Filtration simulations-052621

Report date	May 26, 2021 11:14:07 AM

Contents

1 Global Definitions

Date	May 26, 2021 10:57:21 AM

GLOBAL SETTINGS

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

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

1.1 PARAMETERS

PARAMETERS 1

Name	Expression	Value	Description
cK0	1[mM]	1 mol/m³	initial concentration of K
cCl0	1[mM]	1 mol/m³	initial concentration of Cl
cH3O0	1e-7[M]	1E−4 mol/m³	initial concentration of H3O
cOH0	1e-7[M]	1E−4 mol/m³	initial concentration of OH
cBEAD0	30[fM]	3E−11 mol/m³	initial concentration of microplastics
dK	1.97e-9[m^2/s]	1.97E−9 m²/s	diffusivity of K
dCl	2.033e-9[m^2/s]	2.033E−9 m²/s	diffusivity of Cl
dH3O	9.103E-9[m^2/s]	9.103E−9 m²/s	diffusivity of H3O
dOH	5.286E-9[m^2/s]	5.286E−	diffusivity of

Name	Expression	Value	Description
		9 m^2/s	OH
dBEAD	6.16e-10[m^2/s]	6.16E−10 m^2/s	diffusivity of microplastics
i_elec	440[nA]	4.4E−7 A	steady-state current through the BPE
j_elec	i_elec/(100*50[um^2])	88 A/m^2	current density at the BPE
f_elec	j_elec/F_const	9.1206E−4 $mol/(m^2 \cdot s)$	flux through the BPE
k_fhydro	2e-5[1/s]	2E−5 1/s	forward rate constant for water hydrolysis
k_bhydro	1.4e11[1/(M*s)]	1.4E8 $m^3/(s \cdot mol)$	backward rate constant for water hydrolysis
cH2O0	55.5[M]	55500 mol/m^3	concentration of water

2 Component 1

Date	Jul 28, 2020 6:09:07 PM

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

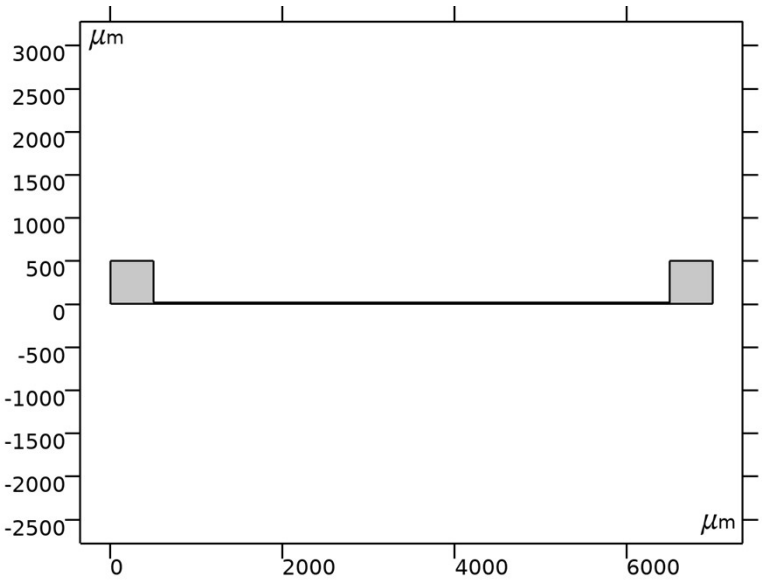
Coordinate system type	Boundary system
Tag	sys1

COORDINATE NAMES

First	Second	Third

First	Second	Third
t1	n	to

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	μm
Angular unit	deg

GEOMETRY STATISTICS

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

2.2.1 Polygon 1 (pol1)

OBJECT TYPE

Description	Value
Type	Solid

COORDINATES

Description	Value
Data source	Table

COORDINATES

x (µm)	y (µm)
0	0
0	500
500	500
500	15
6500	15
6500	500
7000	500
7000	0
0	0

2.2.2 Point 1 (pt1)

POINT

Description	Value
Point coordinate	{2000, 0}

2.2.3 Point 2 (pt2)

POINT

Description	Value
Point coordinate	{2050, 0}

2.2.4 Point 3 (pt3)

POINT

Description	Value
Point coordinate	{4950, 0}

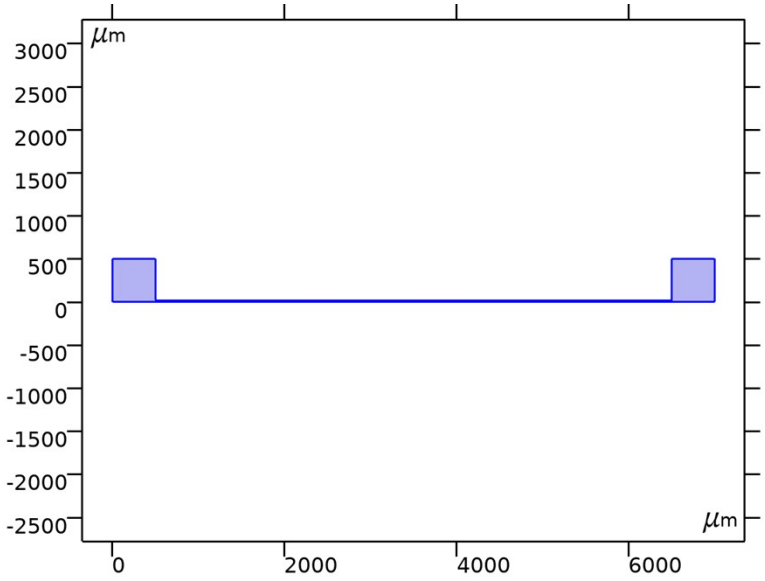
2.2.5 Point 4 (pt4)

POINT

Description	Value
Point coordinate	{5000, 0}

2.3 MATERIALS

2.3.1 Water, liquid



Water, liquid

SELECTION

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

MATERIAL PARAMETERS

Name	Value	Unit
Dynamic viscosity	eta(T)	Pa·s
Density	rho(T)	kg/m³
Relative permittivity	80	1

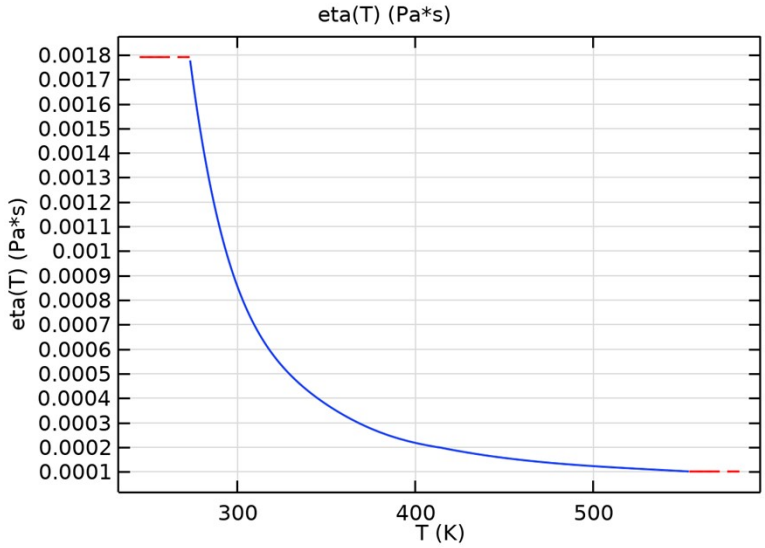
BASIC SETTINGS

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)
thermalexpansioncoefficient_symmetry	3
bulkviscosity_symmetry	0
Dynamic viscosity	eta(T)
dynamicviscosity_symmetry	0
Ratio of specific heats	gamma_w(T)

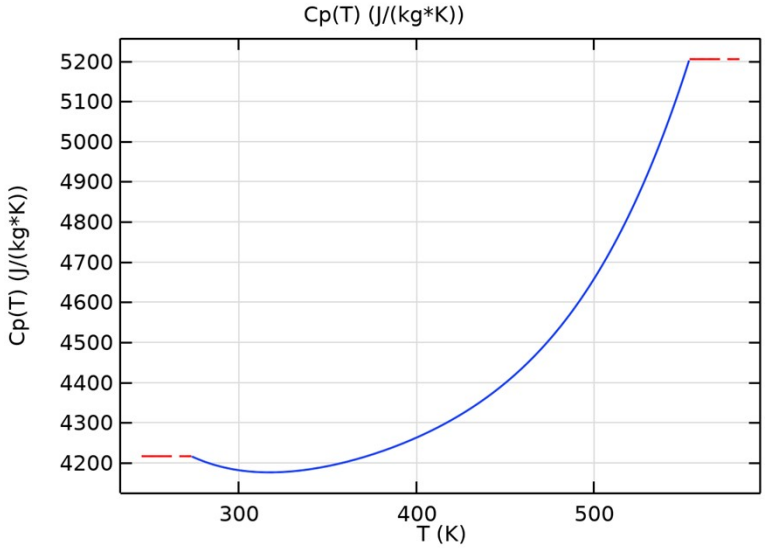
Description	Value
ratioofspecificheat_symmetry	0
Electrical conductivity	{{5.5e-6[S/m], 0, 0}, {0, 5.5e-6[S/m], 0}, {0, 0, 5.5e-6[S/m]}}
electricconductivity_symmetry	3
Heat capacity at constant pressure	Cp(T)
heatcapacity_symmetry	0
Density	rho(T)
density_symmetry	0
Thermal conductivity	{{k(T), 0, 0}, {0, k(T), 0}, {0, 0, k(T)}}
thermalconductivity_symmetry	3
Speed of sound	cs(T)
soundspeed_symmetry	0
Relative permittivity	{{80, 0, 0}, {0, 80, 0}, {0, 0, 80}}
relpermittivity_symmetry	0

FUNCTIONS

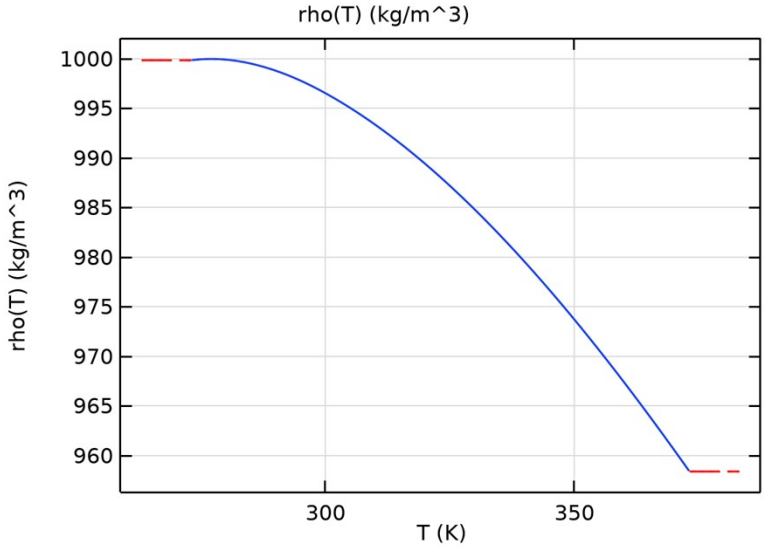
Function name	Type
eta	Piecewise
Cp	Piecewise
rho	Piecewise
k	Piecewise
cs	Interpolation
alpha_p	Analytic
gamma_w	Analytic
muB	Analytic


eta(T) (Pa*s)
0.0018
0.0017
0.0016
0.0015
0.0014
0.0013
0.0012
0.0011
0.001
0.0009
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
eta(T) (Pa*s)
300
400
500
T (K)

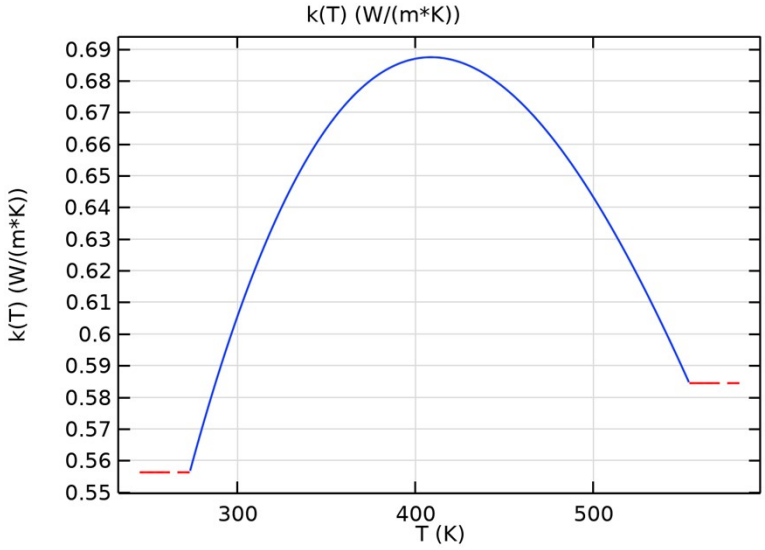
eta


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)

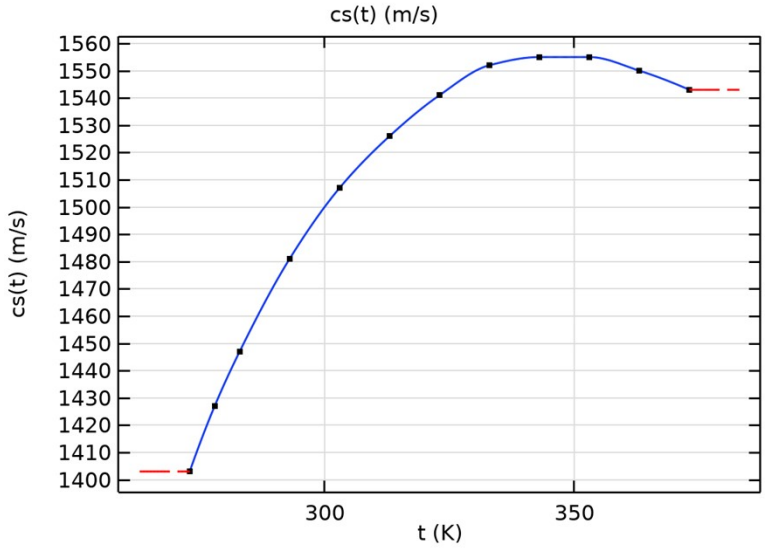
Cp


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

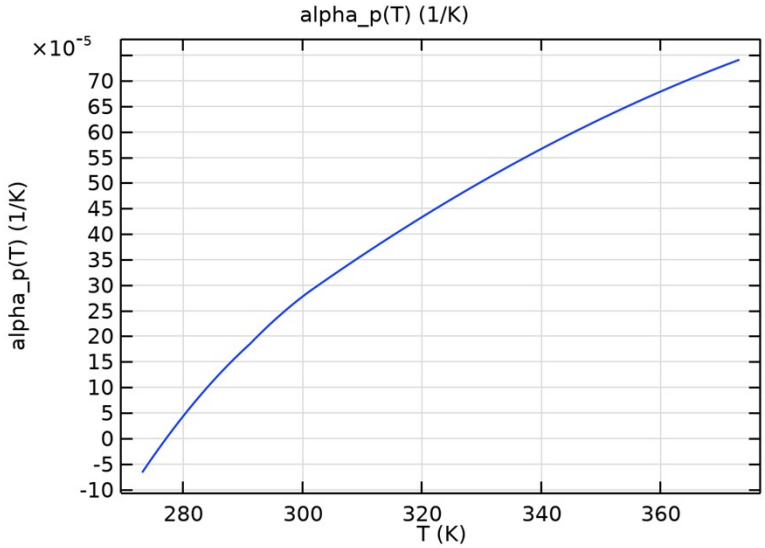
rho


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)

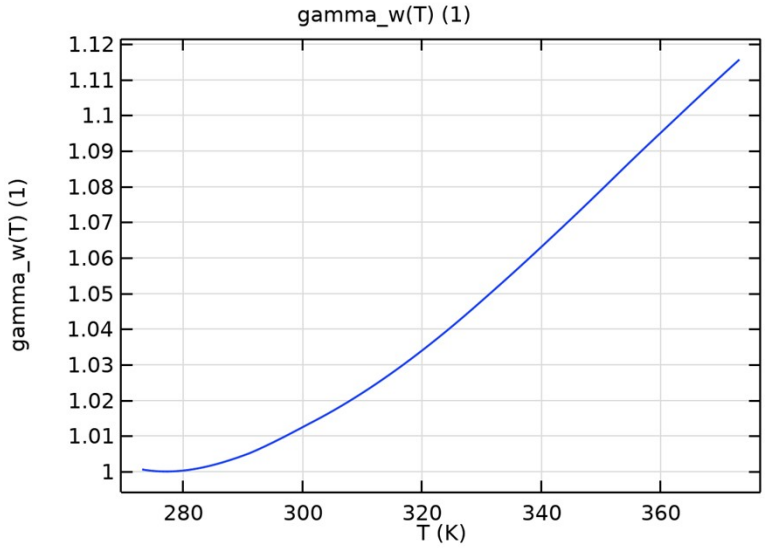
k


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

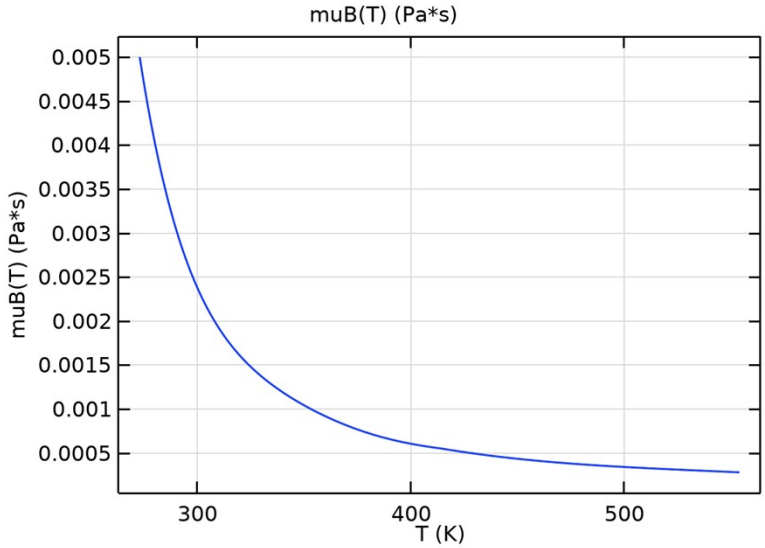
cs


alpha_p(T) (1/K)
×10^-5
alpha_p(T) (1/K)
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
280
300
320
340
360
T (K)

alpha_p



gamma_w



muB

2.4 LAMINAR FLOW

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

Laminar Flow

SELECTION

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

EQUATIONS

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

2.4.1 Interface settings

Discretization

SETTINGS

Description	Value
Discretization of fluids	P2 + P1

Physical model

SETTINGS

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

Description	Value
Reference pressure level	1[atm]

