Supplementary Data for: Electrochemical oxygen reduction at soft interfaces catalyzed by the transfer of hydrated lithium cations

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Table S1: COMSOL simulation parameters

Parameter	Value	Description
v	0.050 V·s^{-1}	Scan rate
$\Delta_o^w\phi_i$	0.000 V	Initial potential
$\Delta_o^w\phi_f$	0.550 V	Upper potential
$\Delta_o^w\phi_{Li^+}^{o'}$	0.696 V	Formal Li^+ transfer potential (ref. [1])
$\Delta_o^w\phi_{OH^-}^{o'}$	−0.696 V	Formal OH^- transfer potential *
$\Delta_o^w\phi_{DMFc^+}^{o'}$	−0.250 V	Formal $DMFc^+$ transfer potential
k^o	0.01 m·s^{-1}	Standard rate constant
α	0.5	Transfer coefficient
$c_{M^+,w}$ / $c_{M^+,o}$	10 mmol·L^{-1}/0 mmol·L^{-1}	Initial metal ion concentration
$c_{DMFc,w}$ / $c_{DMFc,o}$	0 mmol·L^{-1}/5 mmol·L^{-1}	Initial concentration of DMFc
$c_{OH^-,w}$ / $c_{OH^-,o}$	10 mmol·L^{-1}/0 mmol·L^{-1}	Initial hydroxide concentration
$c_{O_2,o}$	1.6 mmol·L^{-1}	Initial oxygen concentration (ref. [2-4])
D_{DMFc}	7.26 × 10^{-6} cm·s^{-1}	Diffusion coefficient of DMFc and $DMFc^+$ (ref. [5])
D_{O_2}	2.76 × 10^{-5} cm·s^{-1}	Diffusion coefficient of O_2 (ref. [2])
D_{M^+}	1.0 × 10^{-5} cm·s^{-1}	Diffusion coefficient of M^+
D_{OH^-}	1.0 × 10^{-5} cm·s^{-1}	Diffusion coefficient of OH^-
k_{cf2} / k_{cb2}(org)	5000 L·mol^{-1}·s^{-1}/1 s^{-1}	Rate of ion-pair formation in the organic phase
k_{cf2} / k_{cb2}(aq)	1 L·mol^{-1}·s^{-1}/1 × 10^5 s^{-1}	Rate of ion-pair formation in the aqueous phase
r_d	0.7 cm	Radius of the ITIES

*A value of −0.656 V is described in the literature (ref. [6]) for $\Delta_o^w\phi_{OH^-}^{o'}$; however, to make the simulated CVs symmetric, and for the sake of convenience, −0.696 V was employed.

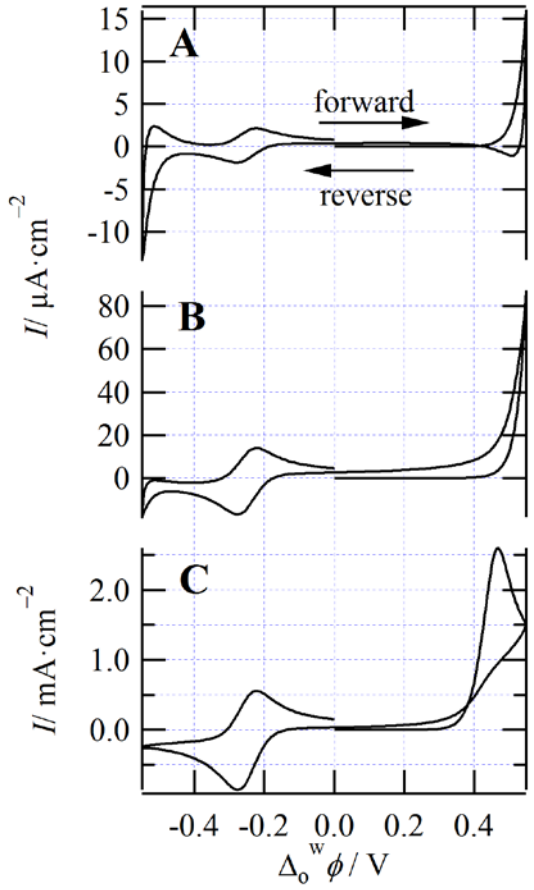


Figure S1: Simulated cyclic voltammograms compiled using the simulation detailed in section 2.0 of the main text with similar parameters as provided for Figure 4 and Table S1; however, with $k_{chem\text{-}1}$, $k_{chem\text{-}2}$, $k_{chem\text{-}3}$, and $k_{chem\text{-}4}$ equal to 1×10^4 L·mol^{-1}·s^{-1}, while k_{cf} /k_{cb} were changed to $1 \times 10^2/1 \times 10^{-2}$, $1 \times 10^4/1$, $1 \times 10^8/1 \times 10^4$ L·mol^{-1}·s^{-1} for panels A, B, and C, respectively.

References

[1] T.J. Stockmann, A.-M. Montgomery, Z. Ding, J. Electroanal. Chem. 684 (2012) 6-12.
[2] A. Schumpe, P. Luehring, J. Chem. Eng. Data 35 (1990) 24-5.
[3] A. Trojánek, J. Langmaier, Z. Samec, Electrochem. Commun. 8 (2006) 475-81.
[4] P. Luehring, A. Schumpe, J. Chem. Eng. Data 34 (1989) 250-2.
[5] T.J. Stockmann, H. Deng, P. Peljo, K. Kontturi, M. Opallo, H. Girault, J. Electroanal. Chem. (2014) Submitted.
[6] M. Zhou, S. Gan, L. Zhong, X. Dong, J. Ulstrup, D. Han, L. Niu, Phys. Chem. Chem. Phys. 14 (2012) 3659-68.

