1

Electric Potential 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1, 4, 9

EQUATIONS

$$V = V_0$$

Constraint settings

SETTINGS

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

Variables

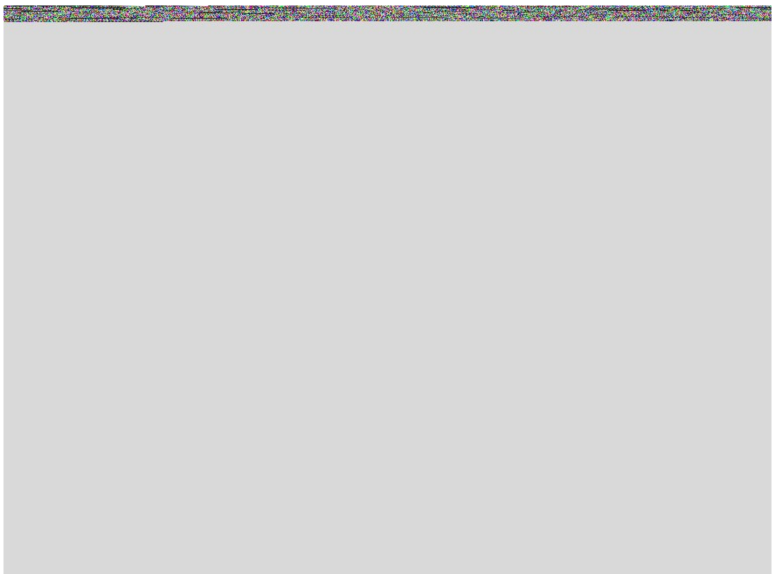
Name	Expression	Unit	Description	Selection
npe.V0	0	V	Electric potential	Boundaries 1, 4, 9

Constraints

Constraint	Constraint force	Shape function	Selection	Details

Constrain t	Constraint force	Shape function	Selection	Details
npe.V0-V	test(npe.V0-V)	Lagrange (Quadratic)	Boundaries 1, 4, 9	Elemental

2.4.19 Reactions 1



Reactions 1

SELECTION

Geometric entity level	Domain
Selection	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 + kfneut*cTrisH - kbneut*cTris*cH3O
Total rate expression	User defined
Total rate expression	kfhydro*cH2O0 - kbhydro*cH3O*cOH + kfneut*cTris -

Description	Value
	kbneut*cTrisH*cOH
Total rate expression	User defined
Total rate expression	-kfneut*cTris + kbneut*cTrisH*cOH + kfneut*cTrisH - kbneut*cTris*cH3O
Total rate expression	User defined
Total rate expression	kfneut*cTris - kbneut*cTrisH*cOH - kfneut*cTrisH + kbneut*cTris*cH3O
Total rate expression	User defined
Total rate expression	0

Variables

Name	Expression	Unit	Description	Selection	Details
npe.R_cH3O	npe.reac1.R_cH3O	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	+ operation
npe.R_cOH	npe.reac1.R_cOH	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	+ operation
npe.R_cTris	npe.reac1.R_cTris	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	+ operation
npe.R_cTrisH	npe.reac1.R_cTrisH	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	+ operation
npe.R_cCl	npe.reac1.R_cCl	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	+ operation
npe.reac1.R_cH3O	model.input.R_cH3O	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	Meta
npe.reac1.R_cOH	model.input.R_cOH	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	Meta
npe.reac1.R_cTris	model.input.R_cTris	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	Meta
npe.reac1.R_cTrisH	model.input.R_cTrisH	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	Meta
npe.reac1.R_cCl	model.input.R_cCl	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	Meta

Weak expressions

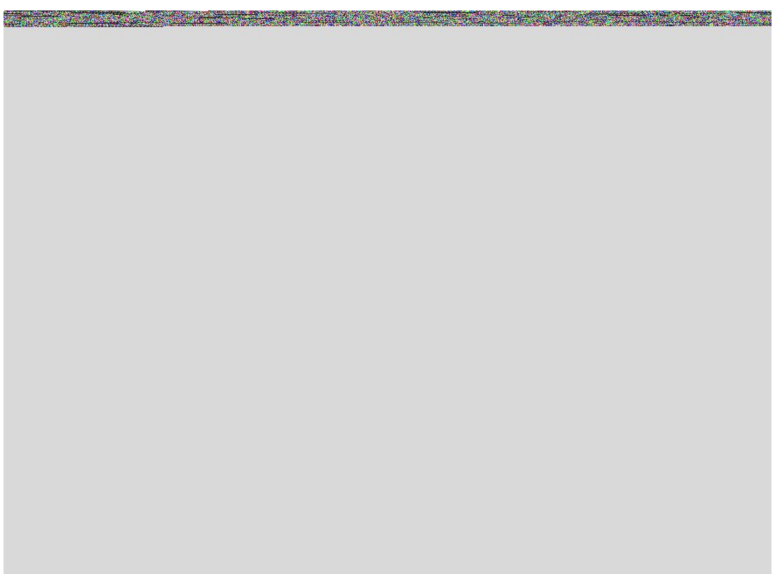
Weak expression	Integration order	Integration frame	Selection
npe.reac1.R_cH3O*test(cH3O)	4	Spatial	Domain 1
F_const*npe.reac1.R_cH3O*npe.z_cH3O*test(V)	4	Spatial	Domain 1

Weak expression	**Integration order**	**Integration frame**	**Selection**
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_cTris*test(cTris)	4	Spatial	Domain 1
F_const*npe.reac1.R_cTris*npe.z_cTris*test(V)	4	Spatial	Domain 1
npe.reac1.R_cTrisH*test(cTrisH)	4	Spatial	Domain 1
F_const*npe.reac1.R_cTrisH*npe.z_cTrisH*test(V)	4	Spatial	Domain 1
F_const*npe.reac1.R_cCl*npe.z_cCl*test(V)	4	Spatial	Domain 1