Turbulence

SETTINGS

Description	Value
Turbulence model type	None

2.4.2 Variables

Name	Expression	Unit	Description	Selection	Details
spf.Tref	model.input.Tref	K	Reference temperature	Global	Meta
spf.dz	1	m	Thickness	Domain 1	
spf.pref	1[atm]	Pa	Reference pressure level	Domain 1	
spf.pA	p+spf.pref	Pa	Absolute pressure	Domain 1	
spf.hasWF	0		Help variable	Boundaries 1–12	
spf.dt_CFL	1/max(spf.maxOp(sqrt(emetric_spatial(u-d(x,TIME),v-d(y,TIME)))),eps)	s	Time step, CFL=1	Global	
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.geometryL	1.25E-4	m	Geometry	Domain 1	

Name	Expression	Unit	Description	Selection	Details
engthScale			length scale		
spf.time_step_inv	max(sqrt(emetric_spatial(u,v)*2^if(gmg_level<2,0,-1+gmg_level)^2),spf.nu/spf.geometryLengthScale^2)	Hz	Inverse time step	Domain 1	
spf.tsti	nojac(spf.time_step_inv/spf.locCFL)	1/s	Help variable	Domain 1	
spf.nx	dnx	1	Normal vector, x component	Boundaries 1–12	
spf.ny	dny	1	Normal vector, y component	Boundaries 1–12	
spf.nz	0	1	Normal vector, z component	Boundaries 1–12	
spf.nxmesh	dnxmesh	1	Normal vector, x component	Boundaries 1–12	
spf.nymesh	dnymesh	1	Normal vector, y component	Boundaries 1–12	
spf.nzmesh	0	1	Normal vector, z component	Boundaries 1–12	

2.4.3 Fluid Properties 1

Fluid Properties 1

SELECTION

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

EQUATIONS

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

Fluid properties

SETTINGS

Description	Value
Density	From material
	Newtonian
Dynamic viscosity	From material

Model input

SETTINGS

Description	Value
Temperature	Common model input

USED PRODUCTS

COMSOL Multiphysics

PROPERTIES FROM MATERIAL

Property	Material	Property group
Density	Water, liquid	Basic
Dynamic viscosity	Water, liquid	Basic

Variables

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

Name	Expression	Unit	Description	Selection	Details
spf.srijzx	0	1/s	Strain rate tensor, zx component	Domain 1	
spf.srijxy	0.5*(uy+vx)	1/s	Strain rate tensor, xy component	Domain 1	
spf.srijyy	vy	1/s	Strain rate tensor, yy component	Domain 1	
spf.srijzy	0	1/s	Strain rate tensor, zy component	Domain 1	
spf.srijxz	0	1/s	Strain rate tensor, xz component	Domain 1	
spf.srijyz	0	1/s	Strain rate tensor, yz component	Domain 1	
spf.srijzz	0	1/s	Strain rate tensor, zz component	Domain 1	
spf.rrijxx	0	1/s	Rotation rate tensor, xx component	Domain 1	
spf.rrijyx	0.5*(vx-uy)	1/s	Rotation rate tensor, yx component	Domain 1	
spf.rrijzx	0	1/s	Rotation rate tensor, zx component	Domain 1	
spf.rrijxy	0.5*(uy-vx)	1/s	Rotation rate tensor, xy component	Domain 1	
spf.rrijyy	0	1/s	Rotation rate tensor, yy component	Domain 1	
spf.rrijzy	0	1/s	Rotation rate tensor,	Domain 1	

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

Name	Expression	Unit	Description	Selection	Details
			force, y component		on
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	
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	Domain 1	+ operati

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

Name	Expression	Unit	Description	Selection	Details
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
spf.K_stress_tensor_testxy	spf.mu_eff*(test(uy)+test(vx))	N/m²	Viscous stress tensor test, xy component	Domain 1	+ operation

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

Name	Expression	Unit	Description	Selection	Details
			tensor, zx component		
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 force, yx component	Domain 1	+ operation
spf.Fst_tensorzx	0	N/m²	Surface tension	Domain 1	+ operation

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

Name	Expression	Unit	Description	Selection	Details
			residual		

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
u	Lagrange (Quadratic)	m/s	Velocity field, x component	Spatial	Domain 1
v	Lagrange (Quadratic)	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)	4	Spatial	Domain 1
spf.Fx*test(u)+spf.Fy*test(v)	4	Spatial	Domain 1
spf.rho*(-(d(u,x)*u+d(u,y)*v)*test(u)-(d(v,x)*u+d(v,y)*v)*test(v))	4	Spatial	Domain 1
-spf.continuityEquation*test(p)	4	Spatial	Domain 1
spf.streamlinens	4	Spatial	Domain 1
spf.crosswindns	4	Spatial	Domain 1
(spf.usePseudoTimeStepping>0)*spf.rho*spf.tsti*(-(u-nojac(u))*test(u)-(v-nojac(v))*test(v))	4	Spatial	Domain 1

2.4.4 Initial Values 1

Initial Values 1

SELECTION

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

Initial values

SETTINGS

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

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

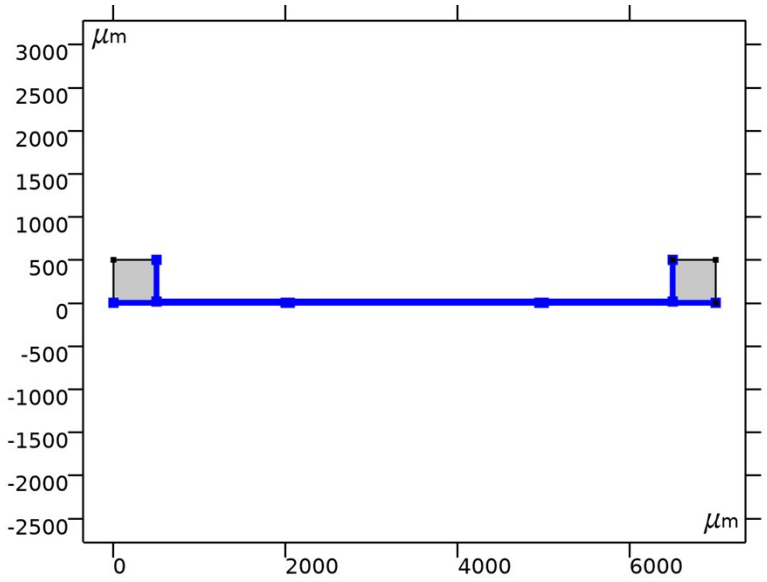
USED PRODUCTS

COMSOL Multiphysics

Variables

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

2.4.5 Wall 1



Wall 1

SELECTION

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

EQUATIONS

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

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

Boundary condition

SETTINGS

Description	Value
Wall condition	Electroosmotic velocity
Electric field	Electric field (es/ccn1)
Electroosmotic mobility	Built - in expression

Description	Value
Zeta potential	(-0.08)[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, 4–10	
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, 4–10	
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, 4–10	
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, 4–10	
spf.KStressTestn_avy	spf.K_stress_tensor_testyx*spf.nx	N/m²	Average viscous	Boundaries 2, 4–10	

Name	Expression	Unit	Description	Selection	Details
	mesh+spf.K_stress_tensor_testyy*spf.nymesh+spf.K_stress_tensor_testyz*spf.nzmesh		stress, y component		
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, 4–10	
spf.ujumpx	spf.u_herex-spf.u_therex	m/s	Velocity jump, x component	Boundaries 2, 4–10	
spf.ujumpy	spf.u_herey-spf.u_therey	m/s	Velocity jump, y component	Boundaries 2, 4–10	
spf.ujumpz	spf.u_herez-spf.u_therez	m/s	Velocity jump, z component	Boundaries 2, 4–10	
spf.meshVol	meshvol_spatial	m		Boundaries 2, 4–10	
spf.meshVolInt	down(meshvol_spatial)	m^2	Volume of interior mesh element	Boundaries 2, 4–10	
spf.c_here	72*nojac(down(spf.mu))*spf.meshVol/spf.meshVolInt	1	Intermediate variable	Boundaries 2, 4–10	
spf.sigma_dg_ns	4*spf.c_here	Pa·s/m		Boundaries 2, 4–10	
spf.rhoFace	down(spf.rho)	kg/m^3	Density face value	Boundaries 2, 4–10	
spf.umxTnFace	(spf.upwind_helpx*spf.nxmesh+spf.upwind_helpy*spf.nymesh+spf.upwind_helpz*spf.nzmesh<0)*(spf.upwind_hel	m/s	Relative velocity on face	Boundaries 2, 4–10	

Name	Expression	Unit	Description	Selection	Details
	px*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, 4–10	
spf.zeta	(-0.08)[V]	V	Zeta potential	Boundaries 2, 4–10	
spf.epsilonr	80	1	Relative permittivity	Boundaries 2, 4–10	
spf.ubndx	spf.ueox+spf.utrx+spf.usx	m/s	Velocity at boundary, x component	Boundaries 2, 4–10	
spf.ubndy	spf.ueoy+spf.utry+spf.usy	m/s	Velocity at boundary, y component	Boundaries 2, 4–10	
spf.ubndz	spf.ueoz+spf.utrz+spf.usz	m/s	Velocity at boundary, z component	Boundaries 2, 4–10	
spf.usx	0	m/s	Velocity of sliding wall, x component	Boundaries 2, 4–10	
spf.usy	0	m/s	Velocity of sliding wall, y component	Boundaries 2, 4–10	
spf.usz	0	m/s	Velocity of sliding wall, z component	Boundaries 2, 4–10	
spf.utrx	0	m/s	Velocity of moving wall, x component	Boundaries 2, 4–10	
spf.utry	0	m/s	Velocity of moving wall,	Boundaries 2, 4–10	

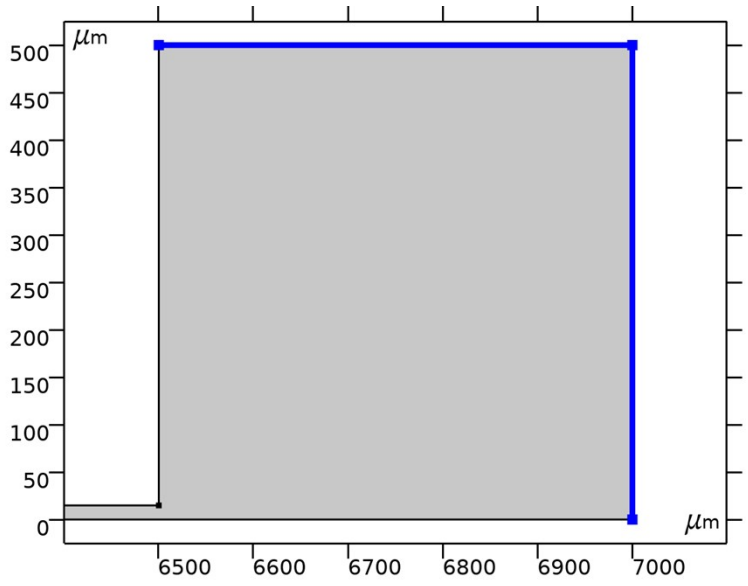
Name	Expression	Unit	Description	Selection	Details
			y component		
spf.utrz	0	m/s	Velocity of moving wall, z component	Boundaries 2, 4–10	
spf.uLeakagex	0	m/s	Leakage velocity, x component	Boundaries 2, 4–10	+ operation
spf.uLeakagey	0	m/s	Leakage velocity, y component	Boundaries 2, 4–10	+ operation
spf.uLeakagez	0	m/s	Leakage velocity, z component	Boundaries 2, 4–10	+ operation
spf.Ex	model.input.E1	V/m	Electric field, x component	Boundaries 2, 4–10	Meta
spf.Ey	model.input.E2	V/m	Electric field, y component	Boundaries 2, 4–10	Meta
spf.Ez	model.input.E3	V/m	Electric field, z component	Boundaries 2, 4–10	Meta
spf.mueo	-spf.zeta*epsilon0_const*spf.epsilonr/spf.mu	$m^2/(V·s)$	Electroosmotic mobility	Boundaries 2, 4–10	
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, 4–10	
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, 4–10	
spf.ueoz	(spf.Ez-spf.nzmesh*(spf.	m/s	Electroosmotic velocity, z	Boundaries 2, 4–10	

Name	Expression	Unit	Description	Selection	Details
	nxmesh*spf.Ex+spf.nymesh*spf.Ey+spf.nzmesh*spf.Ez))*spf.mueo		component		
spf.u_herex	u	m/s	Intermediate variable, x component	Boundaries 2, 4–10	
spf.u_herey	v	m/s	Intermediate variable, y component	Boundaries 2, 4–10	
spf.u_herez	0	m/s	Intermediate variable, z component	Boundaries 2, 4–10	
spf.u_therex	spf.ubndx+spf.uLeakagex	m/s	Intermediate variable, x component	Boundaries 2, 4–10	
spf.u_therey	spf.ubndy+spf.uLeakagey	m/s	Intermediate variable, y component	Boundaries 2, 4–10	
spf.u_therez	spf.ubndz+spf.uLeakagez	m/s	Intermediate variable, z component	Boundaries 2, 4–10	
spf.contCoeffFace	down(spf.contCoeff)	kg/m^3	Help variable	Boundaries 2, 4–10	
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, 4–10	
spf.pFace	p	Pa	Pressure face value	Boundaries 2, 4–10	
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, 4–10	+ 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	4	Spatial	Boundaries 2, 4–10

2.4.6 Inlet 1



Inlet 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 11–12

EQUATIONS

$$\mathbf{n}^{T}\left[-p\mathbf{I}+\mathbf{K}\right]\mathbf{n}=-\hat{p}_{0}$$

$\hat{p_0} \geq p_0$, $\mathbf{u} : \mathbf{t} = 0$

Boundary condition

SETTINGS

Description	Value
Boundary condition	Pressure

Pressure conditions

SETTINGS

Description	Value
Pressure	0
Suppress backflow	On
Flow direction	Normal flow

USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
spf.KStressn_avx	spf.K_stress_tensorxx*spf.nxmesh+spf.K_stress_tensorxy*spf.nymesh+spf.K_stress_tensorxz*spf.nzmesh	N/m²	Average viscous stress, x component	Boundaries 11–12
spf.KStressn_avy	spf.K_stress_tensoryx*spf.nxmesh+spf.K_stress_tensoryy*spf.nymesh+spf.K_stress_tensoryz*spf.nzmesh	N/m²	Average viscous stress, y component	Boundaries 11–12
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 11–12
spf.KStressTestn_avx	spf.K_stress_tensor_testxx*spf.nxmesh+spf.K_stress_tensor_testxy*spf.nymes	N/m²	Average viscous stress, x	Boundaries 11–12

Name	Expression	Unit	Description	Selection
	h+spf.K_stress_tensor_testxz*spf.nzmesh		component	
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/m^2	Average viscous stress, y component	Boundaries 11–12
spf.KStressTestn_avz	spf.K_stress_tensor_testzx*spf.nxmesh+spf.K_stress_tensor_testzy*spf.nymesh+spf.K_stress_tensor_testzz*spf.nzmesh	N/m^2	Average viscous stress, z component	Boundaries 11–12
spf.ujumpx	spf.ut_herex-spf.ut_therex	m/s	Velocity jump, x component	Boundaries 11–12
spf.ujumpy	spf.ut_herey-spf.ut_therey	m/s	Velocity jump, y component	Boundaries 11–12
spf.ujumpz	spf.ut_herez-spf.ut_therez	m/s	Velocity jump, z component	Boundaries 11–12
spf.meshVol	meshvol_spatial	m		Boundaries 11–12
spf.meshVolInt	down(meshvol_spatial)	m^2	Volume of interior mesh element	Boundaries 11–12
spf.c_here	288/spf.epsilon_p	Pa·s/m	Intermediate variable	Boundaries 11–12
spf.sigma_dg_ns	4*spf.ct_here	Pa·s/m		Boundaries 11–12
spf.rhoFace	down(spf.rho)	kg/m^3	Density face value	Boundaries 11–12
spf.umxTnFace	spf.upwind_helpx*spf.nxmesh+spf.upwind_helpy*spf.nymesh+spf.upwind_helpz*spf.nzmesh	m/s	Relative velocity on face	Boundaries 11–12

Name	Expression	Unit	Description	Selection
spf.upwind_ns	spf.backflowPenaltyConv*spf.uNormal	W/m²	Upwind term	Boundaries 11–12
spf.p0	0	Pa	Pressure	Boundaries 11–12
spf.f0	spf.p0+spf.uNormal*(spf.backflowPenaltyDiff+spf.backflowPenaltyConv)*(spf.uNormal>0)	N/m²	Normal stress	Boundaries 11–12
spf.uNormal	u*nojac(spf.nxmesh)+v*nojac(spf.nymesh)	m/s	Normal velocity	Boundaries 11–12
spf.backflowPenaltyDiff	spf.c_here*min((down(spf.mu)+spf.muT)*spf.meshVol/spf.meshVolInt,down(spf.rho)*abs(spf.uNormal)/down(spf.epsilon_p))	kg²/(m⁴·s²)	Backflow penalty parameter, diffusive contribution	Boundaries 11–12
spf.backflowPenaltyConv	spf.rhoFace*spf.umxTnFace/spf.epsilon_p^2	kg/(m²·s)	Backflow penalty parameter, convective contribution	Boundaries 11–12
spf.inl1.Te0xx	0		Viscoelastic stress tensor, xx component	Boundaries 11–12
spf.inl1.Te0xy	0		Viscoelastic stress tensor, xy component	Boundaries 11–12
spf.inl1.Te0xz	0		Viscoelastic stress tensor, xz component	Boundaries 11–12
spf.inl1.Te0yy	0		Viscoelastic stress tensor, yy component	Boundaries 11–12
spf.inl1.Te0yz	0		Viscoelastic stress tensor, yz component	Boundaries 11–12