Contents

1 Global Definitions

1.1 Parameters 1

Parameters

Name	Expression	Description
F	96485[C/mol]	
T	298.15[K]	
R	8.314[J/mol/K]	
fara	F/(R*T)	
Ei	0[V]	
Ef	0.55[V]	
E0	0.696[V]	formal IT of M+
E02	-0.25[V]	formal IT of DMFc+
E03	-0.696[V]	formal IT potential for OH-
nu	0.050[V/s]	
k0	1[cm/s]	
k02	1[cm/s]	k0 for DMFc+ IT
alpha	0.5	
cMaqi	10[mmol/L]	
cMorgi	0[mmol/L]	
cHO2i	0[mmol/L]	
cDMFci	5[mmol/L]	
cDMFcaqi	0[mmol/L]	
cDMFcplusi	0[mmol/L]	
cDMFcplusaqi	0[mmol/L]	
cO2i	1.6[mmol/L]	
cO2aqi	1.6[mmol/L]	
cOHaqi	10[mmol/L]	
cFcHi	0[mmol/L]	
cH2Oi	131[mmol/L]	
cMOHi	0[mmol/L]	

Name	Expression	Description
cHO2minusi	0[mmol/L]	
test1	R*T/F	
n1	1	number of electrons
n2	-1	charge on Cl-
D_DMFc	7.26e-9[m^2/s]	
D_M	1.0e-5[cm^2/s]	
D_DMFcplus	7.26e-6[cm^2/s]	
D_H2O	6.53e-9[m^2/s]	
D_O2	2.76e-5[cm^2/s]	
D_Cl	1e-9[m^2/s]	
D_Horg	1e-9[m^2/s]	
D_H2O2	1e-5[cm^2/s]	
kfo2	0[cm/s]	
kbo2	0[cm/s]	
kcf	10[L/mol/s]	hydride formation
kcb	1[L/mol/s]	
kbFc	1[cm/s]	
kchem1	10 [L/mol/s]	HO2 formation
kchem2	1e+4[L/mol/s]	reaction of DMFcH+ + O2
kchem3	1e+4[L/mol/s]	
kchem4	1e+4 [L/mol/s]	HO2- + M --> H2O2 + MOH
kmohf	1e+8[m/s]	MOH partitioning
kmohb	1[m/s]	
kmf	1e+5[1/s]	complexation in the aqueous phase
kmb	1[L/mol/s]	
kcf2	5000[L/mol/s]	organic phase MOH formation aqueous phase
kcb2	1[1/s]	
cOHorgi	0 [mol/L]	
D_OH	1e-9 [m^2/s]	OH diffusion coefficient

Name	Expression	Description
rd	0.7 [cm]	

1.2 Variables

1.2.1 Variables 1

Selection

Geometric entity level	Entire model

Name	Expression	Description
E_swp	Ei + (2*(Ef - Ei))/pi*asin(sin((pi*nu*t)/(2*(Ef - Ei))))	
E_swp2	(Ei - nu*t)*(t<=25) + (Ef + nu*(t - 25))*(t>25)	
kf	k0*exp(-alpha*fara*n1*(E_swp - E0))	Metal
kb	k0*exp((1 - alpha)*fara*n1*(E_swp - E0))	
E_swp3	Ei	
kf2	k02*exp(-alpha*fara*n1*(E_swp - E02))	DMFc+
kb2	k02*exp((1 - alpha)*fara*n1*(E_swp - E02))	
kf3	k0*exp(-alpha*fara*n2*(E_swp - E03))	hydroxyl
kb3	k0*exp((1 - alpha)*fara*n2*(E_swp - E03))	

1.2.2 Variables 2

Selection

Geometric entity level	Entire model

Name	Expression	Description
Ibar	comp1.intop1(intcpl_source_Ibar)	

2 Component 1 (comp1)

2.1 Definitions

2.1.1 Variables

Variables 3

Selection

Geometric entity level	Boundary
Selection	Boundary 2

Name	Expression	Description
intcpl_source_Ibar	pi*(rd^2)*F*(chds.ndflux_Maq - chds.ndflux_OHaq + chds.ndflux_Fcplusaq)	