2.5 CREEPING FLOW

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module



Creeping Flow

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

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

2.5.1 Interface settings

Discretization

SETTINGS

Description	Value
Discretization of fluids	P1 + P1

Physical model

SETTINGS

Description	Value
Neglect inertial term (Stokes flow)	On
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

Consistent stabilization

SETTINGS

Description	Value
Streamline diffusion	On
Crosswind diffusion	Off

Inconsistent stabilization

SETTINGS

Description	Value
Isotropic diffusion	Off

Advanced settings

SETTINGS

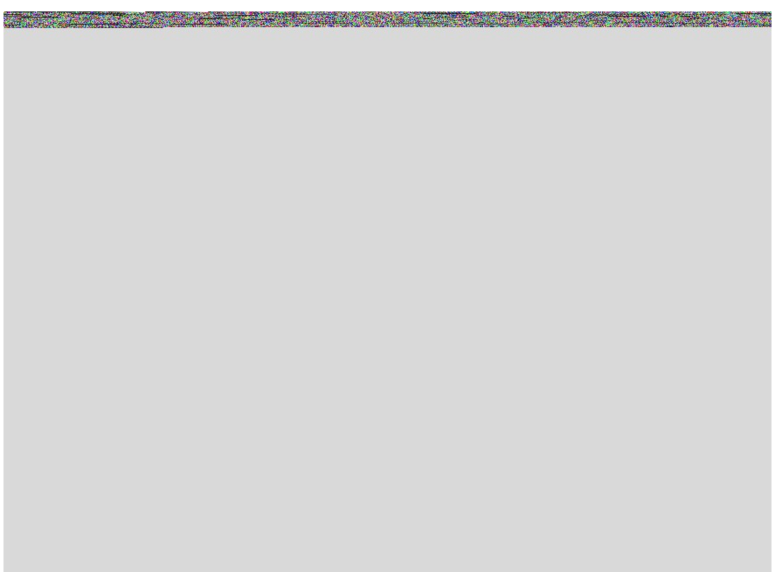
Description	Value
Use pseudo time stepping for stationary equation form	Automatic from physics
CFL number expression	Automatic

2.5.2 Variables

Name	Expression	Unit	Description	Selection	Details
spf.Tref	model.input.Tref	K	Reference 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 1–19	
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	2.58194000000000006E-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	Hz	Inverse time step	Domain 1	

Name	Expression	Unit	Descriptio n	Selection	Details
	^2)				
spf.tsti	nojac(spf.time_step_inv/spf.locCFL)	1/s	Help variable	Domain 1	
spf.nx	dnx	1	Normal vector, x component	Boundaries 1–19	
spf.ny	dny	1	Normal vector, y component	Boundaries 1–19	
spf.nz	0	1	Normal vector, z component	Boundaries 1–19	
spf.nxmesh	dnxmesh	1	Normal vector, x component	Boundaries 1–19	
spf.nymesh	dnymesh	1	Normal vector, y component	Boundaries 1–19	
spf.nzmesh	0	1	Normal vector, z component	Boundaries 1–19	

2.5.3 Fluid Properties 1



Fluid Properties 1

SELECTION

Geometric entity level	Domain
Selection	Domain 1

EQUATIONS

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

Fluid properties

SETTINGS

Description	Value
Density	From material
Dynamic viscosity	From material

Model input

SETTINGS

Description	Value
Temperature	Common model input

PROPERTIES FROM MATERIAL

Property	Material	Property group
Density	Water	Basic
Dynamic viscosity	Water	Basic

Variables

Name	Expression	Unit	Description	Selection	Details
spf.rho	subst(material.rho,spf.fp1.minput_temperature,spf.Trho,spf.fp1.minput_pressure,spf.prho)	kg/m³	Density	Domain 1	Meta
spf.mu	material.mu	Pa·s	Dynamic viscosity	Domain 1	Meta
spf.Trho	spf.Tref	K	Temperatur	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			e for density evaluation		
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/m^3	Reference density	Domain 1	Meta
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	

Name	Expression	Unit	Description	Selection	Details
spf.srijmeanxx	0.5*root.comp1.spf.elemint(2*ux)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, xx component	Domain 1	
spf.srijmeanyx	0.5*root.comp1.spf.elemint(vx+uy)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, yx component	Domain 1	
spf.srijmeanzx	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zx component	Domain 1	
spf.srijmeanxy	0.5*root.comp1.spf.elemint(uy+vx)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, xy component	Domain 1	
spf.srijmeanyy	0.5*root.comp1.spf.elemint(2*vy)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, yy component	Domain 1	
spf.srijmeanzy	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zy component	Domain 1	
spf.srijmeanxz	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, xz component	Domain 1	
spf.srijmeanyz	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, yz component	Domain 1	
spf.srijmeanzz	0.5*root.comp1.spf.elemint(0)/root.comp1.spf.elemint(1)	1/s	Strain rate tensor, zz component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
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, xy component	Domain 1	
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^	1/s	Shear rate	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	2+2*spf.srijzy^2+2*spf.srijzz^2+eps)				
spf.divu	ux+vy	1/s	Divergence of velocity field	Domain 1	
spf.Fx	0	N/m³	Volume force, x component	Domain 1	+ operation
spf.Fy	0	N/m³	Volume force, y component	Domain 1	+ operation
spf.Fz	0	N/m³	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	m²/s	Kinematic viscosity	Domain 1	
spf.betaT	0	1/Pa	Isothermal compressibility coefficient	Domain 1	