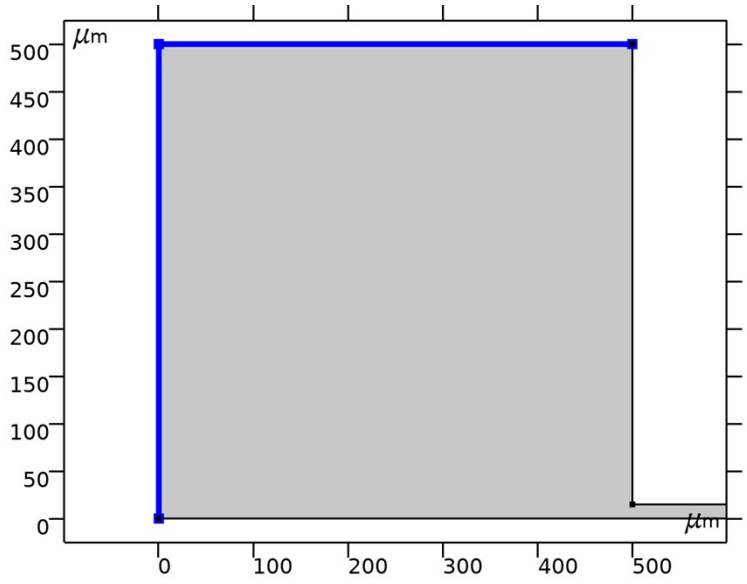
Name	Expression	Unit	Description	Selection
spf.inl1.Te0zz	0		Viscoelastic stress tensor, zz component	Boundaries 11–12
spf.un_here	u*nojac(spf.nxmesh)+v*nojac(spf.nymesh)	m/s	Intermediate variable	Boundaries 11–12
spf.ut_herex	u-spf.un_here*nojac(spf.nxmesh)	m/s	Intermediate variable, x component	Boundaries 11–12
spf.ut_herey	v-spf.un_here*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundaries 11–12
spf.ut_herez	-spf.un_here*nojac(spf.nzmesh)	m/s	Intermediate variable, z component	Boundaries 11–12
spf.un_there	0	m/s	Intermediate variable	Boundaries 11–12
spf.ut_therex	-spf.un_there*nojac(spf.nxmesh)	m/s	Intermediate variable, x component	Boundaries 11–12
spf.ut_therey	-spf.un_there*nojac(spf.nymesh)	m/s	Intermediate variable, y component	Boundaries 11–12
spf.ut_therez	-spf.un_there*nojac(spf.nzmesh)	m/s	Intermediate variable, z component	Boundaries 11–12
spf.ct_here	72*nojac(down((spf.mu+spf.muT)/spf.epsilon_p))*spf.meshVol/spf.meshVolInt	Pa·s/m	Intermediate variable	Boundaries 11–12

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-spf.f0*(test(u)*spf.nxmesh+test(v)*spf.nymesh)	4	Spatial	Boundaries 11–12
spf.KStressn_avx*test(spf.ut_herex)+spf.KStressn_avy*test(spf.ut_here	4	Spatial	Boundaries 11–12

Weak expression	Integration order	Integration frame	Selection
y)+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)			

2.4.7 Outlet 1



Outlet 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 1, 3

EQUATIONS

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

$$\hat{\rho}_0 \le p_0\,,$$

Boundary condition

SETTINGS

Description	Value
Boundary condition	Pressure

Pressure conditions

SETTINGS

Description	Value
Pressure	0
Normal flow	Off
Suppress backflow	On

USED PRODUCTS

COMSOL Multiphysics

Variables

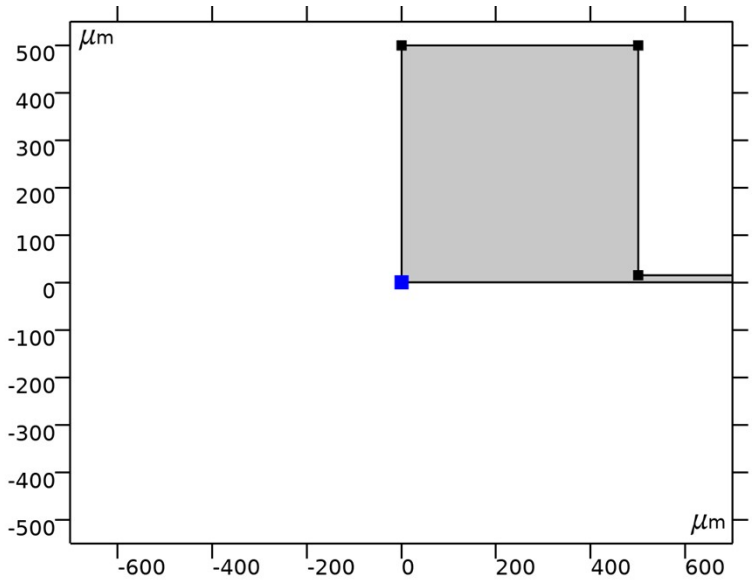
Name	Expression	Unit	Description	Selection
spf.meshVol	meshvol_spatial	m		Boundaries 1, 3
spf.meshVolInt	down(meshvol_spatial)	m^2	Volume of interior mesh element	Boundaries 1, 3
spf.c_here	288/spf.epsilon_p	Pa·s/m	Intermediate variable	Boundaries 1, 3
spf.rhoFace	down(spf.rho)	kg/m^3	Density face value	Boundaries 1, 3
spf.umxTnFace	spf.upwind_helpx*spf.nxmesh+spf.upwind_helpy*spf.nymesh+spf.upwind_helpz*spf.nzmesh	m/s	Relative velocity on face	Boundaries 1, 3
spf.upwind_ns	spf.backflowPenaltyConv*spf.uNormal	Pa	Upwind term	Boundaries 1, 3
spf.p0	0	Pa	Pressure	Boundaries 1, 3
spf.f0	spf.p0+spf.uNormal*(spf.backflowPenaltyDiff-	N/m^2	Normal stress	Boundaries 1, 3

Name	Expression	Unit	Description	Selection
	spf.backflowPenaltyConv)*(spf.uNormal<0)			
spf.uNormal	u*nojac(spf.nxmesh)+v*nojac(spf.nymesh)	m/s	Normal velocity	Boundaries 1, 3
spf.backflowPenaltyDiff	spf.c_here*min((down(spf.mu)+spf.muT)*spf.meshVol/spf.meshVolInt,down(spf.rho)*abs(spf.uNormal)/down(spf.epsilon_p))	$kg^2/(m^4 \cdot s^2)$	Backflow penalty parameter, diffusive contribution	Boundaries 1, 3
spf.backflowPenaltyConv	spf.rhoFace*spf.umxTnFace/spf.epsilon_p^2	$kg/(m^2 \cdot s)$	Backflow penalty parameter, convective contribution	Boundaries 1, 3
spf.out1.Uav	0	m/s	Average velocity	Global
spf.out1.p0avfdf	0	Pa	Average pressure	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)	4	Spatial	Boundaries 1, 3

2.4.8 Pressure Point Constraint 1



Pressure Point Constraint 1

SELECTION

Geometric entity level	Point
Selection	Geometry geom1: Dimension 0: Point 1

EQUATIONS

$p = p_0$

Pressure constraint

SETTINGS

Description	Value
Pressure	0

USED PRODUCTS

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
spf.p0	0	Pa	Pressure	Point 1

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-p+spf.p0	test(-p)	Lagrange (Linear)	Point 1	Elemental

2.5 ELECTROSTATICS

USED PRODUCTS

COMSOL Multiphysics

Electrostatics

SELECTION

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

EQUATIONS

$$\nabla \cdot \mathbf{D} = \rho_v$$
$$\mathbf{E} = -\nabla V$$

2.5.1 Interface settings

Discretization

SETTINGS

Description	Value
Electric potential	Quadratic

Manual terminal sweep settings

SETTINGS

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

2.5.2 Variables

Name	Expression	Unit	Description	Selection
es.d	1.0E-4[m]	m	Out-of-plane thickness	Domain 1
es.nx	dnx		Normal vector, x component	Boundaries 1–12
es.ny	dny		Normal vector, y component	Boundaries 1–12
es.nz	0		Normal vector, z component	Boundaries 1–12
es.nmeshx	dnxmesh		Mesh normal vector, x component	Boundaries 1–12
es.nmeshy	dnymesh		Mesh normal vector, y component	Boundaries 1–12
es.nmeshz	0		Mesh normal vector, z component	Boundaries 1–12
es.unmeshx	unxmesh		Mesh normal vector, upside, x component	Boundaries 1–12
es.unmeshy	unymesh		Mesh normal vector,	Boundaries 1–12

Name	Expression	Unit	Description	Selection
			upside, y component	
es.unmeshz	0		Mesh normal vector, upside, z component	Boundaries 1–12
es.dnmeshx	dnxmesh		Mesh normal vector, downside, x component	Boundaries 1–12
es.dnmeshy	dnymesh		Mesh normal vector, downside, y component	Boundaries 1–12
es.dnmeshz	0		Mesh normal vector, downside, z component	Boundaries 1–12
es.I_sXX	(spatial.invF11*(spatial.invF11*es.I_sxx+spatial.invF21*es.I_syx)+spatial.invF21*(spatial.invF11*es.I_sxy+spatial.invF21*es.I_syy))*spatial.detF	1	Spatial identity matrix, material frame, XX component	Domain 1
es.I_sYX	(spatial.invF11*(spatial.invF12*es.I_sxx+spatial.invF22*es.I_syx)+spatial.invF21*(spatial.invF12*es.I_sxy+spatial.invF22*es.I_syy))*spatial.detF	1	Spatial identity matrix, material frame, YX component	Domain 1
es.I_sZX	(spatial.invF11*es.I_szx+spatial.invF21*es.I_szy)*spatial.detF	1	Spatial identity matrix, material frame, ZX component	Domain 1
es.I_sXY	(spatial.invF12*(spatial.invF11*es.	1	Spatial	Domain 1

Name	Expression	Unit	Description	Selection
	l_sxx+spatial.invF21*es.l_syx)+spatial.invF22*(spatial.invF11*es.l_sxy+spatial.invF21*es.l_syy))*spatial.detF		identity matrix, material frame, XY component	
es.l_sYY	(spatial.invF12*(spatial.invF12*es.l_sxx+spatial.invF22*es.l_syx)+spatial.invF22*(spatial.invF12*es.l_sxy+spatial.invF22*es.l_syy))*spatial.detF	1	Spatial identity matrix, material frame, YY component	Domain 1
es.l_sZY	(spatial.invF12*es.l_szx+spatial.invF22*es.l_szy)*spatial.detF	1	Spatial identity matrix, material frame, ZY component	Domain 1
es.l_sXZ	(spatial.invF11*es.l_sxz+spatial.invF21*es.l_syz)*spatial.detF	1	Spatial identity matrix, material frame, XZ component	Domain 1
es.l_sYZ	(spatial.invF12*es.l_sxz+spatial.invF22*es.l_syz)*spatial.detF	1	Spatial identity matrix, material frame, YZ component	Domain 1
es.l_sZZ	es.l_szz*spatial.detF	1	Spatial identity matrix, material frame, ZZ component	Domain 1
es.l_sxx	1	1	Spatial identity matrix, xx component	Domain 1
es.l_syx	0	1	Spatial identity matrix, yx component	Domain 1
es.l_szx	0	1	Spatial	Domain 1

Name	Expression	Unit	Description	Selection
			identity matrix, zx component	
es.I_sxy	0	1	Spatial identity matrix, xy component	Domain 1
es.I_syy	1	1	Spatial identity matrix, yy component	Domain 1
es.I_szy	0	1	Spatial identity matrix, zy component	Domain 1
es.I_sxz	0	1	Spatial identity matrix, xz component	Domain 1
es.I_syz	0	1	Spatial identity matrix, yz component	Domain 1
es.I_szz	1	1	Spatial identity matrix, zz component	Domain 1
es.unTx	es.unTex	Pa	Maxwell upward surface stress tensor, x component	Boundaries 1–12
es.unTy	es.unTey	Pa	Maxwell upward surface stress tensor, y component	Boundaries 1–12
es.unTz	es.unTez	Pa	Maxwell upward surface stress	Boundaries 1–12

Name	Expression	Unit	Description	Selection
			tensor, z component	
es.dnTx	es.dnTex	Pa	Maxwell downward surface stress tensor, x component	Boundaries 1–12
es.dnTy	es.dnTey	Pa	Maxwell downward surface stress tensor, y component	Boundaries 1–12
es.dnTz	es.dnTez	Pa	Maxwell downward surface stress tensor, z component	Boundaries 1–12
es.unx	unx		Normal vector up direction, x component	Boundaries 1–12
es.uny	uny		Normal vector up direction, y component	Boundaries 1–12
es.unz	0		Normal vector up direction, z component	Boundaries 1–12
es.dnx	dnx		Normal vector down direction, x component	Boundaries 1–12
es.dny	dny		Normal vector down direction, y component	Boundaries 1–12
es.dnz	0		Normal	Boundarie

Name	Expression	Unit	Description	Selection
			vector down direction, z component	s 1–12
es.unTex	0	Pa	Maxwell upward electric surface stress tensor, x component	Boundaries 1–12
es.unTey	0	Pa	Maxwell upward electric surface stress tensor, y component	Boundaries 1–12
es.unTez	0	Pa	Maxwell upward electric surface stress tensor, z component	Boundaries 1–12
es.dnTex	-0.5*es.unx*(real(down(es.Dx))*real(down(es.Ex))+real(down(es.Dy))*real(down(es.Ey))+real(down(es.Dz))*real(down(es.Ez)))+real(down(es.Dx))*(real(down(es.Ex))*es.unx+real(down(es.Ey))*es.uny+real(down(es.Ez))*es.unz)	Pa	Maxwell downward electric surface stress tensor, x component	Boundaries 1–12
es.dnTey	-0.5*es.uny*(real(down(es.Dx))*real(down(es.Ex))+real(down(es.Dy))*real(down(es.Ey))+real(down(es.Dz))*real(down(es.Ez)))+real(down(es.Dy))*(real(down(es.Ex))*es.unx+real(down(es.Ey))*es.uny+real(down(es.Ez))*es.unz)	Pa	Maxwell downward electric surface stress tensor, y component	Boundaries 1–12
es.dnTez	-0.5*es.unz*(real(down(es.Dx))*real(down(es.Ex))+real(down(es.Dy))	Pa	Maxwell downward electric	Boundaries 1–12

Name	Expression	Unit	Description	Selection
	*real(down(es.Ey))+real(down(es.Dz))*real(down(es.Ez)))+real(down(es.Dz))*(real(down(es.Ex))*es.unx+real(down(es.Ey))*es.uny+real(down(es.Ez))*es.unz)		surface stress tensor, z component	
es.intWe	es.int_We(es.d*es.dWe)	J	Total electric energy	Global
es.zref	50[ohm]	Ω	Reference impedance	Global

2.5.3 Charge Conservation 1

Charge Conservation 1

SELECTION

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

EQUATIONS

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

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

Constitutive relation D-E

SETTINGS

Description	Value

Description	Value
Dielectric model	Relative permittivity
Relative permittivity	From material

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

PROPERTIES FROM MATERIAL

Property	Material	Property group
Relative permittivity	Water, liquid	Basic

Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	0	C/m^2	Surface charge density	Boundaries 1–12	+ operation
es.epsilonrXX	material.epsilonr11	1	Relative permittivity, XX component	Domain 1	Meta
es.epsilonrYX	material.epsilonr21	1	Relative permittivity, YX component	Domain 1	Meta
es.epsilonrZX	material.epsilonr31	1	Relative permittivity, ZX component	Domain 1	Meta
es.epsilonrXY	material.epsilonr12	1	Relative permittivity, XY component	Domain 1	Meta
es.epsilonrYY	material.epsilonr22	1	Relative permittivity, YY component	Domain 1	Meta
es.epsilonrZY	material.epsilonr32	1	Relative permittivity, ZY	Domain 1	Meta

Name	Expression	Unit	Description	Selection	Details
			component		
es.epsilonrXZ	material.epsilonr13	1	Relative permittivity, XZ component	Domain 1	Meta
es.epsilonrYZ	material.epsilonr23	1	Relative permittivity, YZ component	Domain 1	Meta
es.epsilonrZZ	material.epsilonr33	1	Relative permittivity, ZZ component	Domain 1	Meta
es.epsilonr_iso	material.epsilonr_iso	1	Relative permittivity, isotropic value	Domain 1	Meta
es.Dx	(spatial.F11*es.DX+spatial.F21*es.DY)*spatial.detInvF	C/m^2	Electric displacement field, x component	Domain 1	
es.Dy	(spatial.F12*es.DX+spatial.F22*es.DY)*spatial.detInvF	C/m^2	Electric displacement field, y component	Domain 1	
es.Dz	es.DZ*spatial.detInvF	C/m^2	Electric displacement field, z component	Domain 1	
es.Px	(spatial.F11*es.PX+spatial.F21*es.PY)*spatial.detInvF	C/m^2	Polarization, x component	Domain 1	
es.Py	(spatial.F12*es.PX+spatial.F22*es.PY)*spatial.detInvF	C/m^2	Polarization, y component	Domain 1	
es.Pz	es.PZ*spatial.detInvF	C/m^2	Polarization, z component	Domain 1	
es.normD	sqrt(realdot(es.Dx,es.Dx)+realdot(es.Dy,es.Dy)+realdot(es.Dz,es.Dz))	C/m^2	Electric displacement field norm	Domain 1	

Name	Expression	Unit	Description	Selection	Details
es.normP	sqrt(realdot(es.Px,es.Px)+realdot(es.Py,es.Py)+realdot(es.Pz,es.Pz))	C/m²	Polarization norm	Domain 1	
es.DX	epsilon0_const*es.l_sXX*es.EX+epsilon0_const*es.l_sXY*es.EY+epsilon0_const*es.l_sXZ*es.EZ+es.PX	C/m²	Electric displacement field, X component	Domain 1	
es.DY	epsilon0_const*es.l_sYX*es.EX+epsilon0_const*es.l_sYY*es.EY+epsilon0_const*es.l_sYZ*es.EZ+es.PY	C/m²	Electric displacement field, Y component	Domain 1	
es.DZ	epsilon0_const*es.l_sZX*es.EX+epsilon0_const*es.l_sZY*es.EY+epsilon0_const*es.l_sZZ*es.EZ+es.PZ	C/m²	Electric displacement field, Z component	Domain 1	
es.PX	epsilon0_const*(es.chiXX*es.EX+es.chiXY*es.EY+es.chiXZ*es.EZ)	C/m²	Polarization, X component	Domain 1	+ operation
es.PY	epsilon0_const*(es.chiYX*es.EX+es.chiYY*es.EY+es.chiYZ*es.EZ)	C/m²	Polarization, Y component	Domain 1	+ operation
es.PZ	epsilon0_const*(es.chiZX*es.EX+es.chiZY*es.EY+es.chiZZ*es.EZ)	C/m²	Polarization, Z component	Domain 1	+ operation
es.chiXX	-1+es.epsilonrXX	1	Electric susceptibility, XX component	Domain 1	
es.chiYX	es.epsilonrYX	1	Electric susceptibility	Domain 1	

Name	Expression	Unit	Description	Selection	Details
			, YX component		
es.chiZX	es.epsilonrZX	1	Electric susceptibility, ZX component	Domain 1	
es.chiXY	es.epsilonrXY	1	Electric susceptibility, XY component	Domain 1	
es.chiYY	-1+es.epsilonrYY	1	Electric susceptibility, YY component	Domain 1	
es.chiZY	es.epsilonrZY	1	Electric susceptibility, ZY component	Domain 1	
es.chiXZ	es.epsilonrXZ	1	Electric susceptibility, XZ component	Domain 1	
es.chiYZ	es.epsilonrYZ	1	Electric susceptibility, YZ component	Domain 1	
es.chiZZ	-1+es.epsilonrZZ	1	Electric susceptibility, ZZ component	Domain 1	
es.Ex	spatial.invF11*es.EX+spatial.invF12*es.EY	V/m	Electric field, x component	Domain 1	
es.Ey	spatial.invF21*es.EX+spatial.invF22*es.EY	V/m	Electric field, y component	Domain 1	
es.Ez	es.EZ	V/m	Electric field, z component	Domain 1	
es.tEx	spatial.invF11*es.tEX+spatial.invF12*es.tEY	V/m	Tangential electric field, x component	Boundaries 1–12	
es.tEy	spatial.invF21*es.tEX+spatial.inv	V/m	Tangential electric field,	Boundaries 1–12	