2.1.2 Component Couplings

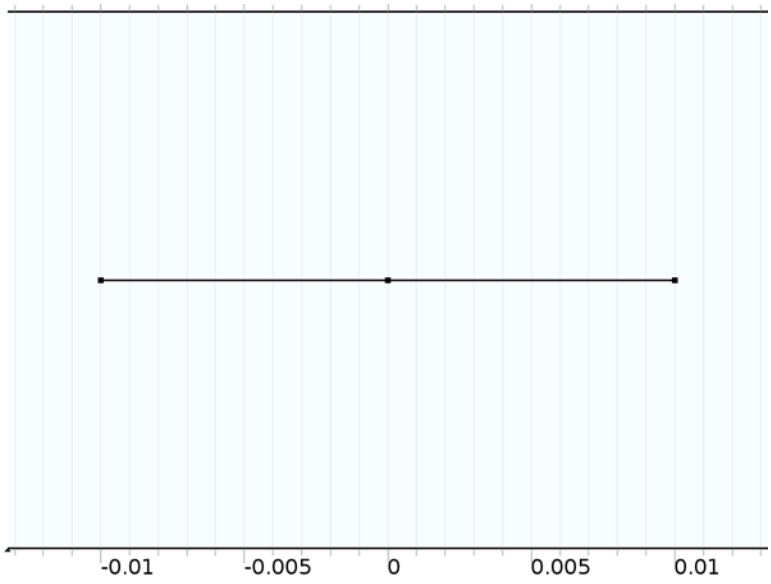
Integration 1

Coupling type	Integration
Operator name	intop1

Source selection

Geometric entity level	Boundary
Selection	Boundary 2

2.2 Geometry 1



Geometry 1

Units

Length unit	m
Angular unit	deg

Geometry statistics

Property	Value
Space dimension	1
Number of domains	2
Number of boundaries	3

2.2.1 Interval 1 (i1)

Selections of resulting entities

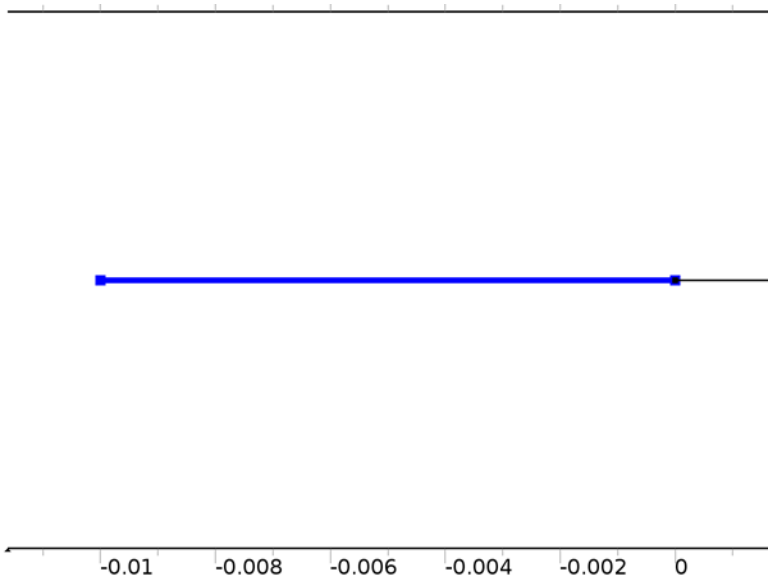
Name	Value
Number of intervals	One
Left endpoint	-0.01
Right endpoint	0

2.2.2 Interval 2 (i2)

Selections of resulting entities

Name	Value
Number of intervals	One
Left endpoint	0
Right endpoint	0.01

2.3 Transport of Diluted Species (chds)



Transport of Diluted Species

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(-D_i \nabla c_i\right) + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\mathbf{N}_i = -D_i \nabla c_i + \mathbf{u} c_i$$

Settings

Description	Value
Concentration	Linear
Compute boundary fluxes	On
Apply smoothing to boundary fluxes	On
Value type when using splitting of complex variables	Real
Migration in electric field	0

Description	Value
Convection	1
Convective term	Non - conservative form
Equation residual	Approximate residual
Enable space-dependent physics interfaces	0
Synchronize with COMSOL Multiphysics	

Used products

COMSOL Multiphysics
Chemical Reaction Engineering Module

Variables

Name	Expression	Unit	Description	Selection
chds.nx	unx		Normal vector, x component	Boundary 1
chds.ny	0		Normal vector, y component	Boundary 1
chds.nz	0		Normal vector, z component	Boundary 1
chds.nx	dnx		Normal vector, x component	Boundary 2
chds.ny	0		Normal vector, y component	Boundary 2
chds.nz	0		Normal vector, z component	Boundary 2

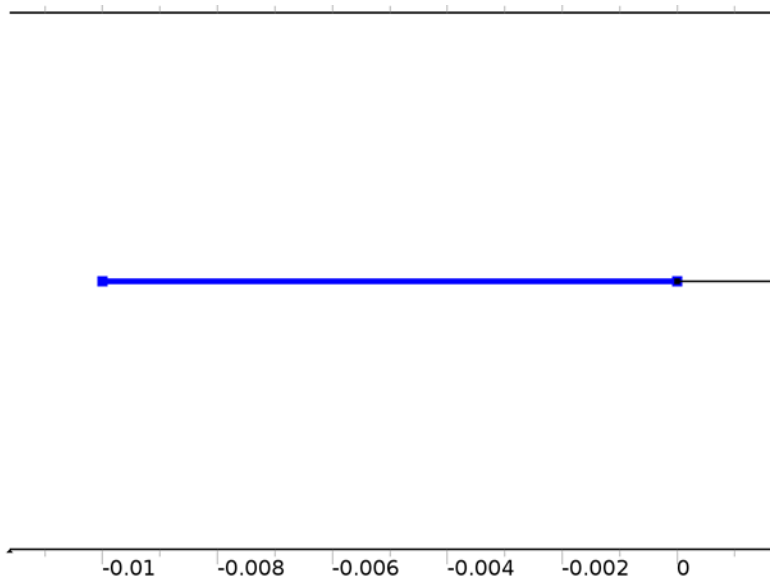
Name	Expression	Unit	Description	Selection
chds.nxmesh	root.unxmesh		Normal vector (mesh), x component	Boundary 1
chds.nymesh	0		Normal vector (mesh), y component	Boundary 1
chds.nzmesh	0		Normal vector (mesh), z component	Boundary 1
chds.nxmesh	root.dnxmesh		Normal vector (mesh), x component	Boundary 2
chds.nymesh	0		Normal vector (mesh), y component	Boundary 2
chds.nzmesh	0		Normal vector (mesh), z component	Boundary 2
chds.R_Maq	0	mol/(m^3*s)	Total rate expression	Domain 1
chds.R_OHaq	0	mol/(m^3*s)	Total rate expression	Domain 1
chds.R_Fcplusaq	0	mol/(m^3*s)	Total rate expression	Domain 1