Name	Expression	Unit	Description	Selection	Details
spf.Qm	0	kg/(m³·s)	Source term	Domain 1	+ operation
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 1–19	+ operation
spf.T_stressy	spf.K_stressy-p*spf.nymesh	N/m²	Total stress, y component	Boundaries 1–19	+ operation
spf.T_stressz	spf.K_stressz-p*spf.nzmesh	N/m²	Total stress, z component	Boundaries 1–19	+ operation
spf.K_stressx	spf.mu_eff*(2*ux*spf.nxmesh+(uy+vx)*spf.nymesh)	N/m²	Viscous stress, x component	Boundaries 1–19	+ operation
spf.K_stressy	spf.mu_eff*((vx+uy)*spf.nxmesh+2*vy*spf.nymesh)	N/m²	Viscous stress, y component	Boundaries 1–19	+ operation
spf.K_stressz	0	N/m²	Viscous stress, z component	Boundaries 1–19	+ operation
spf.K_stress_tensorxx	2*spf.mu_eff*ux	N/m²	Viscous stress tensor, xx component	Domain 1	+ operation
spf.K_stress_tensoryx	spf.mu_eff*(vx+uy)	N/m²	Viscous stress tensor, yx	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			component		
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_testzx	0	N/m²	Viscous stress tensor test, zx component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
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	-d(x,TIME)	m/s	Upwind term, x component	Domain 1	+ operation
spf.upwind_helpy	-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 tensor, xx component	Domain 1	+ operation
spf.tau_vdyx	2*spf.mu*spf.	Pa	Viscous	Domain 1	+ operati

Name	Expression	Unit	Description	Selection	Details
	srijyx		stress tensor, yx component		on
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/m³	Viscous dissipation	Domain 1	+ operation
spf.epsilon_p	1	1	Porosity	Domain 1	
spf.Fst_tensorxx	0	N/m²	Surface tension force, xx component	Domain 1	+ operation
spf.Fst_tensoryx	0	N/m²	Surface tension	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			force, yx component		
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-(d(2*ux,x)+d(uy+vx,y))*spf.mu-spf.Fx	N/m³	Equation residual	Domain 1	
spf.res_v	py-(d(vx+uy,x)+d(2*vy,y))*spf.mu-spf.Fy	N/m³	Equation residual	Domain 1	
spf.res_p	spf.rho*spf.di	kg/(m³·s)	Pressure	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	vu		equation residual		

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.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	Domain 1

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

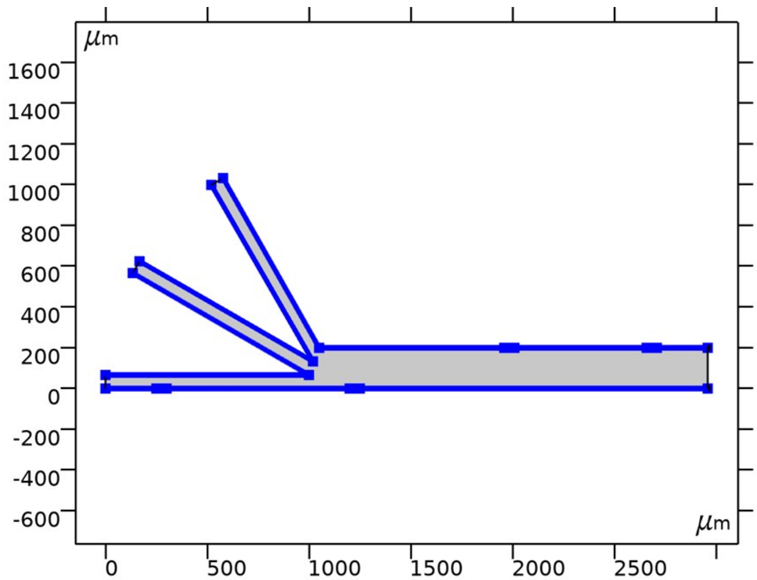
Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection
spf.u_initx	0	m/s	Velocity field, x component	Domain 1

Name	Expression	Unit	Description	Selection
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	Boundaries 2–3, 5–8, 10–18

EQUATIONS

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

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

Boundary condition

SETTINGS

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

Description	Value
Zeta potential	-(0.050)[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 2–3, 5–8, 10–18	
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 2–3, 5–8, 10–18	
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 2–3, 5–8, 10–18	
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 2–3, 5–8, 10–18	
spf.KStressTestn_avy	spf.K_stress_tensor_testyx*spf.nx	N/m²	Average viscous	Boundaries 2–3, 5–8,	

Name	Expression	Unit	Description	Selection	Details
	mesh+spf.K_stress_tensor_testyy*spf.nymesh+spf.K_stress_tensor_testyz*spf.nzmesh		stress, y component	10–18	
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 2–3, 5–8, 10–18	
spf.ujumpx	spf.u_herex-spf.u_therex	m/s	Velocity jump, x component	Boundaries 2–3, 5–8, 10–18	
spf.ujumpy	spf.u_herey-spf.u_therey	m/s	Velocity jump, y component	Boundaries 2–3, 5–8, 10–18	
spf.ujumpz	spf.u_herez-spf.u_therez	m/s	Velocity jump, z component	Boundaries 2–3, 5–8, 10–18	
spf.meshVol	meshvol_spatial	m		Boundaries 2–3, 5–8, 10–18	
spf.meshVolInt	down(meshvol_spatial)	m^2	Volume of interior mesh element	Boundaries 2–3, 5–8, 10–18	
spf.c_here	24*nojac(down(spf.mu))*spf.meshVol/spf.meshVolInt	1	Intermediate variable	Boundaries 2–3, 5–8, 10–18	
spf.sigma_dg_ns	4*spf.c_here	Pa·s/m		Boundaries 2–3, 5–8, 10–18	
spf.rhoFace	down(spf.rho)	kg/m^3	Density face value	Boundaries 2–3, 5–8, 10–18	
spf.umxTnFace	(spf.upwind_helpx*spf.nxmesh+spf.upwind_helpy*spf.nymesh+s	m/s	Relative velocity on face	Boundaries 2–3, 5–8, 10–18	