Name	Expression	Unit	Description	Selection	Details
	F22*es.tEY		y component		
es.tEz	es.tEZ	V/m	Tangential electric field, z component	Boundaries 1–12	
es.EX	-VX	V/m	Electric field, X component	Domain 1	+ operation
es.EY	-VY	V/m	Electric field, Y component	Domain 1	+ operation
es.EZ	0	V/m	Electric field, Z component	Domain 1	+ operation
es.tEX	-VTX	V/m	Tangential electric field, X component	Boundaries 1–12	
es.tEY	-VTY	V/m	Tangential electric field, Y component	Boundaries 1–12	
es.tEZ	0	V/m	Tangential electric field, Z component	Boundaries 1–12	
es.normE	sqrt(realdot(es.Ex,es.Ex)+realdot(es.Ey,es.Ey)+realdot(es.Ez,es.Ez))	V/m	Electric field norm	Domain 1	
es.Jx	(spatial.F11*es.JdX+spatial.F21*es.JdY)*spatial.detInvF	A/m^2	Current density, x component	Domain 1	+ operation
es.Jy	(spatial.F12*es.JdX+spatial.F22*es.JdY)*spatial.detInvF	A/m^2	Current density, y component	Domain 1	+ operation
es.Jz	es.JdZ*spatial.detInvF	A/m^2	Current density, z component	Domain 1	+ operation
es.JX	es.JdX	A/m^2	Current density, X component	Domain 1	+ operation
es.JY	es.JdY	A/m^2	Current density, Y	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			component		
es.JZ	es.JdZ	A/m²	Current density, Z component	Domain 1	+ operation
es.JdX	0	A/m²	Displacement current density, X component	Domain 1	
es.JdY	0	A/m²	Displacement current density, Y component	Domain 1	
es.JdZ	0	A/m²	Displacement current density, Z component	Domain 1	
es.normJ	sqrt(realdot(es.JX,es.JX)+realdot(es.JY,es.JY)+realdot(es.JZ,es.JZ))	A/m²	Current density norm	Domain 1	
es.ccn1.nJ	es.unx*(spatial.invF11*down(es.JX)+spatial.invF12*down(es.JY))+es.uny*(spatial.invF21*down(es.JX)+spatial.invF22*down(es.JY))+es.unz*down(es.JZ)	A/m²	Inward current density	Boundaries 1–12	
es.W	es.We	J/m³	Energy density	Domain 1	+ operation
es.dWe	es.We	J/m³	Integrand for total electric energy	Domain 1	Meta
es.We	0.5*epsilon0_const*(((es.l_sXX+es.chiXX)*es.EX+(es.l_sXY+es.chiXY)*es.EY+(es.l_sXZ+es.chiXZ)*es.EZ)*es.EX+((es.l_sYX+es.chiYX)*es.EX+(es.l_s	J/m³	Electric energy density	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	YY+es.chiYY)*es.EY+(es.l_sYZ+es.chiYZ)*es.EZ)*es.EY+((es.l_sZX+es.chiZX)*es.EX+(es.l_sZY+es.chiZY)*es.EY+(es.l_sZZ+es.chiZZ)*es.EZ)*es.EZ)*spatial.detInvF				

Shape functions

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

Weak expressions

Weak expression	Integration order	Integration frame	Selection
-(es.DX*test(VX)+es.DY*test(VY))*es.d	4	Material	Domain 1

2.5.4 Zero Charge 1

Zero Charge 1

SELECTION

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

EQUATIONS

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

Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	0	C/m^2	Surface charge density	Boundaries 2, 4–10	+ operation

Shape functions

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

2.5.5 Initial Values 1

Initial Values 1

SELECTION

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

SETTINGS

Description	Value
Electric potential	0

2.5.6 Electric Potential 1

Electric Potential 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 11–12

EQUATIONS

$$V = V_0$$

Electric potential

SETTINGS

Description	Value
Electric potential	30

Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	(es.unx*(spatial.F11*down(es.DX)+spatial.F21*down(es.DY))+es.uny*(spatial.F12*down(es.DX)+spatial.F22*down(es.DY))+es.unz*down(es.DZ))*spatial.detInvF	C/m^2	Surface charge density	Boundaries 11–12	+ operation
es.V0	30	V	Electric potential	Boundaries 11–12	

Constraints

Constraint	Constraint force	Shape function	Selection	Details
es.V0-V	test(es.V0-V)	Lagrange (Quadratic)	Boundaries 11–12	Elemental

2.5.7 Ground 1

Ground 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 1, 3

EQUATIONS

$V = 0$

Variables

Name	Expression	Unit	Description	Selection	Details
es.nD	(es.unx*(spatial.F11*down(es.DX)+spatial.F21*down(es.DY))+es.uny*(spatial.F12*down(es.DX)+spatial.F22*down(es.DY))+es.unz*down(es.DZ))*spatial.detInvF	C/m²	Surface charge density	Boundaries 1, 3	+ operation

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-V	test(-V)	Lagrange (Quadratic)	Boundaries 1, 3	Elemental

2.5.8 Space Charge Density 1

Space Charge Density 1

SELECTION

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

EQUATIONS

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

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Variables

Name	Expression	Unit	Description	Selection	Details

Name	Expression	Unit	Description	Selection	Details
es.scd1.rhoq	(cK+cH3O-cCl-cBEAD-cOH)*e_const*N_A_const	C/m³	Space charge density	Domain 1	
es.rhoq	es.scd1.rhoq	C/m³	Space charge density	Domain 1	+ operation

Weak expressions

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

2.6 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics
Chemical Reaction Engineering Module

Transport of Diluted Species

SELECTION

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

EQUATIONS

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

2.6.1 Interface settings

Discretization

SETTINGS

Description	Value
Concentration	Quadratic

Transport mechanisms

SETTINGS

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

2.6.2 Variables

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

Name	Expression	Unit	Description	Selection	Details
			species absorbed to the solid		on
tds.cP_cCl	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
tds.KP_cCl	0	m^3/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
tds.KP_cCl	0	m^3/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
tds.R_cH3O	0	mol/(m^3·s)	Total rate expression	Domain 1	+ operation
tds.cP_cH3O	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
tds.cP_cH3O	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
tds.KP_cH3O	0	m^3/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
tds.KP_cH3O	0	m^3/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
tds.R_cOH	0	mol/(m^3·s)	Total rate expression	Domain 1	+ operation
tds.cP_cOH	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
tds.cP_cOH	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation

Name	Expression	Unit	Description	Selection	Details
tds.KP_cOH	0	m^3/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
tds.KP_cOH	0	m^3/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
tds.R_cBEAD	0	$mol/(m^3 \cdot s)$	Total rate expression	Domain 1	+ operation
tds.cP_cBEAD	0	mol/kg	Concentration species absorbed to the solid	Domain 1	+ operation
tds.cP_cBEAD	0	mol/kg	Concentration species absorbed to the solid	Boundaries 1–12	+ operation
tds.KP_cBEAD	0	m^3/kg	Adsorption isotherm, first concentration derivative	Domain 1	+ operation
tds.KP_cBEAD	0	m^3/kg	Adsorption isotherm, first concentration derivative	Boundaries 1–12	+ operation
tds.epsilon_p	1	1	Porosity	Domain 1	
tds.theta	tds.epsilon_p	1	Liquid volume fraction	Domain 1	
tds.av	0	1	Gas volume fraction	Domain 1	
tds.nx	dnx	1	Normal vector, x component	Boundaries 1–12	
tds.ny	dny	1	Normal vector, y component	Boundaries 1–12	
tds.nz	0	1	Normal vector, z component	Boundaries 1–12	
tds.nxmesh	dnxmesh	1	Normal vector (mesh), x	Boundaries 1–12	

Name	Expression	Unit	Description	Selection	Details
			component		
tds.nymesh	dnymesh	1	Normal vector (mesh), y component	Boundaries 1–12	
tds.nzmesh	0	1	Normal vector (mesh), z component	Boundaries 1–12	
tds.nxc	root.nxc/tds.ncLen	1	Normal vector, x component	Boundaries 1–12	
tds.nyc	root.nyc/tds.ncLen	1	Normal vector, y component	Boundaries 1–12	
tds.nzc	0	1	Normal vector, z component	Boundaries 1–12	
tds.ncLen	sqrt(root.nxc^2+root.nyc^2+eps)	1	Help variable	Boundaries 1–12	
tds.cbf_cK	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	
tds.u	0	m/s	Velocity field, x component	Domain 1	
tds.v	0	m/s	Velocity field, y component	Domain 1	
tds.w	0	m/s	Velocity field, z component	Domain 1	
tds.cbf_cCl	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	
tds.cbf_cH3O	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	
tds.cbf_cOH	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	
tds.cbf_cBEAD	0	mol/(m^2·s)	Convective boundary flux	Boundaries 1–12	

2.6.3 Transport Properties 1

Transport Properties 1

SELECTION

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

EQUATIONS

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

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

Convection

SETTINGS

Description	Value
Velocity field	Velocity field (spf)

Diffusion

SETTINGS

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

Description	Value
Diffusion coefficient	{{dH3O, 0, 0}, {0, dH3O, 0}, {0, 0, dH3O}}
Diffusion coefficient	User defined
Diffusion coefficient	{{dOH, 0, 0}, {0, dOH, 0}, {0, 0, dOH}}
Diffusion coefficient	User defined
Diffusion coefficient	{{dBEAD, 0, 0}, {0, dBEAD, 0}, {0, 0, dBEAD}}

Migration in electric field

SETTINGS

Description	Value
Electric potential	Electric potential (es)
Mobility	Nernst - Einstein relation
Charge number	{1, -1, 1, -1, -1}

Coordinate system selection

SETTINGS

Description	Value
Coordinate system	Global coordinate system

Model input

SETTINGS

Description	Value
Temperature	Common model input

Variables

Name	Expression	Unit	Description	Selection	Details
domflux.cKx	tds.dflux_cKx+tds.mflux_cKx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cKy	tds.dflux_cKy+tds.mflux_cKy	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cClx	tds.dflux_cClx+tds.mflux_cClx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cCly	tds.dflux_cCly+tds.mflux_cC	mol/(m²·s)	Domain flux, y component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	ly				
domflux.cH3Ox	tds.dflux_cH3Ox+tds.mflux_cH3Ox	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cH3Oy	tds.dflux_cH3Oy+tds.mflux_cH3Oy	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cOHx	tds.dflux_cOHx+tds.mflux_cOHx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cOHy	tds.dflux_cOHy+tds.mflux_cOHy	mol/(m²·s)	Domain flux, y component	Domain 1	
domflux.cBEADx	tds.dflux_cBEADx+tds.mflux_cBEADx	mol/(m²·s)	Domain flux, x component	Domain 1	
domflux.cBEADy	tds.dflux_cBEADy+tds.mflux_cBEADy	mol/(m²·s)	Domain flux, y component	Domain 1	
tds.ndflux_cK	tds.dflux_cKx*tds.nxc+tds.dflux_cKy*tds.nyc+tds.dflux_cKz*tds.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	
tds.ncflux_cK	tds.cflux_cKx*tds.nxc+tds.cflux_cKy*tds.nyc+tds.cflux_cKz*tds.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–12	
tds.nmflux_cK	tds.mflux_cKx*tds.nxc+tds.mflux_cKy*tds.nyc+tds.mflux_cKz*tds.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	
tds.ntflux_cK	tds.bndFlux_cK+tds.cflux_cKx*tds.nxc+tds.cflux_cKy*tds.nyc+tds.cflux_cKz*tds.nzc	mol/(m²·s)	Normal total flux	Boundaries 1–12	
tds.ndflux_cCl	tds.dflux_cClx*tds.nxc+tds.dflux_cCly*tds.nyc+tds.dflux	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	

Name	Expression	Unit	Description	Selection	Details
	_cClz*tds.nzc				
tds.ncflux_cCl	tds.cflux_cClx*tds.nxc+tds.cflux_cCly*tds.nyc+tds.cflux_cClz*tds.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–12	
tds.nmflux_cCl	tds.mflux_cClx*tds.nxc+tds.mflux_cCly*tds.nyc+tds.mflux_cClz*tds.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	
tds.ntflux_cCl	tds.bndFlux_cCl+tds.cflux_cClx*tds.nxc+tds.cflux_cCly*tds.nyc+tds.cflux_cClz*tds.nzc	mol/(m²·s)	Normal total flux	Boundaries 1–12	
tds.ndflux_cH3O	tds.dflux_cH3Ox*tds.nxc+tds.dflux_cH3Oy*tds.nyc+tds.dflux_cH3Oz*tds.nzc	mol/(m²·s)	Normal diffusive flux	Boundaries 1–12	
tds.ncflux_cH3O	tds.cflux_cH3Ox*tds.nxc+tds.cflux_cH3Oy*tds.nyc+tds.cflux_cH3Oz*tds.nzc	mol/(m²·s)	Normal convective flux	Boundaries 1–12	
tds.nmflux_cH3O	tds.mflux_cH3Ox*tds.nxc+tds.mflux_cH3Oy*tds.nyc+tds.mflux_cH3Oz*tds.nzc	mol/(m²·s)	Normal electrophoretic flux	Boundaries 1–12	
tds.ntflux_cH3O	tds.bndFlux_cH3O+tds.cflux_cH3Ox*tds.nxc+tds.cflux_cH3Oy*tds.nyc+tds.cflux_cH3Oz*tds.nzc	mol/(m²·s)	Normal total flux	Boundaries 1–12	
tds.ndflux_cO	tds.dflux_cOH	mol/(m	Normal	Boundarie	

Name	Expression	Unit	Description	Selection	Details
H	x*tds.nxc+tds.dflux_cOHy*tds.nyc+tds.dflux_cOHz*tds.nzc	^{2}·s)	diffusive flux	s 1–12	
tds.ncflux_cOH	tds.cflux_cOHx*tds.nxc+tds.cflux_cOHy*tds.nyc+tds.cflux_cOHz*tds.nzc	mol/(m^2·s)	Normal convective flux	Boundaries 1–12	
tds.nmflux_cOH	tds.mflux_cOHx*tds.nxc+tds.mflux_cOHy*tds.nyc+tds.mflux_cOHz*tds.nzc	mol/(m^2·s)	Normal electrophoretic flux	Boundaries 1–12	
tds.ntflux_cOH	tds.bndFlux_cOH+tds.cflux_cOHx*tds.nxc+tds.cflux_cOHy*tds.nyc+tds.cflux_cOHz*tds.nzc	mol/(m^2·s)	Normal total flux	Boundaries 1–12	
tds.ndflux_cBEAD	tds.dflux_cBEADx*tds.nxc+tds.dflux_cBEADy*tds.nyc+tds.dflux_cBEADz*tds.nzc	mol/(m^2·s)	Normal diffusive flux	Boundaries 1–12	
tds.ncflux_cBEAD	tds.cflux_cBEADx*tds.nxc+tds.cflux_cBEADy*tds.nyc+tds.cflux_cBEADz*tds.nzc	mol/(m^2·s)	Normal convective flux	Boundaries 1–12	
tds.nmflux_cBEAD	tds.mflux_cBEADx*tds.nxc+tds.mflux_cBEADy*tds.nyc+tds.mflux_cBEADz*tds.nzc	mol/(m^2·s)	Normal electrophoretic flux	Boundaries 1–12	
tds.ntflux_cBEAD	tds.bndFlux_cBEAD+tds.cflux_cBEADx*td	mol/(m^2·s)	Normal total flux	Boundaries 1–12	

Name	Expression	Unit	Description	Selection	Details
	s.nxc+tds.cflux_cBEADy*tds.nyc+tds.cflux_cBEADz*tds.nzc				
tds.u	model.input.u1	m/s	Velocity field, x component	Domain 1	Meta
tds.v	model.input.u2	m/s	Velocity field, y component	Domain 1	Meta
tds.w	model.input.u3	m/s	Velocity field, z component	Domain 1	Meta
tds.D_cKxx	dK	m^2/s	Diffusion coefficient, xx component	Domain 1	+ operation
tds.D_cKyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	+ operation
tds.D_cKzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	+ operation
tds.D_cKxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	+ operation
tds.D_cKyy	dK	m^2/s	Diffusion coefficient, yy component	Domain 1	+ operation
tds.D_cKzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	+ operation
tds.D_cKxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	+ operation
tds.D_cKyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	+ operation
tds.D_cKzz	dK	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.D_cClxx	dCl	m^2/s	Diffusion coefficient, xx component	Domain 1	+ operation
tds.D_cClyx	0	m^2/s	Diffusion coefficient, yx	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
			component		
tds.D_cClzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	+ operation
tds.D_cClxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	+ operation
tds.D_cClyy	dCl	m^2/s	Diffusion coefficient, yy component	Domain 1	+ operation
tds.D_cClzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	+ operation
tds.D_cClxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	+ operation
tds.D_cClyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	+ operation
tds.D_cClzz	dCl	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.D_cH3Oxx	dH3O	m^2/s	Diffusion coefficient, xx component	Domain 1	+ operation
tds.D_cH3Oyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	+ operation
tds.D_cH3Ozx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	+ operation
tds.D_cH3Oxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	+ operation
tds.D_cH3Oyy	dH3O	m^2/s	Diffusion coefficient, yy component	Domain 1	+ operation
tds.D_cH3Ozy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	+ operation
tds.D_cH3Oxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
tds.D_cH3Oyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	+ operation
tds.D_cH3Ozz	dH3O	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.D_cOHxx	dOH	m^2/s	Diffusion coefficient, xx component	Domain 1	+ operation
tds.D_cOHyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	+ operation
tds.D_cOHzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	+ operation
tds.D_cOHxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	+ operation
tds.D_cOHyy	dOH	m^2/s	Diffusion coefficient, yy component	Domain 1	+ operation
tds.D_cOHzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	+ operation
tds.D_cOHxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	+ operation
tds.D_cOHyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	+ operation
tds.D_cOHzz	dOH	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.D_cBEADxx	dBEAD	m^2/s	Diffusion coefficient, xx component	Domain 1	+ operation
tds.D_cBEADyx	0	m^2/s	Diffusion coefficient, yx component	Domain 1	+ operation
tds.D_cBEADzx	0	m^2/s	Diffusion coefficient, zx component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
tds.D_cBEADxy	0	m^2/s	Diffusion coefficient, xy component	Domain 1	+ operation
tds.D_cBEADyy	dBEAD	m^2/s	Diffusion coefficient, yy component	Domain 1	+ operation
tds.D_cBEADzy	0	m^2/s	Diffusion coefficient, zy component	Domain 1	+ operation
tds.D_cBEADxz	0	m^2/s	Diffusion coefficient, xz component	Domain 1	+ operation
tds.D_cBEADyz	0	m^2/s	Diffusion coefficient, yz component	Domain 1	+ operation
tds.D_cBEADzz	dBEAD	m^2/s	Diffusion coefficient, zz component	Domain 1	+ operation
tds.Dav_cK	0.5*(tds.D_cKxx+tds.D_cKyy)	m^2/s	Average diffusion coefficient	Domain 1	
tds.Dav_cCl	0.5*(tds.D_cClxx+tds.D_cClyy)	m^2/s	Average diffusion coefficient	Domain 1	
tds.Dav_cH3O	0.5*(tds.D_cH3Oxx+tds.D_cH3Oyy)	m^2/s	Average diffusion coefficient	Domain 1	
tds.Dav_cOH	0.5*(tds.D_cOHxx+tds.D_cOHyy)	m^2/s	Average diffusion coefficient	Domain 1	
tds.Dav_cBEAD	0.5*(tds.D_cBEADxx+tds.D_cBEADyy)	m^2/s	Average diffusion coefficient	Domain 1	
tds.tflux_cKx	tds.dflux_cKx+tds.mflux_cKx+tds.cflux_cKx	$mol/(m^2 \cdot s)$	Total flux, x component	Domain 1	+ operation
tds.tflux_cKy	tds.dflux_cKy+tds.mflux_cKy+tds.cflux_cKy	$mol/(m^2 \cdot s)$	Total flux, y component	Domain 1	+ operation
tds.tflux_cKz	tds.dflux_cKz+tds.mflux_cK	$mol/(m^2 \cdot s)$	Total flux, z component	Domain 1	+ operation