Name	Expression	Unit	Description	Selection
chds.R_MOH	0	mol/(m^3*s)	Total rate expression	Domain 1
domflux.Maqx	chds.dfluxx_Maq	mol/(m^2*s)	Domain flux	Domain 1
domflux.OHaqx	chds.dfluxx_OHaq	mol/(m^2*s)	Domain flux	Domain 1
domflux.Fcplusaqx	chds.dfluxx_Fcplusaq	mol/(m^2*s)	Domain flux	Domain 1
domflux.MOHx	chds.dfluxx_MOH	mol/(m^2*s)	Domain flux	Domain 1
chds.bndFlux_Maq	-uflux_spatial(Maq)	mol/(m^2*s)	Boundary flux	Boundary 1
chds.bndFlux_Maq	-dflux_spatial(Maq)	mol/(m^2*s)	Boundary flux	Boundary 2
chds.ntflux_Maq	chds.bndFlux_Maq+chds.cfluxx_Maq*chds.nx+chds.cfluxy_Maq*chds.ny+chds.cfluxz_Maq*chds.nz	mol/(m^2*s)	Normal total flux	Boundaries 1–2
chds.ndflux_Maq	chds.bndFlux_Maq	mol/(m^2*s)	Normal diffusive flux	Boundaries 1–2
chds.ncflux_Maq	chds.cfluxx_Maq*chds.nx+chds.cfluxy_Maq*chds.ny+chds.cfluxz_Maq*chds.nz	mol/(m^2*s)	Normal convective flux	Boundaries 1–2
chds.bndFlux_OHaq	-uflux_spatial(OHaq)	mol/(m^2*s)	Boundary flux	Boundary 1
chds.bndFlux_OHaq	-dflux_spatial(OHaq)	mol/(m^2*s)	Boundary flux	Boundary 2
chds.ntflux_OHaq	chds.bndFlux_OHaq+chds.cfluxx_OHaq*chds.nx+chds.cfluxy_O	mol/(m^2*s)	Normal total flux	Boundaries 1–2

Name	Expression	Unit	Description	Selection
	Haq*chds.ny+chds.cfluxz_OHaq*chds.nz			
chds.ndflux_OHaq	chds.bndFlux_OHaq	mol/(m^2*s)	Normal diffusive flux	Boundaries 1–2
chds.ncflux_OHaq	chds.cfluxx_OHaq*chds.nx+chds.cfluxy_OHaq*chds.ny+chds.cfluxz_OHaq*chds.nz	mol/(m^2*s)	Normal convective flux	Boundaries 1–2
chds.bndFlux_Fcplusaq	-uflux_spatial(Fcplusaq)	mol/(m^2*s)	Boundary flux	Boundary 1
chds.bndFlux_Fcplusaq	-dflux_spatial(Fcplusaq)	mol/(m^2*s)	Boundary flux	Boundary 2
chds.ntflux_Fcplusaq	chds.bndFlux_Fcplusaq+chds.cfluxx_Fcplusaq*chds.nx+chds.cfluxy_Fcplusaq*chds.ny+chds.cfluxz_Fcplusaq*chds.nz	mol/(m^2*s)	Normal total flux	Boundaries 1–2
chds.ndflux_Fcplusaq	chds.bndFlux_Fcplusaq	mol/(m^2*s)	Normal diffusive flux	Boundaries 1–2
chds.ncflux_Fcplusaq	chds.cfluxx_Fcplusaq*chds.nx+chds.cfluxy_Fcplusaq*chds.ny+chds.cfluxz_Fcplusaq*chds.nz	mol/(m^2*s)	Normal convective flux	Boundaries 1–2
chds.bndFlux_MOH	-uflux_spatial(MOH)	mol/(m^2*s)	Boundary flux	Boundary 1

Name	Expression	Unit	Description	Selection
chds.bndFlux_MOH	-dflux_spatial(MOH)	mol/(m^2*s)	Boundary flux	Boundary 2
chds.ntflux_MOH	chds.bndFlux_MOH+chds.cfluxx_MOH*chds.nx+chds.cfluxy_MOH*chds.ny+chds.cfluxz_MOH*chds.nz	mol/(m^2*s)	Normal total flux	Boundaries 1–2
chds.ndflux_MOH	chds.bndFlux_MOH	mol/(m^2*s)	Normal diffusive flux	Boundaries 1–2
chds.ncflux_MOH	chds.cfluxx_MOH*chds.nx+chds.cfluxy_MOH*chds.ny+chds.cfluxz_MOH*chds.nz	mol/(m^2*s)	Normal convective flux	Boundaries 1–2

2.3.1 Convection and Diffusion 1



Convection and Diffusion 1

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(-D_i \nabla c_i\right) + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\mathbf{N}_i = -D_i \nabla c_i + \mathbf{u} c_i$$