Name	Expression	Unit	Description	Selection	Details
	pf.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 2–3, 5–8, 10–18	
spf.zeta	(-0.05)[V]	V	Zeta potential	Boundaries 2–3, 5–8, 10–18	
spf.epsilonr	80	1	Relative permittivity	Boundaries 2–3, 5–8, 10–18	
spf.ubndx	spf.ueox	m/s	Velocity at boundary, x component	Boundaries 2–3, 5–8, 10–18	+ operation
spf.ubndy	spf.ueoy	m/s	Velocity at boundary, y component	Boundaries 2–3, 5–8, 10–18	+ operation
spf.ubndz	spf.ueoz	m/s	Velocity at boundary, z component	Boundaries 2–3, 5–8, 10–18	+ operation
spf.uLeakagex	0	m/s	Leakage velocity, x component	Boundaries 2–3, 5–8, 10–18	+ operation
spf.uLeakagey	0	m/s	Leakage velocity, y component	Boundaries 2–3, 5–8, 10–18	+ operation
spf.uLeakagez	0	m/s	Leakage velocity, z component	Boundaries 2–3, 5–8, 10–18	+ operation
spf.Ex	model.input.E1	V/m	Electric field, x component	Boundaries 2–3, 5–8, 10–18	Meta
spf.Ey	model.input.E2	V/m	Electric field,	Boundarie	Meta

Name	Expression	Unit	Description	Selection	Details
			y component	s 2–3, 5–8, 10–18	
spf.Ez	model.input.E3	V/m	Electric field, z component	Boundaries 2–3, 5–8, 10–18	Meta
spf.mueo	-spf.zeta*epsilon0_const*spf.epsilonr/spf.mu	$m^2/(V\cdot s)$	Electroosmotic mobility	Boundaries 2–3, 5–8, 10–18	
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 2–3, 5–8, 10–18	
spf.ueoy	(spf.Ey-spf.nymesh*(spf.nxmesh*spf.Ex+spf.nymesh*spf.Ey+spf.nzmesh*spf.Ez))*spf.mueo	m/s	Electroosmotic velocity, y component	Boundaries 2–3, 5–8, 10–18	
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 2–3, 5–8, 10–18	
spf.u_herex	u	m/s	Intermediate variable, x component	Boundaries 2–3, 5–8, 10–18	
spf.u_herey	v	m/s	Intermediate variable, y component	Boundaries 2–3, 5–8, 10–18	
spf.u_herez	0	m/s	Intermediate variable, z component	Boundaries 2–3, 5–8, 10–18	
spf.u_therex	spf.ubndx+spf.uLeakagex	m/s	Intermediate variable, x component	Boundaries 2–3, 5–8, 10–18	
spf.u_therey	spf.ubndy+spf.uLeakagey	m/s	Intermediate variable, y	Boundaries 2–3, 5–8,	

Name	Expression	Unit	Description	Selection	Details
			component	10–18	
spf.u_therez	spf.ubndz+spf.uLeakagez	m/s	Intermediate variable, z component	Boundaries 2–3, 5–8, 10–18	
spf.contCoeffFace	down(spf.contCoeff)	kg/m^3	Help variable	Boundaries 2–3, 5–8, 10–18	
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 2–3, 5–8, 10–18	
spf.pFace	p	Pa	Pressure face value	Boundaries 2–3, 5–8, 10–18	
spf.consFlux	spf.pFace*(-test(spf.u_herex)*spf.nxmesh-test(spf.u_herey)*spf.nymesh-test(spf.u_herez)*spf.nzmesh)	W/m^2	Conservative flux	Boundaries 2–3, 5–8, 10–18	+ operation

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 2–3, 5–8, 10–18

2.5.6 Inlet 1

Inlet 1

SELECTION

Geometric entity level	Boundary
Selection	Boundary 19

EQUATIONS

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

$$\hat{p}_0 \geq p_0, \quad \mathbf{u}\cdot\mathbf{t} = 0$$

Boundary condition

SETTINGS

Description	**Value**
Boundary condition	Pressure

Pressure conditions

SETTINGS

Description	**Value**
Pressure	0
Suppress backflow	On
Flow direction	Normal flow

Constraint settings

SETTINGS

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

Variables

Name	Expression	Unit	Description	Selection
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 19
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 19
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	Boundary 19
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 19
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 19
spf.KStressTestn_avz	spf.K_stress_tensor_testzx*spf.nxmes	N/m²	Average viscous	Boundary 19

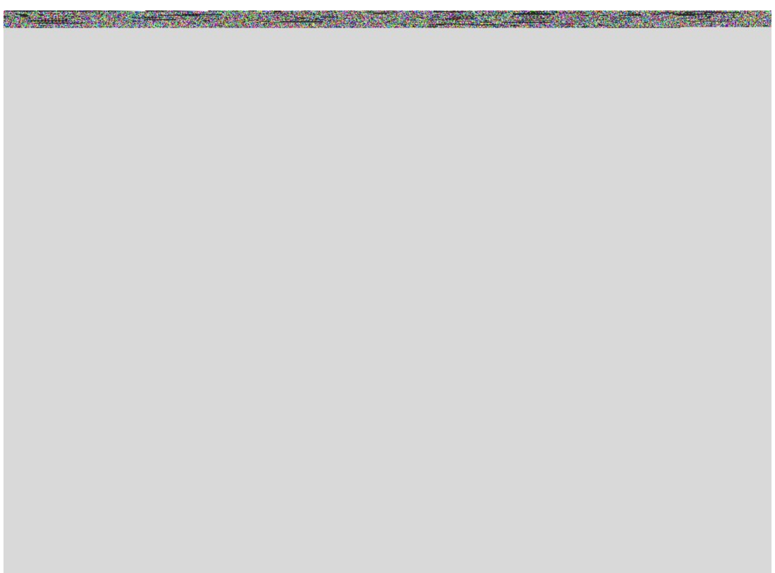
Name	Expression	Unit	Description	Selection
	h+spf.K_stress_tensor_testzy*spf.nymesh+spf.K_stress_tensor_testzz*spf.nzmesh		stress, z component	
spf.ujumpx	spf.ut_herex-spf.ut_therex	m/s	Velocity jump, x component	Boundary 19
spf.ujumpy	spf.ut_herey-spf.ut_therey	m/s	Velocity jump, y component	Boundary 19
spf.ujumpz	spf.ut_herez-spf.ut_therez	m/s	Velocity jump, z component	Boundary 19
spf.meshVol	meshvol_spatial	m		Boundary 19
spf.meshVolInt	down(meshvol_spatial)	m²	Volume of interior mesh element	Boundary 19
spf.c_here	96/spf.epsilon_p	1	Intermediate variable	Boundary 19
spf.sigma_dg_ns	4*spf.ct_here	Pa·s/m		Boundary 19
spf.rhoFace	down(spf.rho)	kg/m³	Density face value	Boundary 19
spf.umxTnFace	spf.upwind_helpx*spf.nxmesh+spf.upwind_helpy*spf.nymesh+spf.upwind_helpz*spf.nzmesh	m/s	Relative velocity on face	Boundary 19
spf.upwind_ns	spf.backflowPenaltyConv*spf.uNormal	Pa	Upwind term	Boundary 19
spf.p0	0	Pa	Pressure	Boundary 19
spf.f0	spf.p0+spf.uNormal*(spf.backflowPenaltyDiff+spf.backflowPenaltyConv)*(spf.uNormal>0)	N/m²	Normal stress	Boundary 19
spf.un_here	u*nojac(spf.nxmes	m/s	Intermediat	Boundary