Name	Expression	Unit	Description	Selection	Details
	z+tds.cflux_cKz				
tds.dfluxMag_cK	sqrt(tds.dflux_cKx^2+tds.dflux_cKy^2+tds.dflux_cKz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cK	sqrt(tds.tflux_cKx^2+tds.tflux_cKy^2+tds.tflux_cKz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
tds.mflux_cKx	tds.z_cK*F_const*cK*(-tds.um_cKxx*d(tds.V,x)-tds.um_cKxy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
tds.mflux_cKy	tds.z_cK*F_const*cK*(-tds.um_cKyx*d(tds.V,x)-tds.um_cKyy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
tds.mflux_cKz	tds.z_cK*F_const*cK*(-tds.um_cKzx*d(tds.V,x)-tds.um_cKzy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
tds.tflux_cClx	tds.dflux_cClx+tds.mflux_cClx+tds.cflux_cClx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
tds.tflux_cCly	tds.dflux_cCly+tds.mflux_cCly+tds.cflux_cCly	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
tds.tflux_cClz	tds.dflux_cClz+tds.mflux_cClz+tds.cflux_cClz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cCl	sqrt(tds.dflux_cClx^2+tds.dflux_cCly^2+t	mol/(m²·s)	Diffusive flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	ds.dflux_cClz^2)				
tds.tfluxMag_cCl	sqrt(tds.tflux_cClx^2+tds.tflux_cCly^2+tds.tflux_cClz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	
tds.mflux_cClx	tds.z_cCl*F_const*cCl*(-tds.um_cClxx*d(tds.V,x)-tds.um_cClxy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
tds.mflux_cCly	tds.z_cCl*F_const*cCl*(-tds.um_cClyx*d(tds.V,x)-tds.um_cClyy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
tds.mflux_cClz	tds.z_cCl*F_const*cCl*(-tds.um_cClzx*d(tds.V,x)-tds.um_cClzy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
tds.tflux_cH3Ox	tds.dflux_cH3Ox+tds.mflux_cH3Ox+tds.cflux_cH3Ox	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
tds.tflux_cH3Oy	tds.dflux_cH3Oy+tds.mflux_cH3Oy+tds.cflux_cH3Oy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
tds.tflux_cH3Oz	tds.dflux_cH3Oz+tds.mflux_cH3Oz+tds.cflux_cH3Oz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cH3O	sqrt(tds.dflux_cH3Ox^2+tds.dflux_cH3Oy^2+tds.dflux_cH3Oz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cH3O	sqrt(tds.tflux_cH3Ox^2+tds	mol/(m²·s)	Total flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	.tflux_cH3Oy^2+tds.tflux_cH3Oz^2)				
tds.mflux_cH3Ox	tds.z_cH3O*F_const*cH3O*(-tds.um_cH3Oxx*d(tds.V,x)-tds.um_cH3Oxy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
tds.mflux_cH3Oy	tds.z_cH3O*F_const*cH3O*(-tds.um_cH3Oyx*d(tds.V,x)-tds.um_cH3Oyy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
tds.mflux_cH3Oz	tds.z_cH3O*F_const*cH3O*(-tds.um_cH3Ozx*d(tds.V,x)-tds.um_cH3Ozy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
tds.tflux_cOHx	tds.dflux_cOHx+tds.mflux_cOHx+tds.cflux_cOHx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
tds.tflux_cOHy	tds.dflux_cOHy+tds.mflux_cOHy+tds.cflux_cOHy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
tds.tflux_cOHz	tds.dflux_cOHz+tds.mflux_cOHz+tds.cflux_cOHz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cOH	sqrt(tds.dflux_cOHx^2+tds.dflux_cOHy^2+tds.dflux_cOHz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cOH	sqrt(tds.tflux_cOHx^2+tds.tflux_cOHy^2+tds.tflux_cO	mol/(m²·s)	Total flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	Hz^2)				
tds.mflux_cOHx	tds.z_cOH*F_const*cOH*(-tds.um_cOHxx*d(tds.V,x)-tds.um_cOHxy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
tds.mflux_cOHy	tds.z_cOH*F_const*cOH*(-tds.um_cOHyx*d(tds.V,x)-tds.um_cOHyy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
tds.mflux_cOHz	tds.z_cOH*F_const*cOH*(-tds.um_cOHzx*d(tds.V,x)-tds.um_cOHzy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
tds.tflux_cBEADx	tds.dflux_cBEADx+tds.mflux_cBEADx+tds.cflux_cBEADx	mol/(m²·s)	Total flux, x component	Domain 1	+ operation
tds.tflux_cBEADy	tds.dflux_cBEADy+tds.mflux_cBEADy+tds.cflux_cBEADy	mol/(m²·s)	Total flux, y component	Domain 1	+ operation
tds.tflux_cBEADz	tds.dflux_cBEADz+tds.mflux_cBEADz+tds.cflux_cBEADz	mol/(m²·s)	Total flux, z component	Domain 1	+ operation
tds.dfluxMag_cBEAD	sqrt(tds.dflux_cBEADx^2+tds.dflux_cBEADy^2+tds.dflux_cBEADz^2)	mol/(m²·s)	Diffusive flux magnitude	Domain 1	
tds.tfluxMag_cBEAD	sqrt(tds.tflux_cBEADx^2+tds.tflux_cBEADy^2+tds.tflux_cBEADz^2)	mol/(m²·s)	Total flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
tds.mflux_cBEADx	tds.z_cBEAD*F_const*cBEAD*(-tds.um_cBEADxx*d(tds.V,x)-tds.um_cBEADxy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, x component	Domain 1	
tds.mflux_cBEADy	tds.z_cBEAD*F_const*cBEAD*(-tds.um_cBEADyx*d(tds.V,x)-tds.um_cBEADyy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, y component	Domain 1	
tds.mflux_cBEADz	tds.z_cBEAD*F_const*cBEAD*(-tds.um_cBEADzx*d(tds.V,x)-tds.um_cBEADzy*d(tds.V,y))	mol/(m²·s)	Electrophoretic flux, z component	Domain 1	
tds.dflux_cKx	-tds.D_cKxx*cKx-tds.D_cKxy*cKy	mol/(m²·s)	Diffusive flux, x component	Domain 1	
tds.dflux_cKy	-tds.D_cKyx*cKx-tds.D_cKyy*cKy	mol/(m²·s)	Diffusive flux, y component	Domain 1	
tds.dflux_cKz	-tds.D_cKzx*cKx-tds.D_cKzy*cKy	mol/(m²·s)	Diffusive flux, z component	Domain 1	
tds.grad_cKx	cKx	mol/m⁴	Concentration gradient, x component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
tds.grad_cKy	cKy	mol/m^4	Concentration gradient, y component	Domain 1	
tds.grad_cKz	0	mol/m^4	Concentration gradient, z component	Domain 1	
tds.dflux_cClx	-tds.D_cClxx*cClx-tds.D_cClxy*cCly	mol/(m^2·s)	Diffusive flux, x component	Domain 1	
tds.dflux_cCly	-tds.D_cClyx*cClx-tds.D_cClyy*cCly	mol/(m^2·s)	Diffusive flux, y component	Domain 1	
tds.dflux_cClz	-tds.D_cClzx*cClx-tds.D_cClzy*cCly	mol/(m^2·s)	Diffusive flux, z component	Domain 1	
tds.grad_cClx	cClx	mol/m^4	Concentration gradient, x component	Domain 1	
tds.grad_cCly	cCly	mol/m^4	Concentration gradient, y component	Domain 1	
tds.grad_cClz	0	mol/m^4	Concentration gradient, z component	Domain 1	
tds.dflux_cH3Ox	-tds.D_cH3Oxx*cH3Ox-tds.D_cH3Oxy*cH3Oy	mol/(m^2·s)	Diffusive flux, x component	Domain 1	
tds.dflux_cH3Oy	-tds.D_cH3Oyx*cH3Ox-tds.D_cH3Oyy*cH3Oy	mol/(m^2·s)	Diffusive flux, y component	Domain 1	
tds.dflux_cH3Oz	-tds.D_cH3Ozx*cH3Ox-tds.D_cH3Ozy	mol/(m^2·s)	Diffusive flux, z component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	*cH3Oy				
tds.grad_cH3Ox	cH3Ox	mol/m^4	Concentration gradient, x component	Domain 1	
tds.grad_cH3Oy	cH3Oy	mol/m^4	Concentration gradient, y component	Domain 1	
tds.grad_cH3Oz	0	mol/m^4	Concentration gradient, z component	Domain 1	
tds.dflux_cOHx	-tds.D_cOHxx*cOHx-tds.D_cOHxy*cOHy	mol/(m^2·s)	Diffusive flux, x component	Domain 1	
tds.dflux_cOHy	-tds.D_cOHyx*cOHx-tds.D_cOHyy*cOHy	mol/(m^2·s)	Diffusive flux, y component	Domain 1	
tds.dflux_cOHz	-tds.D_cOHzx*cOHx-tds.D_cOHzy*cOHy	mol/(m^2·s)	Diffusive flux, z component	Domain 1	
tds.grad_cOHx	cOHx	mol/m^4	Concentration gradient, x component	Domain 1	
tds.grad_cOHy	cOHy	mol/m^4	Concentration gradient, y component	Domain 1	
tds.grad_cOHz	0	mol/m^4	Concentration gradient, z component	Domain 1	
tds.dflux_cBEADx	-tds.D_cBEADxx*cBEADx-tds.D_cBEADxy*cBEADy	mol/(m^2·s)	Diffusive flux, x component	Domain 1	
tds.dflux_cBEADy	-tds.D_cBEADyx*cBEADx-tds.D_cBEADyy*cBEADy	mol/(m^2·s)	Diffusive flux, y component	Domain 1	

Name	Expression	Unit	Description	Selection	Details
tds.dflux_cBEADz	-tds.D_cBEADzx*cBEADx-tds.D_cBEADzy*cBEADy	mol/(m^2·s)	Diffusive flux, z component	Domain 1	
tds.grad_cBEADx	cBEADx	mol/m^4	Concentration gradient, x component	Domain 1	
tds.grad_cBEADy	cBEADy	mol/m^4	Concentration gradient, y component	Domain 1	
tds.grad_cBEADz	0	mol/m^4	Concentration gradient, z component	Domain 1	
tds.um_cKxx	tds.D_cKxx/(R_const*tds.T)	s·mol/kg	Mobility, xx component	Domain 1	
tds.um_cKyx	tds.D_cKyx/(R_const*tds.T)	s·mol/kg	Mobility, yx component	Domain 1	
tds.um_cKzx	tds.D_cKzx/(R_const*tds.T)	s·mol/kg	Mobility, zx component	Domain 1	
tds.um_cKxy	tds.D_cKxy/(R_const*tds.T)	s·mol/kg	Mobility, xy component	Domain 1	
tds.um_cKyy	tds.D_cKyy/(R_const*tds.T)	s·mol/kg	Mobility, yy component	Domain 1	
tds.um_cKzy	tds.D_cKzy/(R_const*tds.T)	s·mol/kg	Mobility, zy component	Domain 1	
tds.um_cKxz	tds.D_cKxz/(R_const*tds.T)	s·mol/kg	Mobility, xz component	Domain 1	
tds.um_cKyz	tds.D_cKyz/(R_const*tds.T)	s·mol/kg	Mobility, yz component	Domain 1	
tds.um_cKzz	tds.D_cKzz/(R_const*tds.T)	s·mol/kg	Mobility, zz component	Domain 1	
tds.z_cK	1	1	Charge number	Domain 1	
tds.um_cClxx	tds.D_cClxx/(R_const*tds.T)	s·mol/kg	Mobility, xx component	Domain 1	
tds.um_cClyx	tds.D_cClyx/(R_const*tds.T)	s·mol/kg	Mobility, yx component	Domain 1	
tds.um_cClzx	tds.D_cClzx/(R_const*tds.T)	s·mol/kg	Mobility, zx component	Domain 1	
tds.um_cClxy	tds.D_cClxy/(	s·mol/k	Mobility, xy	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	R_const*tds.T)	g	component		
tds.um_cClyy	tds.D_cClyy/(R_const*tds.T)	s·mol/kg	Mobility, yy component	Domain 1	
tds.um_cClzy	tds.D_cClzy/(R_const*tds.T)	s·mol/kg	Mobility, zy component	Domain 1	
tds.um_cClxz	tds.D_cClxz/(R_const*tds.T)	s·mol/kg	Mobility, xz component	Domain 1	
tds.um_cClyz	tds.D_cClyz/(R_const*tds.T)	s·mol/kg	Mobility, yz component	Domain 1	
tds.um_cClzz	tds.D_cClzz/(R_const*tds.T)	s·mol/kg	Mobility, zz component	Domain 1	
tds.z_cCl	-1	1	Charge number	Domain 1	
tds.um_cH3Oxx	tds.D_cH3Oxx/(R_const*tds.T)	s·mol/kg	Mobility, xx component	Domain 1	
tds.um_cH3Oyx	tds.D_cH3Oyx/(R_const*tds.T)	s·mol/kg	Mobility, yx component	Domain 1	
tds.um_cH3Ozx	tds.D_cH3Ozx/(R_const*tds.T)	s·mol/kg	Mobility, zx component	Domain 1	
tds.um_cH3Oxy	tds.D_cH3Oxy/(R_const*tds.T)	s·mol/kg	Mobility, xy component	Domain 1	
tds.um_cH3Oyy	tds.D_cH3Oyy/(R_const*tds.T)	s·mol/kg	Mobility, yy component	Domain 1	
tds.um_cH3Ozy	tds.D_cH3Ozy/(R_const*tds.T)	s·mol/kg	Mobility, zy component	Domain 1	
tds.um_cH3Oxz	tds.D_cH3Oxz/(R_const*tds.T)	s·mol/kg	Mobility, xz component	Domain 1	
tds.um_cH3Oyz	tds.D_cH3Oyz/(R_const*tds.T)	s·mol/kg	Mobility, yz component	Domain 1	
tds.um_cH3Ozz	tds.D_cH3Ozz/(R_const*tds.T)	s·mol/kg	Mobility, zz component	Domain 1	
tds.z_cH3O	1	1	Charge number	Domain 1	

Name	Expression	Unit	Description	Selection	Details
tds.um_cOHxx	tds.D_cOHxx/(R_const*tds.T)	s·mol/kg	Mobility, xx component	Domain 1	
tds.um_cOHyx	tds.D_cOHyx/(R_const*tds.T)	s·mol/kg	Mobility, yx component	Domain 1	
tds.um_cOHzx	tds.D_cOHzx/(R_const*tds.T)	s·mol/kg	Mobility, zx component	Domain 1	
tds.um_cOHxy	tds.D_cOHxy/(R_const*tds.T)	s·mol/kg	Mobility, xy component	Domain 1	
tds.um_cOHyy	tds.D_cOHyy/(R_const*tds.T)	s·mol/kg	Mobility, yy component	Domain 1	
tds.um_cOHzy	tds.D_cOHzy/(R_const*tds.T)	s·mol/kg	Mobility, zy component	Domain 1	
tds.um_cOHxz	tds.D_cOHxz/(R_const*tds.T)	s·mol/kg	Mobility, xz component	Domain 1	
tds.um_cOHyz	tds.D_cOHyz/(R_const*tds.T)	s·mol/kg	Mobility, yz component	Domain 1	
tds.um_cOHzz	tds.D_cOHzz/(R_const*tds.T)	s·mol/kg	Mobility, zz component	Domain 1	
tds.z_cOH	-1	1	Charge number	Domain 1	
tds.um_cBEADxx	tds.D_cBEADxx/(R_const*tds.T)	s·mol/kg	Mobility, xx component	Domain 1	
tds.um_cBEADyx	tds.D_cBEADyx/(R_const*tds.T)	s·mol/kg	Mobility, yx component	Domain 1	
tds.um_cBEADzx	tds.D_cBEADzx/(R_const*tds.T)	s·mol/kg	Mobility, zx component	Domain 1	
tds.um_cBEADxy	tds.D_cBEADxy/(R_const*tds.T)	s·mol/kg	Mobility, xy component	Domain 1	
tds.um_cBEADyy	tds.D_cBEADyy/(R_const*tds.T)	s·mol/kg	Mobility, yy component	Domain 1	
tds.um_cBEA	tds.D_cBEADz	s·mol/k	Mobility, zy	Domain 1	