Settings

Settings

Description	Value
Velocity field	User defined
Velocity field	{0, 0, 0}
Electric potential	User defined
Electric potential	0
Diffusion coefficient	User defined
Diffusion coefficient	{{D_M, 0, 0}, {0, D_M, 0}, {0, 0, D_M}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_Cl, 0, 0}, {0, D_Cl, 0}, {0, 0, D_Cl}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_DMFcplus, 0, 0}, {0, D_DMFcplus, 0}, {0, 0, D_DMFcplus}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_M, 0, 0}, {0, D_M, 0}, {0, 0, D_M}}
Bulk material	None

Used products

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
chds.cbf_Maq	0	mol/(m^2*s)	Convective boundary flux	Boundaries 1–2
chds.cbf_OHaq	0	mol/(m^2*s)	Convective boundary flux	Boundaries 1–2
chds.cbf_Fcplusaq	0	mol/(m^2*s)	Convective boundary flux	Boundaries 1–2

Name	Expression	Unit	Description	Selection
chds.cbf_MOH	0	mol/(m^2*s)	Convective boundary flux	Boundaries 1–2
chds.Dxx_Maq	D_M	m^2/s	Diffusion coefficient, xx component	Domain 1
chds.Dyx_Maq	0	m^2/s	Diffusion coefficient, yx component	Domain 1
chds.Dzx_Maq	0	m^2/s	Diffusion coefficient, zx component	Domain 1
chds.Dxy_Maq	0	m^2/s	Diffusion coefficient, xy component	Domain 1
chds.Dyy_Maq	D_M	m^2/s	Diffusion coefficient, yy component	Domain 1
chds.Dzy_Maq	0	m^2/s	Diffusion coefficient, zy component	Domain 1
chds.Dxz_Maq	0	m^2/s	Diffusion coefficient, xz component	Domain 1
chds.Dyz_Maq	0	m^2/s	Diffusion coefficient, yz component	Domain 1
chds.Dzz_Maq	D_M	m^2/s	Diffusion coefficient, zz component	Domain 1

Name	Expression	Unit	Description	Selection
chds.Dav_Maq	chds.Dxx_Maq	m^2/s	Average diffusion coefficient	Domain 1
chds.tfluxx_Maq	-chds.Dxx_Maq*Maqx+chds.cfluxx_Maq	mol/(m^2*s)	Total flux, x component	Domain 1
chds.tfluxy_Maq	-chds.Dyx_Maq*Maqx+chds.cfluxy_Maq	mol/(m^2*s)	Total flux, y component	Domain 1
chds.tfluxz_Maq	-chds.Dzx_Maq*Maqx+chds.cfluxz_Maq	mol/(m^2*s)	Total flux, z component	Domain 1
chds.dfluxx_Maq	-chds.Dxx_Maq*Maqx	mol/(m^2*s)	Diffusive flux, x component	Domain 1
chds.dfluxy_Maq	-chds.Dyx_Maq*Maqx	mol/(m^2*s)	Diffusive flux, y component	Domain 1
chds.dfluxz_Maq	-chds.Dzx_Maq*Maqx	mol/(m^2*s)	Diffusive flux, z component	Domain 1
chds.gradx_Maq	Maqx	mol/m^4	Concentration gradient, x component	Domain 1
chds.grady_Maq	0	mol/m^4	Concentration gradient, y component	Domain 1
chds.gradz_Maq	0	mol/m^4	Concentration gradient, z component	Domain 1

Name	Expression	Unit	Description	Selection
chds.dfluxMag_Maq	sqrt(chds.dfluxx_Maq^2+chds.dfluxy_Maq^2+chds.dfluxz_Maq^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 1
chds.tfluxMag_Maq	sqrt(chds.tfluxx_Maq^2+chds.tfluxy_Maq^2+chds.tfluxz_Maq^2)	mol/(m^2*s)	Total flux magnitude	Domain 1
chds.Dxx_OHaq	D_Cl	m^2/s	Diffusion coefficient, xx component	Domain 1
chds.Dyx_OHaq	0	m^2/s	Diffusion coefficient, yx component	Domain 1
chds.Dzx_OHaq	0	m^2/s	Diffusion coefficient, zx component	Domain 1
chds.Dxy_OHaq	0	m^2/s	Diffusion coefficient, xy component	Domain 1
chds.Dyy_OHaq	D_Cl	m^2/s	Diffusion coefficient, yy component	Domain 1
chds.Dzy_OHaq	0	m^2/s	Diffusion coefficient, zy component	Domain 1
chds.Dxz_OHaq	0	m^2/s	Diffusion coefficient, xz component	Domain 1
chds.Dyz_OHaq	0	m^2/s	Diffusion coefficient, yz component	Domain 1

Name	Expression	Unit	Description	Selection
chds.Dzz_OHaq	D_Cl	m^2/s	Diffusion coefficient, zz component	Domain 1
chds.Dav_OHaq	chds.Dxx_OHaq	m^2/s	Average diffusion coefficient	Domain 1
chds.tfluxx_OHaq	-chds.Dxx_OHaq*OHaqx+chds.cfluxx_OHaq	mol/(m^2*s)	Total flux, x component	Domain 1
chds.tfluxy_OHaq	-chds.Dyx_OHaq*OHaqx+chds.cfluxy_OHaq	mol/(m^2*s)	Total flux, y component	Domain 1
chds.tfluxz_OHaq	-chds.Dzx_OHaq*OHaqx+chds.cfluxz_OHaq	mol/(m^2*s)	Total flux, z component	Domain 1
chds.dfluxx_OHaq	-chds.Dxx_OHaq*OHaqx	mol/(m^2*s)	Diffusive flux, x component	Domain 1
chds.dfluxy_OHaq	-chds.Dyx_OHaq*OHaqx	mol/(m^2*s)	Diffusive flux, y component	Domain 1
chds.dfluxz_OHaq	-chds.Dzx_OHaq*OHaqx	mol/(m^2*s)	Diffusive flux, z component	Domain 1
chds.gradx_OHaq	OHaqx	mol/m^4	Concentration gradient, x component	Domain 1
chds.grady_OHaq	0	mol/m^4	Concentration gradient, y component	Domain 1