Name	Expression	Unit	Description	Selection
	h)+v*nojac(spf.ny mesh)		e variable	19
spf.ut_herex	u- spf.un_here*nojac(spf.nxmesh)	m/s	Intermediat e variable, x component	Boundary 19
spf.ut_herey	v- spf.un_here*nojac(spf.nymesh)	m/s	Intermediat e variable, y component	Boundary 19
spf.ut_herez	- spf.un_here*nojac(spf.nzmesh)	m/s	Intermediat e variable, z component	Boundary 19
spf.un_there	0	m/s	Intermediat e variable	Boundary 19
spf.ut_therex	- spf.un_there*nojac (spf.nxmesh)	m/s	Intermediat e variable, x component	Boundary 19
spf.ut_therey	- spf.un_there*nojac (spf.nymesh)	m/s	Intermediat e variable, y component	Boundary 19
spf.ut_therez	- spf.un_there*nojac (spf.nzmesh)	m/s	Intermediat e variable, z component	Boundary 19
spf.ct_here	24*nojac(down((s pf.mu+spf.muT)/s pf.epsilon_p))*spf. meshVol/spf.mesh VolInt	Pa·s/m	Intermediat e variable	Boundary 19
spf.uNormal	u*nojac(spf.nxmes h)+v*nojac(spf.ny mesh)	m/s	Normal velocity	Boundary 19
spf.backflowPen altyDiff	spf.c_here*min((d own(spf.mu)+spf. muT)*spf.meshVol /spf.meshVolInt,d own(spf.rho)*abs(s pf.uNormal)/down (spf.epsilon_p))	$kg^2/(m^4 \cdot s^2)$	Backflow penalty parameter, diffusive contribution	Boundary 19
spf.backflowPen altyConv	spf.rhoFace*spf.u mxTnFace/spf.epsi lon_p^2	$kg/(m^2 \cdot s)$	Backflow penalty parameter, convective contribution	Boundary 19

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-spf.f0*(test(u)*spf.nxmesh+test(v)*spf.nymesh)	2	Spatial	Boundary 19
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 19

2.5.7 Outlet 1



Outlet 1

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 1, 4, 9

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

Constraint settings

SETTINGS

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

Variables

Name	Expression	Unit	Description	Selection
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, 4, 9
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, 4, 9
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, 4, 9

Name	Expression	Unit	Description	Selection
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 1, 4, 9
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, 4, 9
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, 4, 9
spf.ujumpx	spf.ut_herex-spf.ut_therex	m/s	Velocity jump, x component	Boundaries 1, 4, 9
spf.ujumpy	spf.ut_herey-spf.ut_therey	m/s	Velocity jump, y component	Boundaries 1, 4, 9
spf.ujumpz	spf.ut_herez-spf.ut_therez	m/s	Velocity jump, z component	Boundaries 1, 4, 9
spf.meshVol	meshvol_spatial	m		Boundaries 1, 4, 9
spf.meshVolInt	down(meshvol_spatial)	m²	Volume of interior mesh element	Boundaries 1, 4, 9
spf.sigma_dg_ns	4*spf.ct_here	Pa·s/m		Boundaries 1, 4, 9
spf.p0	0	Pa	Pressure	Boundaries 1, 4, 9
spf.f0	spf.p0	N/m²	Normal stress	Boundaries 1, 4, 9
spf.un_here	u*nojac(spf.nxmesh)+v*nojac(spf.nymesh)	m/s	Intermediate variable	Boundaries 1, 4, 9
spf.ut_herex	u-spf.un_here*nojac(spf.	m/s	Intermediate variable, x	Boundaries 1, 4, 9

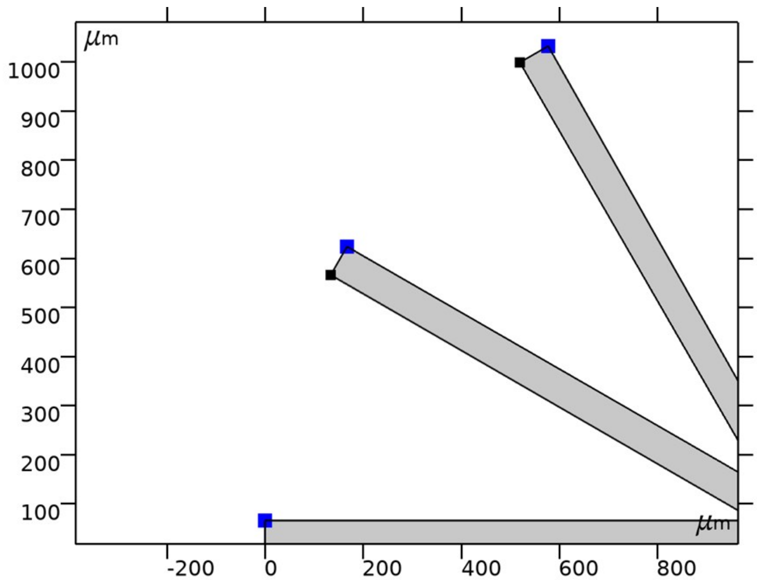
Name	Expression	Unit	Description	Selection
	nxmesh)		component	
spf.ut_herey	v-spf.un_here*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundaries 1, 4, 9
spf.ut_herez	-spf.un_here*nojac(spf.nzmesh)	m/s	Intermediate variable, z component	Boundaries 1, 4, 9
spf.un_there	0	m/s	Intermediate variable	Boundaries 1, 4, 9
spf.ut_therex	-spf.un_there*nojac(spf.nxmesh)	m/s	Intermediate variable, x component	Boundaries 1, 4, 9
spf.ut_therey	-spf.un_there*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundaries 1, 4, 9
spf.ut_therez	-spf.un_there*nojac(spf.nzmesh)	m/s	Intermediate variable, z component	Boundaries 1, 4, 9
spf.ct_here	24*nojac(down((spf.mu+spf.muT)/spf.epsilon_p))*spf.meshVol/spf.meshVolInt	Pa·s/m	Intermediate variable	Boundaries 1, 4, 9
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, 4, 9
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-	2	Spatial	Boundaries 1, 4, 9