Name	Expression	Unit	Description	Selection	Details
Dzy	y/(R_const*tds.T)	g	component		
tds.um_cBEADxz	tds.D_cBEADxz/(R_const*tds.T)	s·mol/kg	Mobility, xz component	Domain 1	
tds.um_cBEADyz	tds.D_cBEADyz/(R_const*tds.T)	s·mol/kg	Mobility, yz component	Domain 1	
tds.um_cBEADzz	tds.D_cBEADzz/(R_const*tds.T)	s·mol/kg	Mobility, zz component	Domain 1	
tds.z_cBEAD	-1	1	Charge number	Domain 1	
tds.V	model.input.V	V	Electric potential	Domain 1	Meta
tds.T	tds.cdm1.minput_temperature	K	Temperature	Domain 1	
tds.cflux_cKx	cK*tds.u	mol/(m²·s)	Convective flux, x component	Domain 1	
tds.cflux_cKy	cK*tds.v	mol/(m²·s)	Convective flux, y component	Domain 1	
tds.cflux_cKz	cK*tds.w	mol/(m²·s)	Convective flux, z component	Domain 1	
tds.cfluxMag_cK	sqrt(tds.cflux_cKx^2+tds.cflux_cKy^2+tds.cflux_cKz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
tds.cflux_cClx	cCl*tds.u	mol/(m²·s)	Convective flux, x component	Domain 1	
tds.cflux_cCly	cCl*tds.v	mol/(m²·s)	Convective flux, y component	Domain 1	
tds.cflux_cClz	cCl*tds.w	mol/(m²·s)	Convective flux, z component	Domain 1	
tds.cfluxMag_cCl	sqrt(tds.cflux_cClx^2+tds.cflux_cCly^2+t	mol/(m²·s)	Convective flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	ds.cflux_cClz^2)				
tds.cflux_cH3Ox	cH3O*tds.u	mol/(m²·s)	Convective flux, x component	Domain 1	
tds.cflux_cH3Oy	cH3O*tds.v	mol/(m²·s)	Convective flux, y component	Domain 1	
tds.cflux_cH3Oz	cH3O*tds.w	mol/(m²·s)	Convective flux, z component	Domain 1	
tds.cfluxMag_cH3O	sqrt(tds.cflux_cH3Ox^2+tds.cflux_cH3Oy^2+tds.cflux_cH3Oz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
tds.cflux_cOHx	cOH*tds.u	mol/(m²·s)	Convective flux, x component	Domain 1	
tds.cflux_cOHy	cOH*tds.v	mol/(m²·s)	Convective flux, y component	Domain 1	
tds.cflux_cOHz	cOH*tds.w	mol/(m²·s)	Convective flux, z component	Domain 1	
tds.cfluxMag_cOH	sqrt(tds.cflux_cOHx^2+tds.cflux_cOHy^2+tds.cflux_cOHz^2)	mol/(m²·s)	Convective flux magnitude	Domain 1	
tds.cflux_cBEADx	cBEAD*tds.u	mol/(m²·s)	Convective flux, x component	Domain 1	
tds.cflux_cBEADy	cBEAD*tds.v	mol/(m²·s)	Convective flux, y component	Domain 1	
tds.cflux_cBEADz	cBEAD*tds.w	mol/(m²·s)	Convective flux, z component	Domain 1	
tds.cfluxMag_cBEAD	sqrt(tds.cflux_cBEADx^2+tds.cflux_cBEADy^2+tds.cflux	mol/(m²·s)	Convective flux magnitude	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	_cBEADz^2)				
tds.bndFlux_cK	-dflux_spatial(cK)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
tds.bndFlux_cCl	-dflux_spatial(cCl)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
tds.bndFlux_cH3O	-dflux_spatial(cH3O)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
tds.bndFlux_cOH	-dflux_spatial(cOH)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
tds.bndFlux_cBEAD	-dflux_spatial(cBEAD)	mol/(m²·s)	Boundary flux	Boundaries 1–12	
tds.Res_cK	-tds.D_cKxx*cKxx-tds.D_cKxy*cKxy-tds.D_cKyx*cKyx-tds.D_cKyy*cKyy+d(cK*tds.z_cK*F_const*(-tds.um_cKxx*d(tds.V,x)-tds.um_cKxy*d(tds.V,y)),x)+d(cK*tds.z_cK*F_const*(-tds.um_cKyx*d(tds.V,x)-tds.um_cKyy*d(tds.V,y)),y)+tds.u*cKx+tds.v*cKy-tds.R_cK	mol/(m³·s)	Equation residual	Domain 1	
tds.Res_cCl	-tds.D_cClxx*cClxx-tds.D_cClxy*cClxy-	mol/(m³·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	tds.D_cClyx*cClyx-tds.D_cClyy*cClyy+d(cCl*tds.z_cCl*F_const*(-tds.um_cClxx*d(tds.V,x)-tds.um_cClxy*d(tds.V,y)),x)+d(cCl*tds.z_cCl*F_const*(-tds.um_cClyx*d(tds.V,x)-tds.um_cClyy*d(tds.V,y)),y)+tds.u*cClx+tds.v*cCly-tds.R_cCl				
tds.Res_cH3O	-tds.D_cH3Oxx*cH3Oxx-tds.D_cH3Oxy*cH3Oxy-tds.D_cH3Oyx*cH3Oyx-tds.D_cH3Oyy*cH3Oyy+d(cH3O*tds.z_cH3O*F_const*(-tds.um_cH3Oxx*d(tds.V,x)-tds.um_cH3Oxy*d(tds.V,y)),x)+d(cH3O*tds.z_cH3O*F_const*(-tds.um_cH3Oyx*d(tds.V,x)-tds.um_cH3Oyy*d(tds.V,y)),y)+tds.u*cH3Ox+tds.v*cH3Oy-tds.R_cH3O	mol/(m³·s)	Equation residual	Domain 1	
tds.Res_cOH	-tds.D_cOHxx*	mol/(m³·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	cOHxx-tds.D_cOHxy*cOHxy-tds.D_cOHyx*cOHyx-tds.D_cOHyy*cOHyy+d(cOH*tds.z_cOH*F_const*(-tds.um_cOHxx*d(tds.V,x)-tds.um_cOHxy*d(tds.V,y)),x)+d(cOH*tds.z_cOH*F_const*(-tds.um_cOHyx*d(tds.V,x)-tds.um_cOHyy*d(tds.V,y)),y)+tds.u*cOHx+tds.v*cOHy-tds.R_cOH				
tds.Res_cBEAD	-tds.D_cBEADxx*cBEADxx-tds.D_cBEADxy*cBEADxy-tds.D_cBEADyx*cBEADyx-tds.D_cBEADyy*cBEADyy+d(cBEAD*tds.z_cBEAD*F_const*(-tds.um_cBEADxx*d(tds.V,x)-tds.um_cBEADxy*d(tds.V,y)),x)+d(cBEAD*tds.z_cBEAD*F_const*(-tds.um_cBEADyx*d(tds.V,x)-tds.um_cBEA	mol/(m³·s)	Equation residual	Domain 1	

Name	Expression	Unit	Description	Selection	Details
	Dyy*d(tds.V,y),y)+tds.u*cBEADx+tds.v*cBEADy-tds.R_cBEAD				

Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
cK	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
cCl	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
cH3O	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
cOH	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1
cBEAD	Lagrange (Quadratic)	mol/m³	Concentration	Spatial	Domain 1

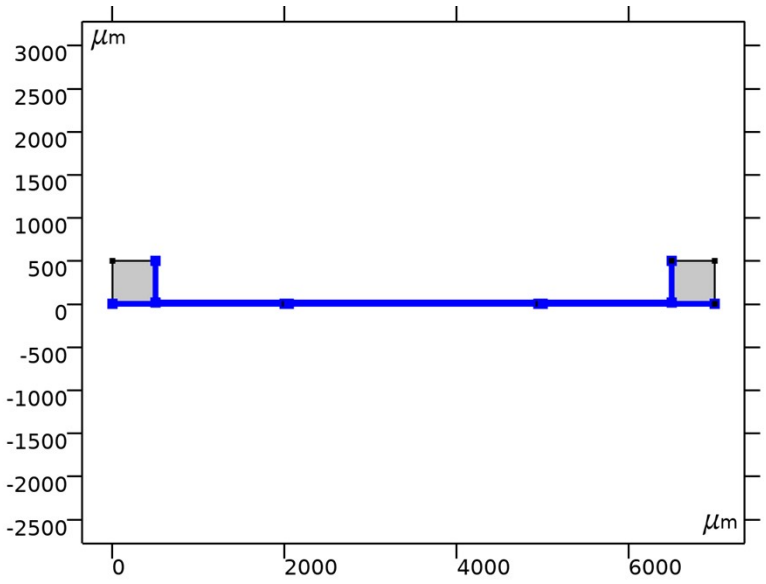
Weak expressions

Weak expression	Integration order	Integration frame	Selection
tds.dflux_cKx*test(cKx)+tds.dflux_cKy*test(cKy)	4	Spatial	Domain 1
tds.dflux_cClx*test(cClx)+tds.dflux_cCly*test(cCly)	4	Spatial	Domain 1
tds.dflux_cH3Ox*test(cH3Ox)+tds.dflux_cH3Oy*test(cH3Oy)	4	Spatial	Domain 1
tds.dflux_cOHx*test(cOHx)+tds.dflux_cOHy*test(cOHy)	4	Spatial	Domain 1
tds.dflux_cBEADx*test(cBEADx)+tds.dflux_cBEADy*test(cBEADy)	4	Spatial	Domain 1
tds.z_cK*F_const*cK*((-tds.um_cKxx*d(tds.V,x)-tds.um_cKxy*d(tds.V,y))*test(cKx)+(-tds.um_cKyx*d(tds.V,x)-tds.um_cKyy*d(tds.V,y))	4	Spatial	Domain 1

Weak expression	Integration order	Integration frame	Selection
*test(cKy))			
tds.z_cCl*F_const*cCl*((-tds.um_cClxx*d(tds.V,x)-tds.um_cClxy*d(tds.V,y))*test(cClx)+(-tds.um_cClyx*d(tds.V,x)-tds.um_cClyy*d(tds.V,y))*test(cCly))	4	Spatial	Domain 1
tds.z_cH3O*F_const*cH3O*((-tds.um_cH3Oxx*d(tds.V,x)-tds.um_cH3Oxy*d(tds.V,y))*test(cH3Ox)+(-tds.um_cH3Oyx*d(tds.V,x)-tds.um_cH3Oyy*d(tds.V,y))*test(cH3Oy))	4	Spatial	Domain 1
tds.z_cOH*F_const*cOH*((-tds.um_cOHxx*d(tds.V,x)-tds.um_cOHxy*d(tds.V,y))*test(cOHx)+(-tds.um_cOHyx*d(tds.V,x)-tds.um_cOHyy*d(tds.V,y))*test(cOHy))	4	Spatial	Domain 1
tds.z_cBEAD*F_const*cBEAD*((-tds.um_cBEADxx*d(tds.V,x)-tds.um_cBEADxy*d(tds.V,y))*test(cBEADx)+(-tds.um_cBEADyx*d(tds.V,x)-tds.um_cBEADyy*d(tds.V,y))*test(cBEADy))	4	Spatial	Domain 1
-(tds.u*cKx+tds.v*cKy)*test(cK)*(isScalingSystemDomain==0)	4	Spatial	Domain 1
tds.cbf_cK*test(cK)	4	Spatial	Boundaries 1–

Weak expression	Integration order	Integration frame	Selection
			12
-(tds.u*cClx+tds.v*cCly)*test(cCl)*(isScalingSystemDomain==0)	4	Spatial	Domain 1
tds.cbf_cCl*test(cCl)	4	Spatial	Boundaries 1–12
-(tds.u*cH3Ox+tds.v*cH3Oy)*test(cH3O)*(isScalingSystemDomain==0)	4	Spatial	Domain 1
tds.cbf_cH3O*test(cH3O)	4	Spatial	Boundaries 1–12
-(tds.u*cOHx+tds.v*cOHy)*test(cOH)*(isScalingSystemDomain==0)	4	Spatial	Domain 1
tds.cbf_cOH*test(cOH)	4	Spatial	Boundaries 1–12
-(tds.u*cBEADx+tds.v*cBEADy)*test(cBEAD)*(isScalingSystemDomain==0)	4	Spatial	Domain 1
tds.cbf_cBEAD*test(cBEAD)	4	Spatial	Boundaries 1–12
tds.streamline*(isScalingSystemDomain==0)	4	Spatial	Domain 1
tds.crosswind*(isScalingSystemDomain==0)	6	Spatial	Domain 1

2.6.4 No Flux 1



No Flux 1

SELECTION

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

EQUATIONS

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

Convection

SETTINGS

Description	Value
Include	Off

2.6.5 Initial Values 1

Initial Values 1

SELECTION

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

Initial values

SETTINGS

Description	Value
Concentration	{cK0 + cBEAD0, cCl0, cH3O0, cOH0, cBEAD0}

2.6.6 Inflow 1

Inflow 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 11–12

EQUATIONS

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

Concentration

SETTINGS

Description	Value
Concentration	{cK0 + cBEAD0, cCl0, cH3O0, cOH0, cBEAD0}

Boundary condition type

SETTINGS

Description	Value
Boundary condition type	Concentration constraint

Variables

Name	Expression	Unit	Description	Selection	Details
tds.c0_cK	cK0+cBEAD0	mol/m³	Concentration	Boundaries 11–12	+ operation

Name	Expression	Unit	Description	Selection	Details
tds.c0_cCl	cCl0	mol/m³	Concentration	Boundaries 11–12	+ operation
tds.c0_cH3O	cH3O0	mol/m³	Concentration	Boundaries 11–12	+ operation
tds.c0_cOH	cOH0	mol/m³	Concentration	Boundaries 11–12	+ operation
tds.c0_cBEAD	cBEAD0	mol/m³	Concentration	Boundaries 11–12	+ operation
tds.in1.c0_avg_cK	tds.in1.int(cK*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.in1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global	
tds.in1.c0_avg_cCl	tds.in1.int(cCl*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.in1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global	
tds.in1.c0_avg_cH3O	tds.in1.int(cH3O*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.in1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global	
tds.in1.c0_avg_cOH	tds.in1.int(cOH*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.in1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global	
tds.in1.c0_avg_cBEAD	tds.in1.int(cBEAD*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.in1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global	

Constraints

Constraint	Constraint force	Shape function	Selection	Details
-cK+tds.c0_cK	-test(cK)	Lagrange (Quadratic)	Boundaries 11–12	Elemental
-cCl+tds.c0_cCl	-test(cCl)	Lagrange (Quadratic)	Boundaries 11–12	Elemental
-cH3O+tds.c0_cH3O	-test(cH3O)	Lagrange (Quadratic)	Boundaries 11–12	Elemental
-cOH+tds.c0_cOH	-test(cOH)	Lagrange (Quadratic)	Boundaries 11–12	Elemental
-cBEAD+tds.c0_cBEAD	-test(cBEAD)	Lagrange (Quadratic)	Boundaries 11–12	Elemental

2.6.7 Outflow 1

Outflow 1

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 1, 3

EQUATIONS

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

Variables

Name	Expression	Unit	Description	Selection
tds.out1.c0_avg_cK	tds.out1.int(cK*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.out1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global
tds.out1.c0_avg_cCl	tds.out1.int(cCl*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.out1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global
tds.out1.c0_avg_cH3O	tds.out1.int(cH3O*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.out1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global
tds.out1.c0_avg_cOH	tds.out1.int(cOH*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.out1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global
tds.out1.c0_avg_cBEAD	tds.out1.int(cBEAD*(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz))/tds.out1.int(tds.u*tds.nx+tds.v*tds.ny+tds.w*tds.nz)	mol/m³	Concentration	Global

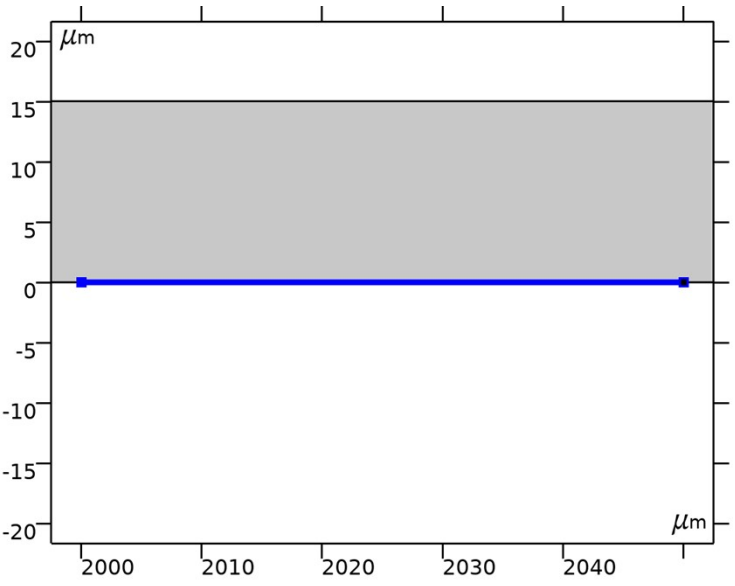
Weak expressions

Weak expression	Integration order	Integration frame	Selection
0	4	Spatial	Boundaries 1, 3
-tds.z_cK*F_const*cK*(-tds.nx*(tds.um_cKxx*mean(d(tds.V,x))+tds.um_cKxy*mean(d(tds.V,y))+tds.um_cKxz*mean(0))-tds.ny*(tds.um_cKyx*mean(d(tds.V,x))+tds.um_cKyy*mean(d(tds.V,y))+tds.um_cKyz*mean(0))-tds.nz*(tds.um_cKzx*mean(d(tds.V,x))+tds.um_cKzy*mean(d(tds.V,y))+tds.um_cKzz*mean(0)))*test(cK)	4	Spatial	Boundaries 1, 3
0	4	Spatial	Boundaries 1, 3
-tds.z_cCl*F_const*cCl*(-tds.nx*(tds.um_cClxx*m	4	Spatial	Boundaries 1, 3

Weak expression	Integration order	Integration frame	Selection
ean(d(tds.V,x))+tds.um_cClxy*mean(d(tds.V,y))+tds.um_cClxz*mean(0))-tds.ny*(tds.um_cClyx*mean(d(tds.V,x))+tds.um_cClyy*mean(d(tds.V,y))+tds.um_cClyz*mean(0))-tds.nz*(tds.um_cClzx*mean(d(tds.V,x))+tds.um_cClzy*mean(d(tds.V,y))+tds.um_cClzz*mean(0)))*test(cCl)			
0	4	Spatial	Boundaries 1, 3
-tds.z_cH3O*F_const*cH3O*(-tds.nx*(tds.um_cH3Oxx*mean(d(tds.V,x))+tds.um_cH3Oxy*mean(d(tds.V,y))+tds.um_cH3Oxz*mean(0))-tds.ny*(tds.um_cH3Oyx*mean(d(tds.V,x))+tds.um_cH3Oyy*mean(d(tds.V,y))+tds.um_cH3Oyz*mean(0))-tds.nz*(tds.um_cH3Ozx*mean(d(tds.V,x))+tds.um_cH3Ozy*mean(d(tds.V,y))+tds.um_cH3Ozz*mean(0)))*test(cH3O)	4	Spatial	Boundaries 1, 3
0	4	Spatial	Boundaries 1, 3
-tds.z_cOH*F_const*cOH*(-tds.nx*(tds.um_cOHxx*mean(d(tds.V,x))+tds.um_cOHxy*mean(d(tds.V,y))+tds.um_cOHxz*mean(0))-tds.ny*(tds.um_cOHyx*mean(d(tds.V,x))+tds.um_cOHyy*mean(d(tds.V,y))+tds.um_cOHyz*mean(0))-	4	Spatial	Boundaries 1, 3