Name	Expression	Unit	Description	Selection
chds.gradz_OHaq	0	mol/m^4	Concentration gradient, z component	Domain 1
chds.dfluxMag_OHaq	sqrt(chds.dfluxx_OHaq^2+chds.dfluxy_OHaq^2+chds.dfluxz_OHaq^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 1
chds.tfluxMag_OHaq	sqrt(chds.tfluxx_OHaq^2+chds.tfluxy_OHaq^2+chds.tfluxz_OHaq^2)	mol/(m^2*s)	Total flux magnitude	Domain 1
chds.Dxx_Fcplusaq	D_DMFcplus	m^2/s	Diffusion coefficient, xx component	Domain 1
chds.Dyx_Fcplusaq	0	m^2/s	Diffusion coefficient, yx component	Domain 1
chds.Dzx_Fcplusaq	0	m^2/s	Diffusion coefficient, zx component	Domain 1
chds.Dxy_Fcplusaq	0	m^2/s	Diffusion coefficient, xy component	Domain 1
chds.Dyy_Fcplusaq	D_DMFcplus	m^2/s	Diffusion coefficient, yy component	Domain 1
chds.Dzy_Fcplusaq	0	m^2/s	Diffusion coefficient, zy component	Domain 1
chds.Dxz_Fcplusaq	0	m^2/s	Diffusion coefficient, xz component	Domain 1

Name	Expression	Unit	Description	Selection
chds.Dyz_Fcplusaq	0	m^2/s	Diffusion coefficient, yz component	Domain 1
chds.Dzz_Fcplusaq	D_DMFcplus	m^2/s	Diffusion coefficient, zz component	Domain 1
chds.Dav_Fcplusaq	chds.Dxx_Fcplusaq	m^2/s	Average diffusion coefficient	Domain 1
chds.tfluxx_Fcplusaq	-chds.Dxx_Fcplusaq*Fcplusaqx+chds.cfluxx_Fcplusaq	mol/(m^2*s)	Total flux, x component	Domain 1
chds.tfluxy_Fcplusaq	-chds.Dyx_Fcplusaq*Fcplusaqx+chds.cfluxy_Fcplusaq	mol/(m^2*s)	Total flux, y component	Domain 1
chds.tfluxz_Fcplusaq	-chds.Dzx_Fcplusaq*Fcplusaqx+chds.cfluxz_Fcplusaq	mol/(m^2*s)	Total flux, z component	Domain 1
chds.dfluxx_Fcplusaq	-chds.Dxx_Fcplusaq*Fcplusaqx	mol/(m^2*s)	Diffusive flux, x component	Domain 1
chds.dfluxy_Fcplusaq	-chds.Dyx_Fcplusaq*Fcplusaqx	mol/(m^2*s)	Diffusive flux, y component	Domain 1
chds.dfluxz_Fcplusaq	-chds.Dzx_Fcplusaq*Fcplusaqx	mol/(m^2*s)	Diffusive flux, z component	Domain 1
chds.gradx_Fcplusaq	Fcplusaqx	mol/m^4	Concentration gradient, x component	Domain 1

Name	Expression	Unit	Description	Selection
chds.grady_Fcplusaq	0	mol/m^4	Concentration gradient, y component	Domain 1
chds.gradz_Fcplusaq	0	mol/m^4	Concentration gradient, z component	Domain 1
chds.dfluxMag_Fcplusaq	sqrt(chds.dfluxx_Fcplusaq^2+chds.dfluxy_Fcplusaq^2+chds.dfluxz_Fcplusaq^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 1
chds.tfluxMag_Fcplusaq	sqrt(chds.tfluxx_Fcplusaq^2+chds.tfluxy_Fcplusaq^2+chds.tfluxz_Fcplusaq^2)	mol/(m^2*s)	Total flux magnitude	Domain 1
chds.Dxx_MOH	D_M	m^2/s	Diffusion coefficient, xx component	Domain 1
chds.Dyx_MOH	0	m^2/s	Diffusion coefficient, yx component	Domain 1
chds.Dzx_MOH	0	m^2/s	Diffusion coefficient, zx component	Domain 1
chds.Dxy_MOH	0	m^2/s	Diffusion coefficient, xy component	Domain 1
chds.Dyy_MOH	D_M	m^2/s	Diffusion coefficient, yy component	Domain 1
chds.Dzy_MOH	0	m^2/s	Diffusion coefficient, zy component	Domain 1