Weak expression	Integration order	Integration frame	Selection
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)			

2.5.8 Pressure Point Constraint 1



Pressure Point Constraint 1

SELECTION

Geometric entity level	Point
Selection	Points 2, 4, 8

EQUATIONS

$$p = p_0$$

Pressure constraint

SETTINGS

Description	Value
Pressure	0

Constraint settings

SETTINGS

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

Variables

Name	Expression	Unit	Description	Selection
spf.p0	0	Pa	Pressure	Points 2, 4, 8

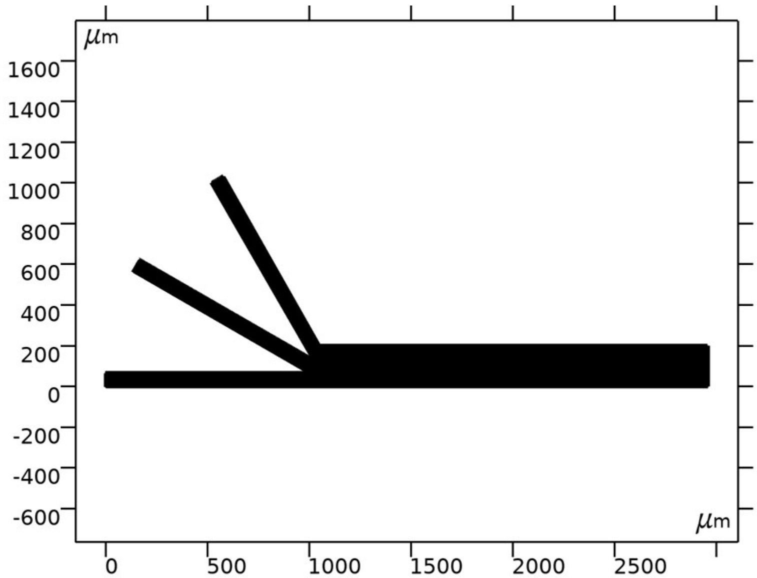
Constraints

Constraint	Constraint force	Shape function	Selection	Details
-p+spf.p0	test(-p)	Lagrange (Linear)	Points 2, 4, 8	Elemental

2.6 MESH 1

MESH STATISTICS

Description	Value
Minimum element quality	0.5352
Average element quality	0.9682
Triangle	48519
Quad	963
Edge element	1853
Vertex element	19



Mesh 1

2.6.1 Size (size)

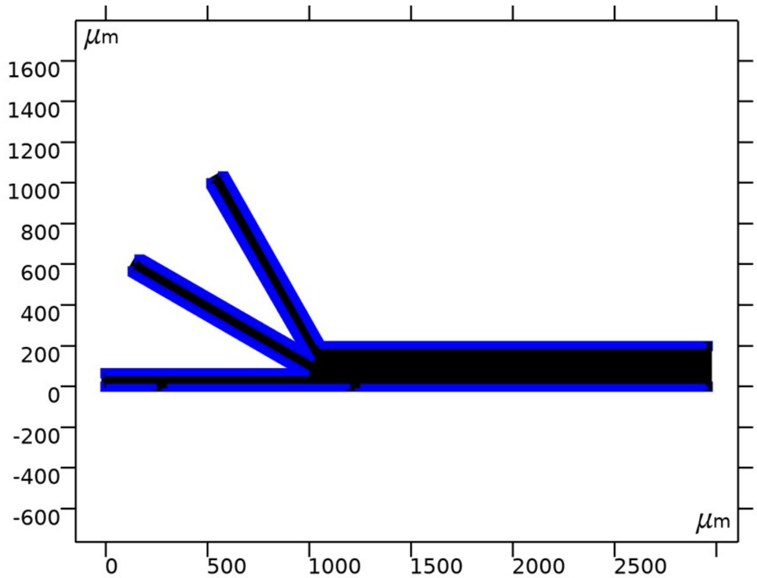
SETTINGS

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	6.92
Minimum element size	0.0207
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	Boundaries 2–3, 5–6, 8, 10–12, 14–18