Weak expression	Integration order	Integration frame	Selection
tds.nz*(tds.um_cOHzx*mean(d(tds.V,x))+tds.um_cOHzy*mean(d(tds.V,y))+tds.um_cOHzz*mean(0)))*test(cOH)			
0	4	Spatial	Boundaries 1, 3
-tds.z_cBEAD*F_const*cBEAD*(-tds.nx*(tds.um_cBEADxx*mean(d(tds.V,x))+tds.um_cBEADxy*mean(d(tds.V,y))+tds.um_cBEADxz*mean(0))-tds.ny*(tds.um_cBEADyx*mean(d(tds.V,x))+tds.um_cBEADyy*mean(d(tds.V,y))+tds.um_cBEADyz*mean(0))-tds.nz*(tds.um_cBEADzx*mean(d(tds.V,x))+tds.um_cBEADzy*mean(d(tds.V,y))+tds.um_cBEADzz*mean(0)))*test(cBEAD)	4	Spatial	Boundaries 1, 3

2.6.8 Flux 1



Flux 1

SELECTION

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

EQUATIONS

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

Convection

SETTINGS

Description	Value
Include	Off

Inward flux

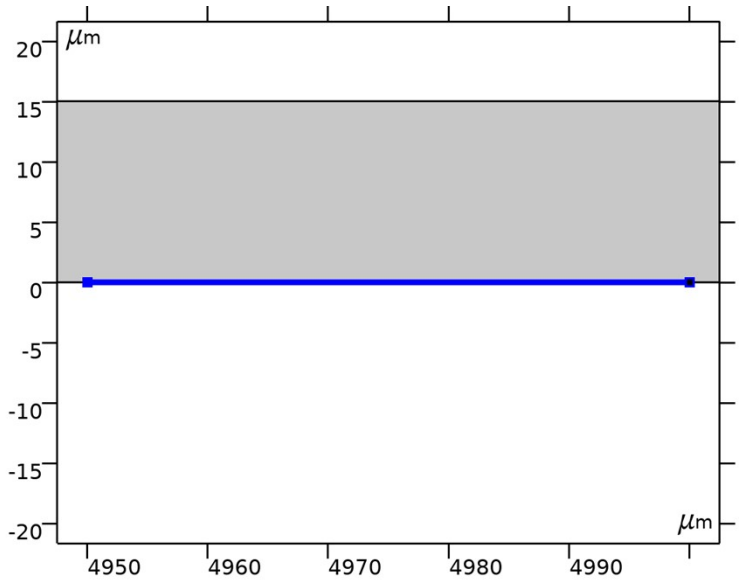
SETTINGS

Description	Value
Flux type	General inward flux
Species cK	Off
Species cCl	Off
Species cH3O	On
Species cOH	Off
Species cBEAD	Off

Weak expressions

Weak expression	Integration order	Integration frame	Selection
0	4	Spatial	Boundary 6
0	4	Spatial	Boundary 6
f_elec*test(cH3O)	4	Spatial	Boundary 6
0	4	Spatial	Boundary 6
0	4	Spatial	Boundary 6

2.6.9 Flux 2



Flux 2

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundary 8

EQUATIONS

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

Convection

SETTINGS

Description	Value
Include	Off

Inward flux

SETTINGS

Description	Value
Flux type	General inward flux
Species cK	Off
Species cCl	Off
Species cH3O	Off
Species cOH	On
Species	Off

Description	Value
cBEAD	

Weak expressions

Weak expression	Integration order	Integration frame	Selection
0	4	Spatial	Boundary 8
0	4	Spatial	Boundary 8
0	4	Spatial	Boundary 8
f_elec*test(cOH)	4	Spatial	Boundary 8
0	4	Spatial	Boundary 8

2.6.10 Reactions 1

Reactions 1

SELECTION

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

EQUATIONS

$$\nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = \underbrace{R_i}_{\cdots} + S_i$$

Reaction rates

SETTINGS

Description	Value
Total rate expression	User defined
Total rate expression	0
Total rate expression	User defined
Total rate expression	0
Total rate expression	User defined
Total rate expression	k_fhydro*cH2O0 - k_bhydro*cOH*cH3O
Total rate expression	User defined
Total rate expression	k_fhydro*cH2O0 - k_bhydro*cOH*cH3O
Total rate expression	User defined
Total rate expression	0

Variables

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

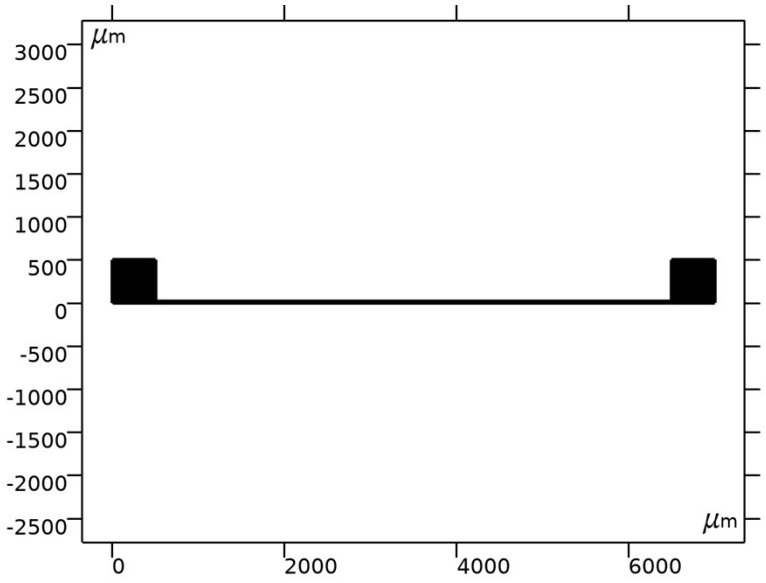
Weak expressions

Weak expression	Integration order	Integration frame	Selection
tds.reac1.R_cK*test(cK)	4	Spatial	Domain 1
tds.reac1.R_cCl*test(cCl)	4	Spatial	Domain 1
tds.reac1.R_cH3O*test(cH3O)	4	Spatial	Domain 1
tds.reac1.R_cOH*test(cOH)	4	Spatial	Domain 1
tds.reac1.R_cBEAD*test(cBEAD)	4	Spatial	Domain 1

2.7 MESH 1

MESH STATISTICS

Description	Value
Minimum element quality	0.6386
Average element quality	0.9686
Triangle	76191
Edge element	5773
Vertex element	12



Mesh 1

2.7.1 Size (size)

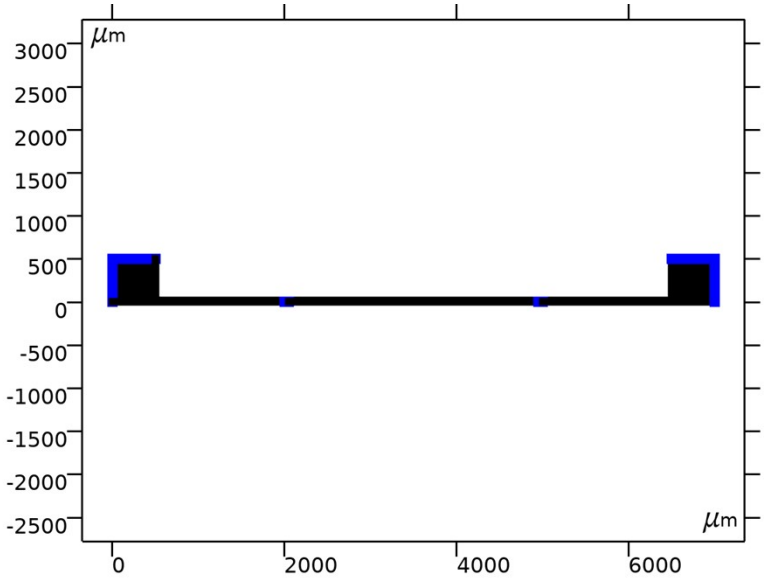
SETTINGS

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	22.5
Minimum element size	1
Curvature factor	0.3
Maximum element growth rate	1.15

2.7.2 Size 1 (size1)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 1, 3, 6, 8, 11–12



Size 1

SETTINGS

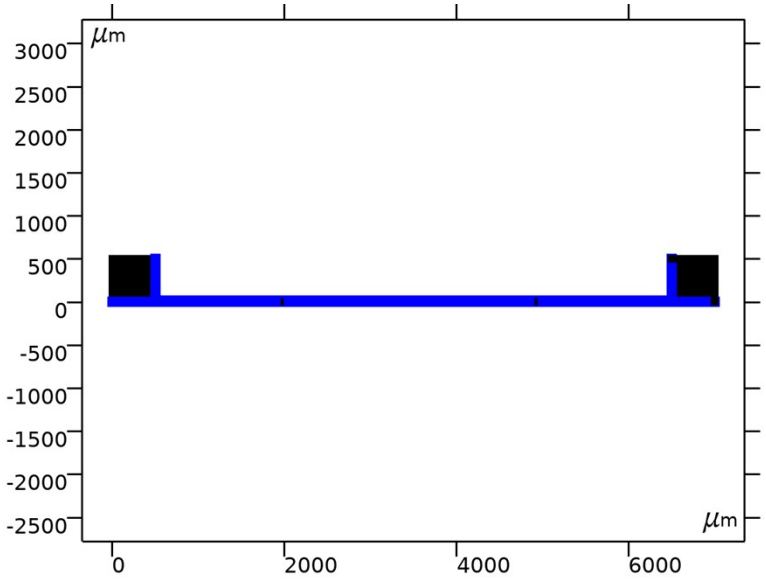
Description	Value
Calibrate for	Fluid dynamics
Minimum element size	0.08
Curvature factor	0.25
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.08

Description	Value
Predefined size	Extra fine
Custom element size	Custom

2.7.3 Size 2 (size2)

SELECTION

Geometric entity level	Boundary
Selection	Geometry geom1: Dimension 1: Boundaries 2, 4–5, 7, 9–10



Size 2

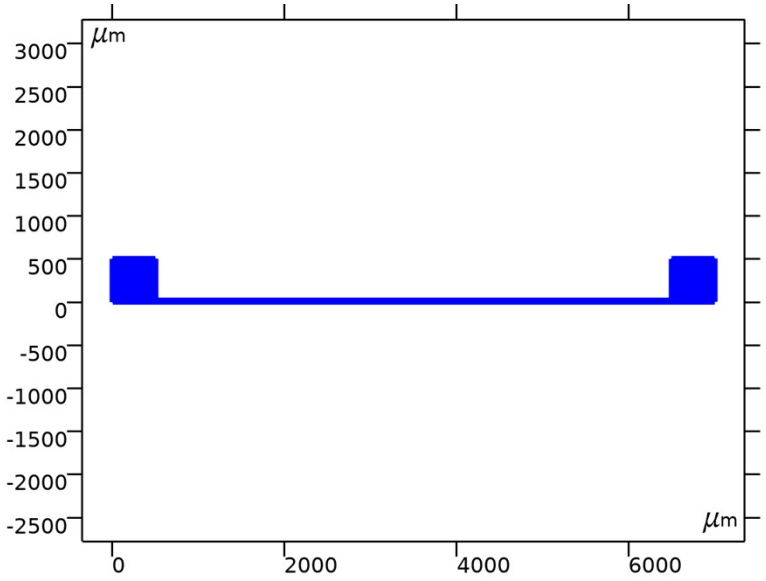
SETTINGS

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	4
Minimum element size	0.25
Curvature factor	0.25
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.12
Predefined size	Finer
Custom element size	Custom

2.7.4 Free Triangular 1 (ftri1)

SELECTION

Geometric entity level	Domain
Selection	Remaining



Free Triangular 1

3 Study 1

COMPUTATION INFORMATION

Computation time	5 min 33 s
CPU	Intel64 Family 6 Model 44 Stepping 2, 12 cores
Operating system	Windows 7

3.1 STATIONARY

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

PHYSICS AND VARIABLES SELECTION

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

MESH SELECTION

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.2 SOLVER CONFIGURATIONS

3.2.1 Solution 2

Compile Equations: Stationary (st1)

STUDY AND STEP

Description	Value
Use study	
Use study step	

LOG

```
<---- Compile Equations: Stationary in Study 1/Solution 2 (sol2) ----------
--
Started at May 26, 2021 11:00:50 AM.
Geometry shape order: Linear
Running on Intel64 Family 6 Model 44 Stepping 2, GenuineIntel.
Using 1 socket with 12 cores in total on CNS-R-WEL870984.
Available memory: 110.59 GB.
Time: 5 s.
Physical memory: 2.24 GB
Virtual memory: 2.46 GB
Ended at May 26, 2021 11:00:55 AM.
----- Compile Equations: Stationary in Study 1/Solution 2 (sol2) ----------
->
```

Dependent Variables 1 (v1)

INITIAL VALUES OF VARIABLES SOLVED FOR

Description	Value
Method	Solution
Solution	

LOG

```
<---- Dependent Variables 1 in Study 1/Solution 2 (sol2) ----------
--
Started at May 26, 2021 11:00:58 AM.
Initial values of variables solved for: Solution 2 (sol2).
Solution time: 0 s.
Physical memory: 2.1 GB
Virtual memory: 2.29 GB
Ended at May 26, 2021 11:00:59 AM.
----- Dependent Variables 1 in Study 1/Solution 2 (sol2) ----------
->
```

Concentration (comp1.cBEAD) (comp1_cBEAD)

GENERAL

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

Concentration (comp1.cCl) (comp1_cCl)

GENERAL

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

Concentration (comp1.cH3O) (comp1_cH3O)

GENERAL

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

Concentration (comp1.cK) (comp1_cK)

GENERAL

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

Concentration (comp1.cOH) (comp1_cOH)

GENERAL

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

Pressure (comp1.p) (comp1_p)

GENERAL

Description	Value
Field components	comp1.p

Velocity field (comp1.u) (comp1_u)

GENERAL

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

Electric potential (comp1.V) (comp1_V)

GENERAL

Description	Value
Field components	comp1.V

Stationary Solver 1 (s1)

GENERAL

Description	Value
Defined by study step	

LOG

```
<---- Stationary Solver 1 in Study 1/Solution 2 (sol2) ----------------------
--
Started at May 26, 2021 11:00:59 AM.
Nonlinear solver
Number of degrees of freedom solved for: 1306231 (plus 57791 internal DOFs).
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (comp1.cBEAD): 5.3e+06
Concentration (comp1.cCl): 1.7e+03
Concentration (comp1.cH3O): 63
Concentration (comp1.cK): 2.2e+03
Concentration (comp1.cOH): 44
Pressure (comp1.p): 40
Velocity field (comp1.u): 5.2e+02
Electric potential (comp1.V): 3.5e+04
Orthonormal null-space function used.
Iter      SolEst      ResEst     Damping    Stepsize #Res #Jac #Sol   LinErr
 LinRes
   1       4e-07     5.5e+03   0.0100000       4e-07    2    1    2  4.1e-
12  9.2e-15
   2     1.2e-06     9.2e+02   1.0000000        0.11    4    2    4  3.9e-
12    1e-14
   3     3.9e-07     8.9e+02   1.0000000     8.3e-07    6    3    6  1.9e-
11  1.7e-14
Solution time: 325 s. (5 minutes, 25 seconds)
Physical memory: 11.45 GB
Virtual memory: 12.76 GB
Ended at May 26, 2021 11:06:24 AM.
----- Stationary Solver 1 in Study 1/Solution 2 (sol2) ----------------------
->
```

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

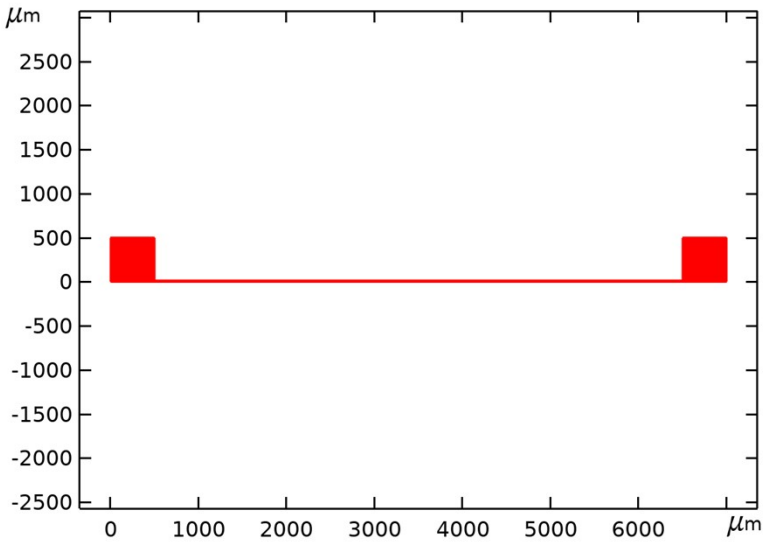
4 Results

4.1 DATASETS

4.1.1 Study 1/Solution 2

SOLUTION

Description	Value
Solution	
Component	Save Point Geometry 1



Dataset: Study 1/Solution 2

4.1.2 Cut Line 2D 1

DATA

Description	Value
Dataset	

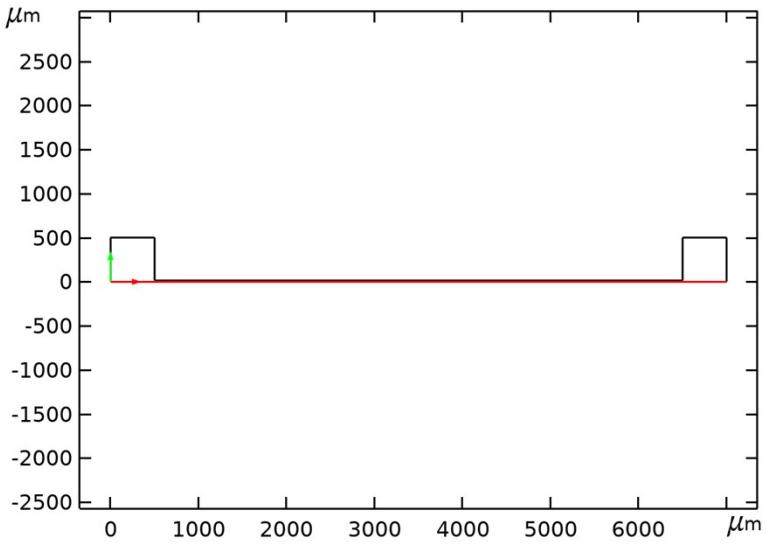
LINE DATA

Description	Value
Line entry method	Two points
Points	{{0, 0}, {0, 0}}
Bounded by	Off