Name	Expression	Unit	Description	Selection
chds.Dxz_MOH	0	m^2/s	Diffusion coefficient, xz component	Domain 1
chds.Dyz_MOH	0	m^2/s	Diffusion coefficient, yz component	Domain 1
chds.Dzz_MOH	D_M	m^2/s	Diffusion coefficient, zz component	Domain 1
chds.Dav_MOH	chds.Dxx_MOH	m^2/s	Average diffusion coefficient	Domain 1
chds.tfluxx_MOH	-chds.Dxx_MOH*MOHx+chds.cfluxx_MOH	mol/(m^2*s)	Total flux, x component	Domain 1
chds.tfluxy_MOH	-chds.Dyx_MOH*MOHx+chds.cfluxy_MOH	mol/(m^2*s)	Total flux, y component	Domain 1
chds.tfluxz_MOH	-chds.Dzx_MOH*MOHx+chds.cfluxz_MOH	mol/(m^2*s)	Total flux, z component	Domain 1
chds.dfluxx_MOH	-chds.Dxx_MOH*MOHx	mol/(m^2*s)	Diffusive flux, x component	Domain 1
chds.dfluxy_MOH	-chds.Dyx_MOH*MOHx	mol/(m^2*s)	Diffusive flux, y component	Domain 1
chds.dfluxz_MOH	-chds.Dzx_MOH*MOHx	mol/(m^2*s)	Diffusive flux, z component	Domain 1

Name	Expression	Unit	Description	Selection
chds.gradx_MOH	MOHx	mol/m^4	Concentration gradient, x component	Domain 1
chds.grady_MOH	0	mol/m^4	Concentration gradient, y component	Domain 1
chds.gradz_MOH	0	mol/m^4	Concentration gradient, z component	Domain 1
chds.dfluxMag_MOH	sqrt(chds.dfluxx_MOH^2+chds.dfluxy_MOH^2+chds.dfluxz_MOH^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 1
chds.tfluxMag_MOH	sqrt(chds.tfluxx_MOH^2+chds.tfluxy_MOH^2+chds.tfluxz_MOH^2)	mol/(m^2*s)	Total flux magnitude	Domain 1
chds.u	model.input.u1	m/s	Velocity field, x component	Domain 1
chds.v	model.input.u2	m/s	Velocity field, y component	Domain 1
chds.w	model.input.u3	m/s	Velocity field, z component	Domain 1
chds.cfluxx_Maq	Maq*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 1
chds.cfluxy_Maq	Maq*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 1

Name	Expression	Unit	Description	Selection
chds.cfluxz_Maq	Maq*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 1
chds.cfluxMag_Maq	sqrt(chds.cfluxx_Maq^2+chds.cfluxy_Maq^2+chds.cfluxz_Maq^2)	mol/(m^2*s)	Convective flux magnitude	Domain 1
chds.cfluxx_OHaq	OHaq*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 1
chds.cfluxy_OHaq	OHaq*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 1
chds.cfluxz_OHaq	OHaq*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 1
chds.cfluxMag_OHaq	sqrt(chds.cfluxx_OHaq^2+chds.cfluxy_OHaq^2+chds.cfluxz_OHaq^2)	mol/(m^2*s)	Convective flux magnitude	Domain 1
chds.cfluxx_Fcplusaq	Fcplusaq*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 1
chds.cfluxy_Fcplusaq	Fcplusaq*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 1
chds.cfluxz_Fcplusaq	Fcplusaq*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 1
chds.cfluxMag_Fcplusaq	sqrt(chds.cfluxx_Fcplusaq^2+chds.cfluxy_Fcplusaq^2+chds.cfluxz_Fcplusaq^2)	mol/(m^2*s)	Convective flux magnitude	Domain 1

Name	Expression	Unit	Description	Selection
chds.cfluxx_MOH	MOH*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 1
chds.cfluxy_MOH	MOH*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 1
chds.cfluxz_MOH	MOH*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 1
chds.cfluxMag_MOH	sqrt(chds.cfluxx_MOH^2+chds.cfluxy_MOH^2+chds.cfluxz_MOH^2)	mol/(m^2*s)	Convective flux magnitude	Domain 1
chds.helem	h	m	Element size	Domain 1
chds.Res_Maq	chds.u*Maqx-chds.R_Maq	mol/(m^3*s)	Equation residual	Domain 1
chds.Res_OHaq	chds.u*OHaqx-chds.R_OHaq	mol/(m^3*s)	Equation residual	Domain 1
chds.Res_Fcplusaq	chds.u*Fcplusaqx-chds.R_Fcplusaq	mol/(m^3*s)	Equation residual	Domain 1
chds.Res_MOH	chds.u*MOHx-chds.R_MOH	mol/(m^3*s)	Equation residual	Domain 1

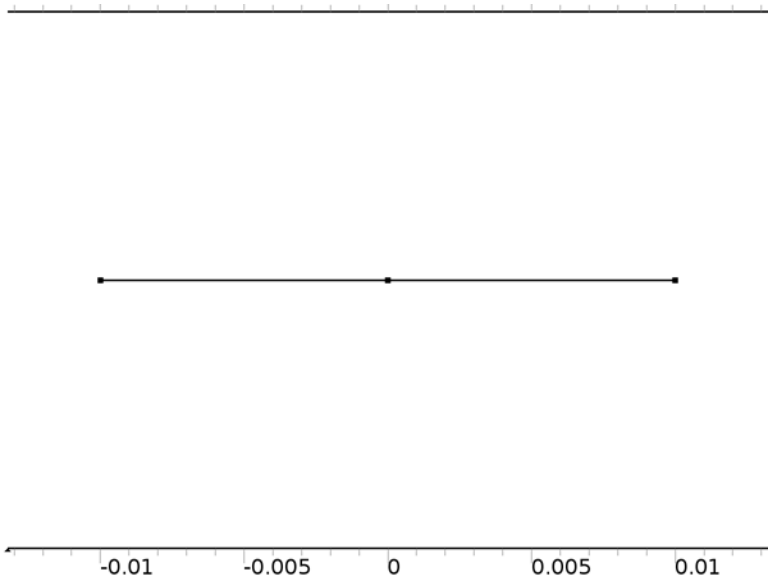
Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
Maq	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 1
OHaq	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 1
Fcplusaq	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 1
MOH	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 1