Size 1

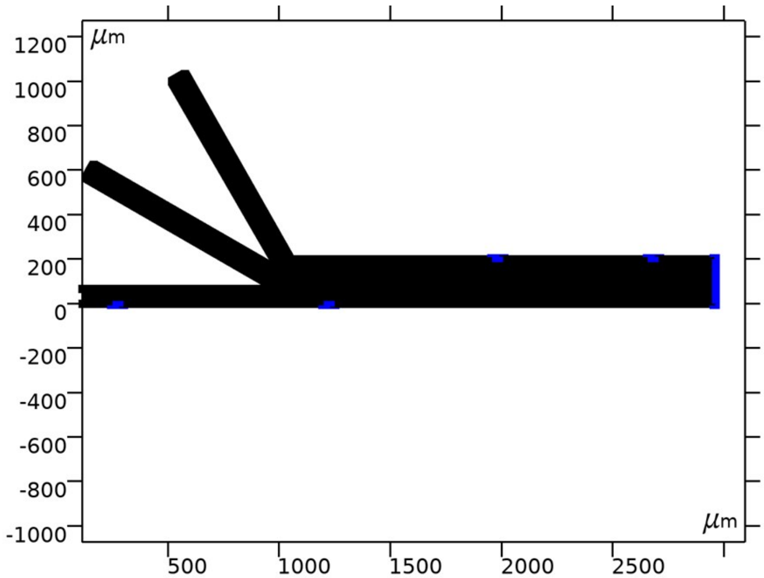
SETTINGS

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	6.92
Minimum element size	0.0207
Curvature factor	0.2
Maximum element growth rate	1.05
Predefined size	Extremely fine

2.6.3 Size 2 (size2)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 7, 13, 15, 17, 19



Size 2

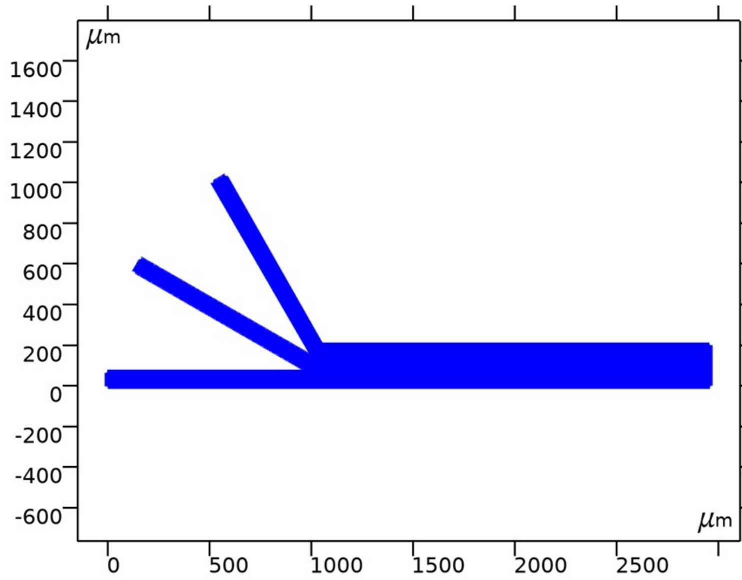
SETTINGS

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	Domain 1

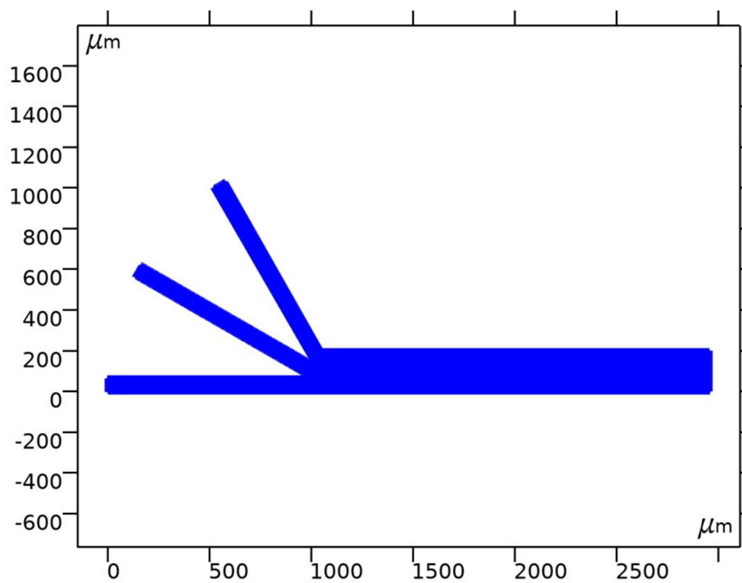


Corner Refinement 1

2.6.5 Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Remainin g



Free Triangular 1

2.6.6 Boundary Layers 1 (bl1)

SELECTION

Geometric entity level	Domain
Selection	Domain 1

Boundary Layers 1

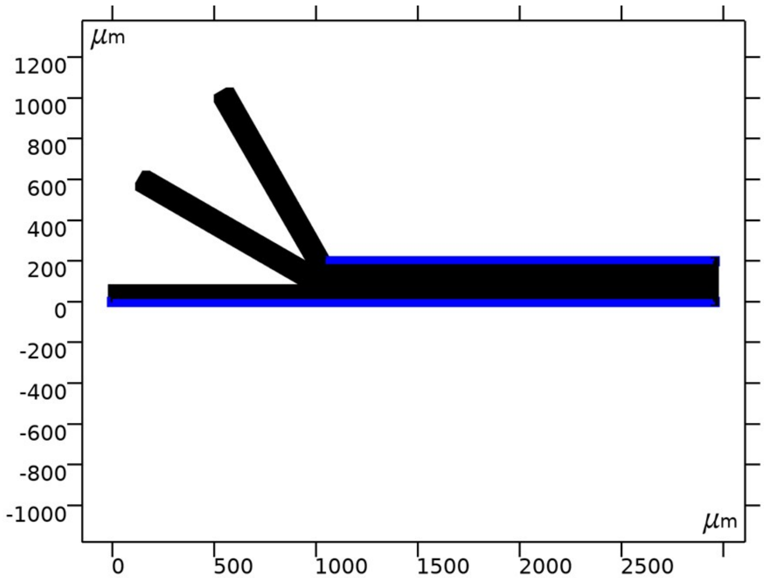
SETTINGS

Description	Value
Handling of sharp corners	Trimming

Boundary Layer Properties 1 (blp1)

SELECTION

Geometric entity level	Boundary
Selection	Boundaries 2, 7–8, 12–18



Boundary Layer Properties 1

SETTINGS

Description	Value
Number of boundary layers	1
Thickness adjustment factor	10

3 Study 1

COMPUTATION INFORMATION

Computation time	7 min 32 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

MESH SELECTION

Geometry	Mesh
mesh1	mesh1

PHYSICS AND VARIABLES SELECTION

Physics interface	Discretization
Nernst-Planck Equations (npe)	physics
Creeping Flow (spf)	physics