Description	Value
points	

ADVANCED

Description	Value
Space variable	cln1x
Normal variables	{cln1nx, cln1ny}



Dataset: Cut Line 2D 1

4.1.3 Cut Line 2D 2

DATA

Description	Value
Dataset	

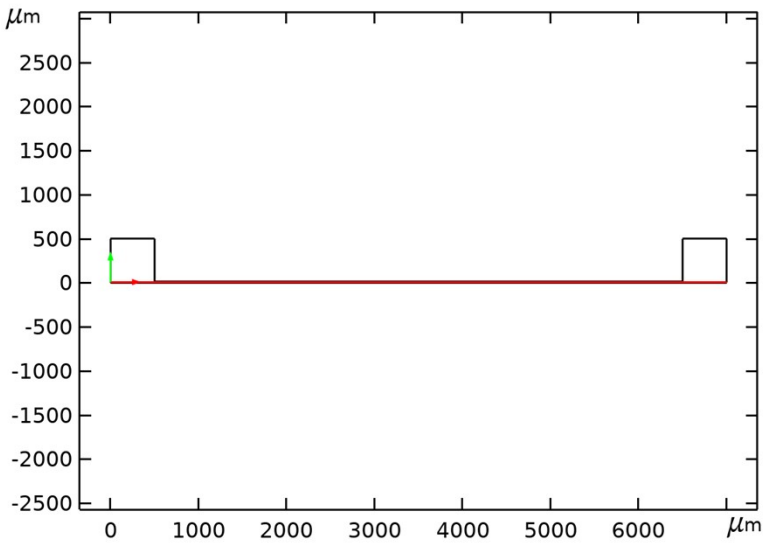
LINE DATA

Description	Value
Line entry method	Two points
Points	{{0, 7.5}, {0, 7.5}}
Bounded by points	Off

ADVANCED

Description	Value

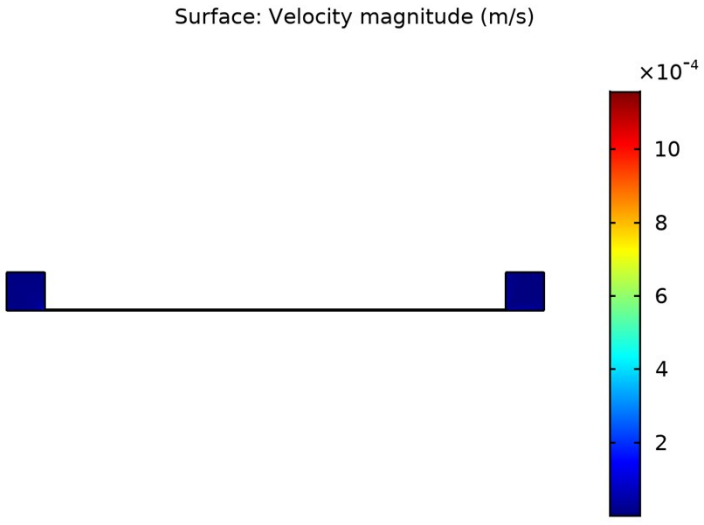
Description	Value
Space variable	cln1x
Normal variables	{cln1nx, cln1ny}



Dataset: Cut Line 2D 2

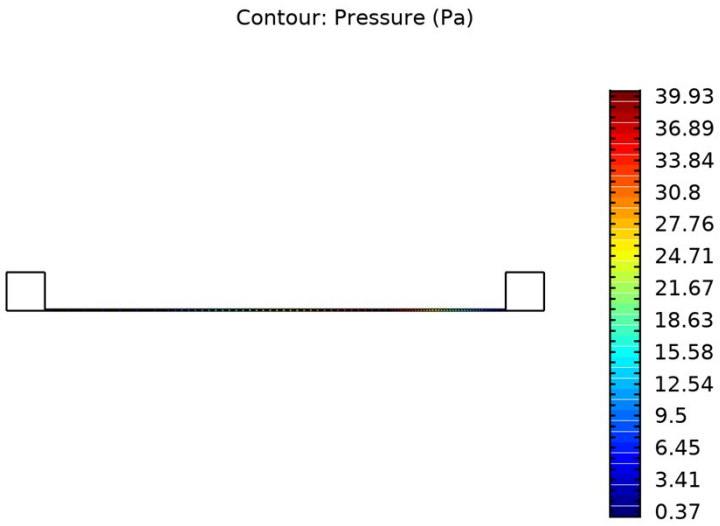
4.2 PLOT GROUPS

4.2.1 Velocity (spf) 1



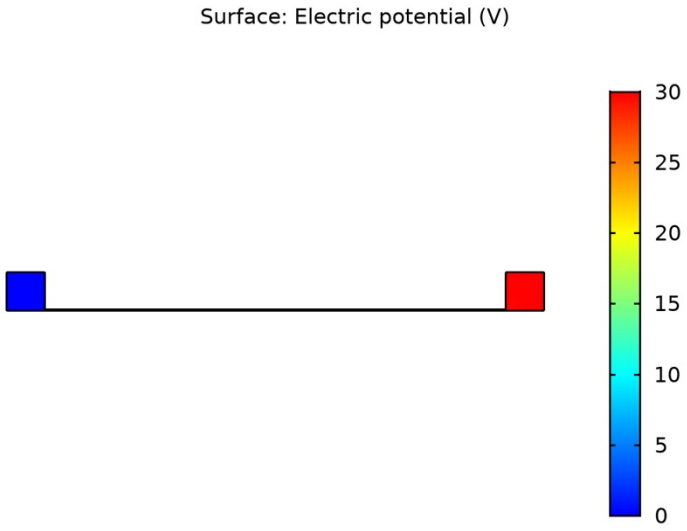
Surface: Velocity magnitude (m/s)

4.2.2 Pressure (spf) 1



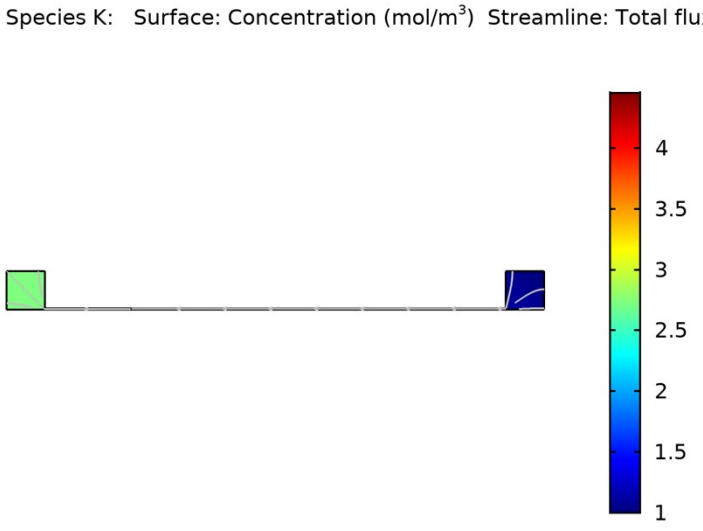
Contour: Pressure (Pa)

4.2.3 Electric Potential (es) 1



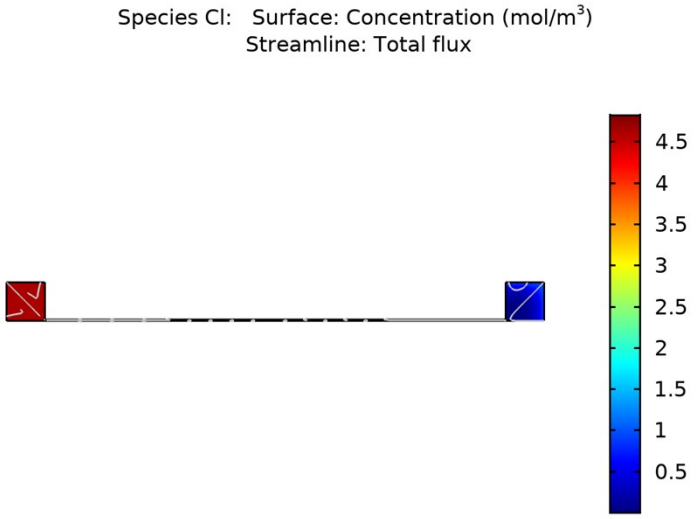
Surface: Electric potential (V)

4.2.4 Concentration, K (tds) 1



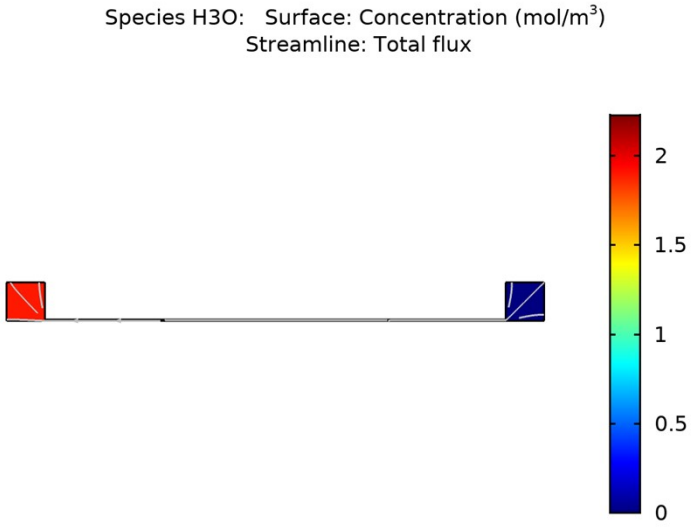
Species K: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.5 Concentration, Cl (tds) 1



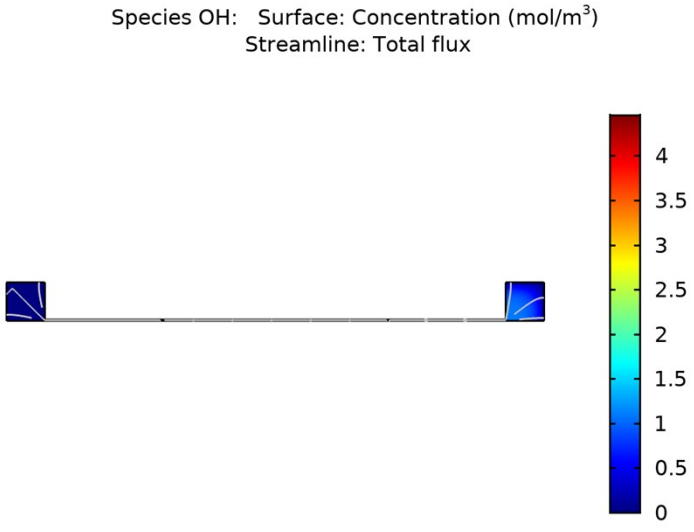
Species Cl: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.6 Concentration, H3O (tds) 1



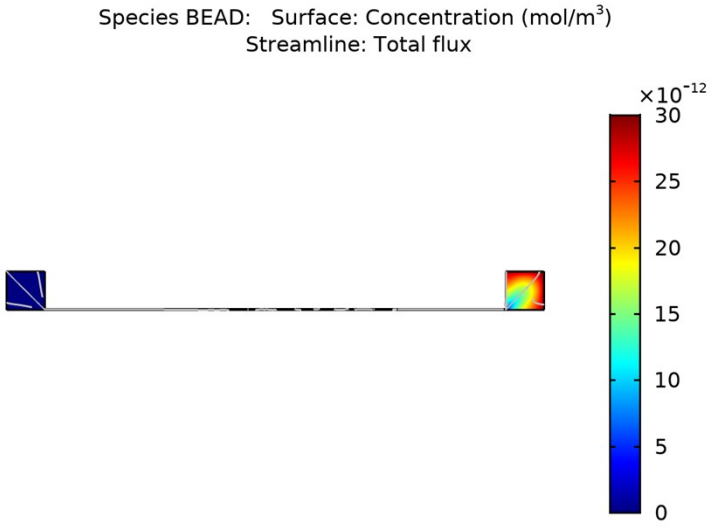
Species H3O: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.7 Concentration, OH (tds) 1



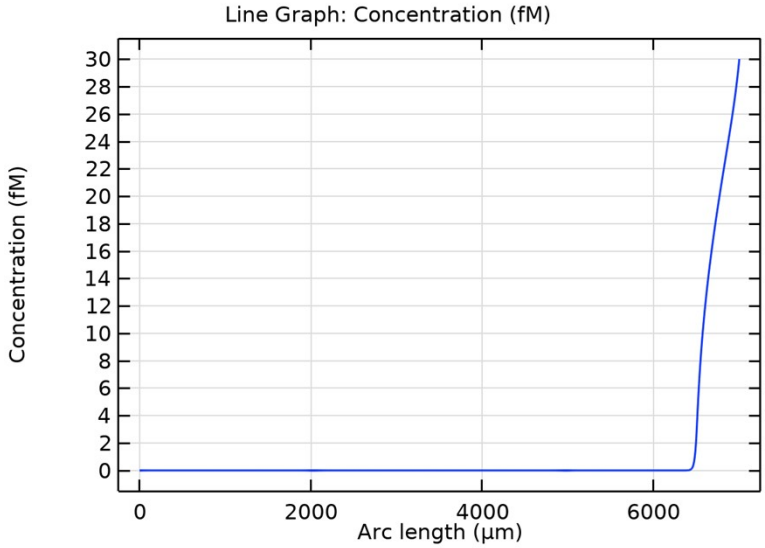
Species OH: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.8 Concentration, BEAD (tds) 1



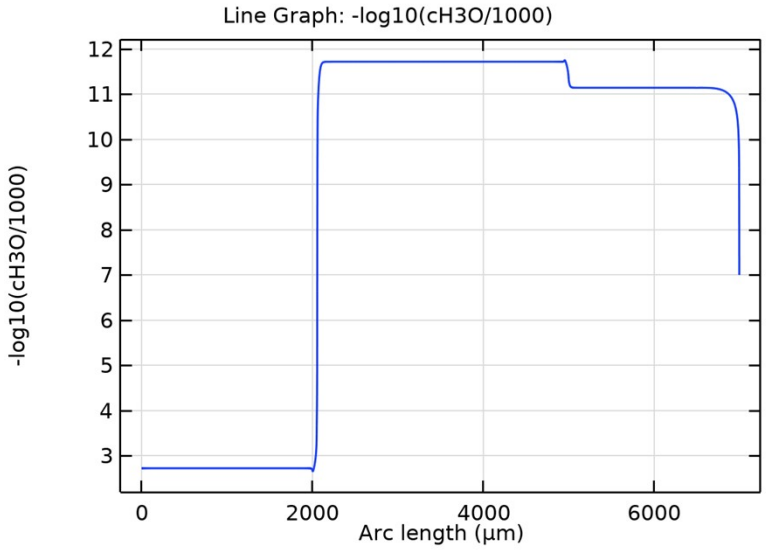
Species BEAD: Surface: Concentration (mol/m³) Streamline: Total flux

4.2.9 Microplastic concentration



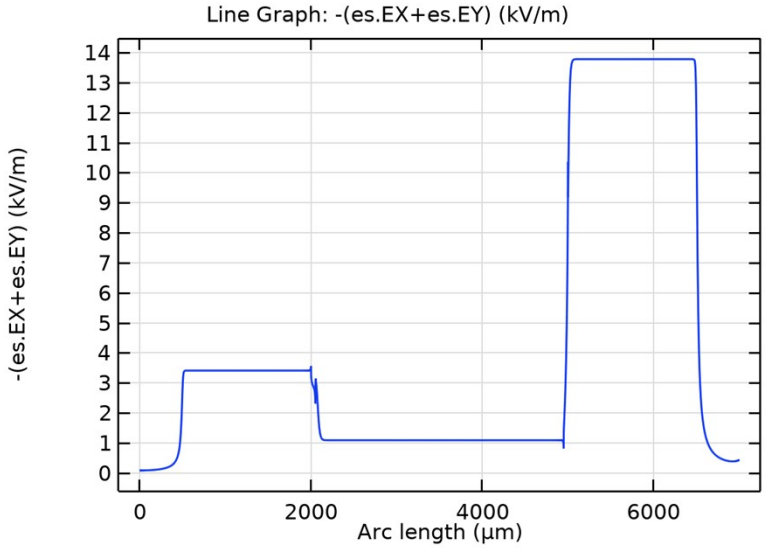
Line Graph: Concentration (fM)

4.2.10 pH



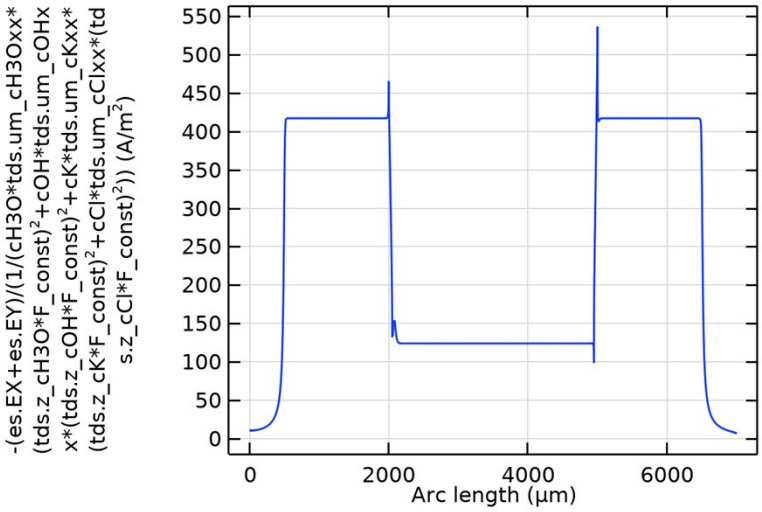
Line Graph: -log10(cH3O/1000)

4.2.11 Electric field



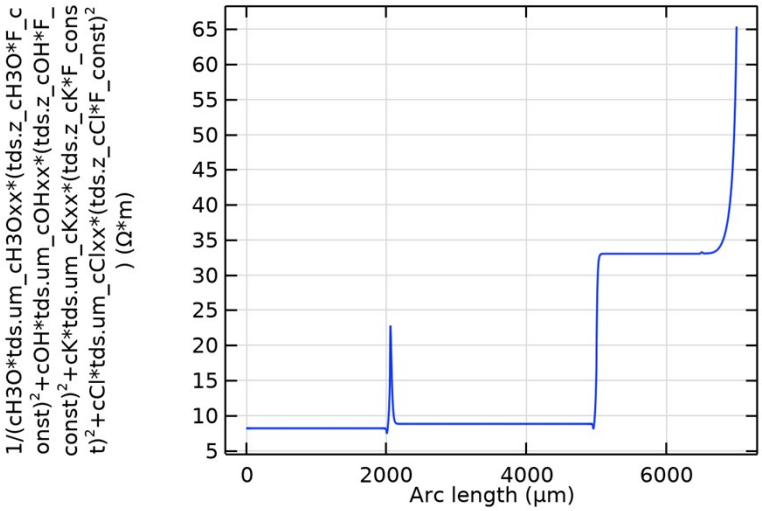
Line Graph: -(es.EX+es.EY) (kV/m)

4.2.12 Ionic current density



*Line Graph: -(es.EX+es.EY)/(1/(cH3O*tds.um_cH3Oxx*(tds.z_cH3O*F_const)^2+cOH*tds.um_cOHxx*(tds.z_cOH*F_const)^2+cK*tds.um_cKxx*(tds.z_cK*F_const)^2+cCl*tds.um_cClxx*(tds.z_cCl*F_const)^2)) (A/m^2)*

4.2.13 Solution resistivity



*Line Graph: 1/(cH3O*tds.um_cH3Oxx*(tds.z_cH3O*F_const)^2+cOH*tds.um_cOHxx*(tds.z_cOH*F_const)^2+cK*tds.um_cKxx*(tds.z_cK*F_const)^2+cCl*tds.um_cClxx*(tds.z_cCl*F_const)^2) (Ω*m)*