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.1.1 Study extensions

STUDY EXTENSIONS

Description	Value
Sweep type	Specified combinations

PARAMETERS

Parameter name	Parameter value list	Parameter unit
issBPE2 (steady-state current through	range(0.6,0.01,0.74)	uA

Parameter name	Parameter value list	Parameter unit
BPE 2)		

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 Mar 14, 2020 7:38:09 PM.
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: 2.48 GB
Virtual memory: 2.68 GB
Ended at Mar 14, 2020 7:38:12 PM.
----- Compile Equations: Stationary in Study 1/Solution 1 (sol1) -------------
->
```

Dependent Variables 1 (v1)

INITIAL VALUES OF VARIABLES SOLVED FOR

Description	Value
Method	Solution
Solution	

INITIAL VALUE CALCULATION CONSTANTS

Constant name	Initial value source
issBPE2	range(0.6,0.01,0.74)[uA]

LOG

```
<---- Dependent Variables 1 in Study 1/Solution 1 (sol1) ---------------------
--
Started at Mar 14, 2020 7:38:13 PM.
Initial values of variables solved for: Solution 1 (sol1), issBPE=6E-7 [Last].
Solution time: 0 s.
Physical memory: 2.02 GB
Virtual memory: 2.21 GB
Ended at Mar 14, 2020 7:38:13 PM.
----- Dependent Variables 1 in Study 1/Solution 1 (sol1) ---------------------
->
```

Concentration (comp1.cH3O) (comp1_cH3O)

GENERAL

Description	Value
Field components	comp1.cH3O

Concentration (comp1.cOH) (comp1_cOH)

GENERAL

Description	Value
Field components	comp1.cOH

Concentration (comp1.cTris) (comp1_cTris)

GENERAL

Description	Value
Field components	comp1.cTris

Concentration (comp1.cTrisH) (comp1_cTrisH)

GENERAL

Description	Value
Field components	comp1.cTrisH

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}

Electric potential (comp1.V) (comp1_V)

GENERAL

Description	Value
Field components	comp1.V

Stationary Solver 1 (s1)

GENERAL

Description	Value
Defined by study step	

RESULTS WHILE SOLVING

Description	Value
Probes	None

LOG

```
<---- Stationary Solver 1 in Study 1/Solution 1 (sol1) -----------------------
--
Started at Mar 14, 2020 7:38:13 PM.
Continuation solver
Nonlinear solver
Number of degrees of freedom solved for: 592170 (plus 18626 internal DOFs).

Continuation parameter issBPE2 = 6e-07.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (comp1.cH3O): 6.5e+03
Concentration (comp1.cOH): 1.8e+04
Concentration (comp1.cTris): 6.1e+05
Concentration (comp1.cTrisH): 1.6e+04
Pressure (comp1.p): 1.7e+02
Velocity field (comp1.u): 10
Electric potential (comp1.V): 30
Orthonormal null-space function used.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1       5e-06     6.1e+03   0.0100000     5.1e-06    2    1    2  1.7e-
11  1.3e-14
   2     1.2e-08       4e+02   1.0000000     1.2e-05    4    2    4  6.7e-
12    6e-14

Continuation parameter issBPE2 = 6.1e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.9e-05         4.8   1.0000000     0.00087    9    3    7    3e-
11  1.7e-13

Continuation parameter issBPE2 = 6.2e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.9e-05         4.5   1.0000000      0.0009   14    4   10  3.1e-
11  1.6e-13

Continuation parameter issBPE2 = 6.3e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.9e-05         4.6   1.0000000      0.0009   19    5   13  2.9e-
11  1.7e-13

Continuation parameter issBPE2 = 6.4e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.8e-05         4.3   1.0000000     0.00088   24    6   16  3.2e-
11  1.8e-13

Continuation parameter issBPE2 = 6.5e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.8e-05         4.2   1.0000000     0.00087   29    7   19    2e-
11  1.8e-13

Continuation parameter issBPE2 = 6.6e-07.
```

```
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.7e-05           4   1.0000000     0.00086   34    8   22  2.4e-
11  1.8e-13

Continuation parameter issBPE2 = 6.7e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.6e-05         3.9   1.0000000     0.00084   39    9   25  2.9e-
11  1.9e-13

Continuation parameter issBPE2 = 6.8e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.5e-05         3.7   1.0000000     0.00083   44   10   28  2.7e-
11    2e-13

Continuation parameter issBPE2 = 6.9e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.4e-05         3.7   1.0000000     0.00081   49   11   31  2.6e-
11    2e-13

Continuation parameter issBPE2 = 7e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.4e-05         3.6   1.0000000      0.0008   54   12   34  3.3e-
11  2.1e-13

Continuation parameter issBPE2 = 7.1e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.4e-05         3.5   1.0000000      0.0008   59   13   37  3.7e-
11  2.1e-13

Continuation parameter issBPE2 = 7.2e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.3e-05         3.5   1.0000000     0.00078   64   14   40  1.9e-
11  2.1e-13

Continuation parameter issBPE2 = 7.3e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.4e-05         3.5   1.0000000     0.00077   69   15   43  3.3e-
11  2.2e-13

Continuation parameter issBPE2 = 7.4e-07.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1     2.4e-05         3.5   1.0000000     0.00076   74   16   46  2.5e-
11  2.2e-13
Solution time: 448 s. (7 minutes, 28 seconds)
Physical memory: 7.92 GB
Virtual memory: 9.11 GB
Ended at Mar 14, 2020 7:45:41 PM.
```

```
----- 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

Parametric (pDef)

GENERAL

Description	Value
Defined by study step	

PARAMETERS

Parameter name	Parameter value list	Parameter unit
issBPE2	range(0.6,0.01,0.74)	uA

LEAST-SQUARES DATA

Description	Value
Use least-squares parameters from file	Off