Weak expressions

Weak expression	Integration frame	Selection
-d(Maq,t)*test(Maq)- chds.Dxx_Maq*Maqx*test(Maqx)	Material	Domain 1
-d(OHaq,t)*test(OHaq)- chds.Dxx_OHaq*OHaqx*test(OHaqx)	Material	Domain 1
-d(Fcplusaq,t)*test(Fcplusaq)- chds.Dxx_Fcplusaq*Fcplusaqx*test(Fcplusaqx)	Material	Domain 1
-d(MOH,t)*test(MOH)- chds.Dxx_MOH*MOHx*test(MOHx)	Material	Domain 1
-chds.u*Maqx*test(Maq)	Material	Domain 1
chds.cbf_Maq*test(Maq)	Material	Boundaries 1–2
-chds.u*OHaqx*test(OHaq)	Material	Domain 1
chds.cbf_OHaq*test(OHaq)	Material	Boundaries 1–2
-chds.u*Fcplusaqx*test(Fcplusaq)	Material	Domain 1
chds.cbf_Fcplusaq*test(Fcplusaq)	Material	Boundaries 1–2
-chds.u*MOHx*test(MOH)	Material	Domain 1
chds.cbf_MOH*test(MOH)	Material	Boundaries 1–2
chds.streamline	Material	Domain 1
chds.crosswind	Material	Domain 1

2.3.2 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	No boundaries

Equations

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

Settings

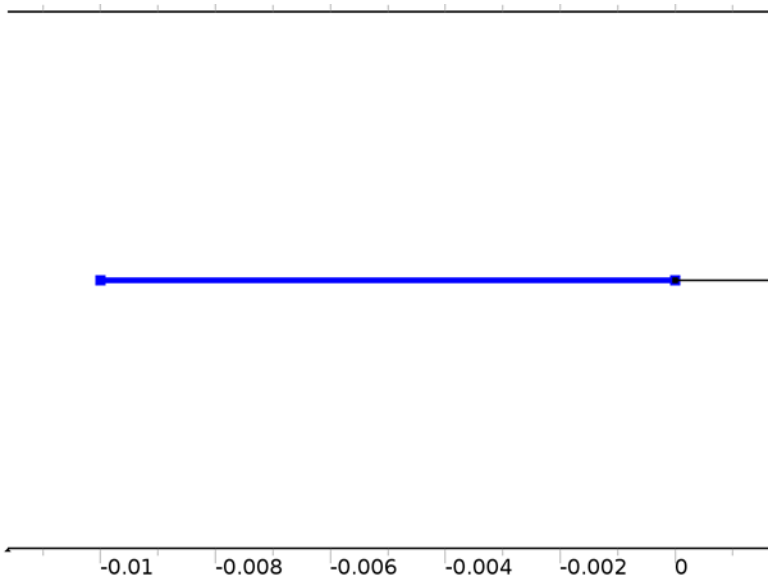
Settings

Description	Value
Apply for all species	Apply for all species

Used products

COMSOL Multiphysics

2.3.3 Initial Values 1



Initial Values 1

Selection

Geometric entity level	Domain
Selection	Domain 1

Settings

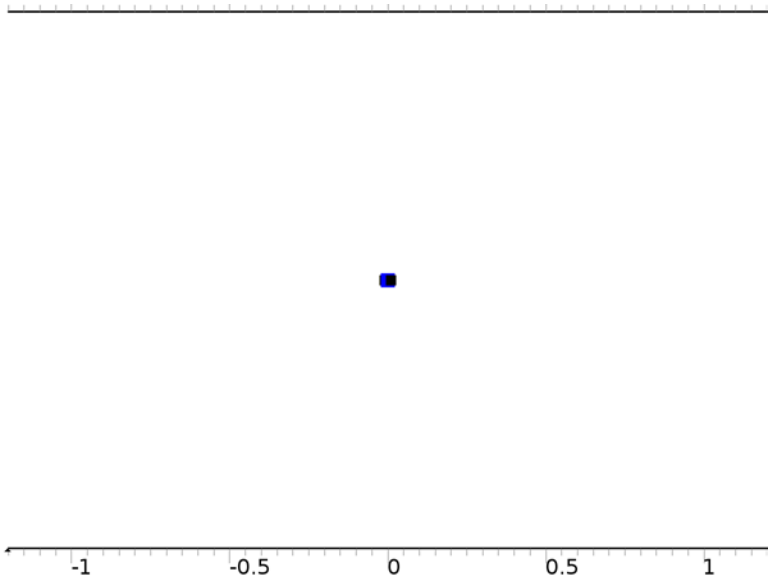
Settings

Description	Value
Concentration	cMaqi
Concentration	cOHaqi
Concentration	cDMFcplusaqi
Concentration	cMOHi

Used products

COMSOL Multiphysics

2.3.4 Flux 1



Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundary 2

Equations

$$-\mathbf{n} \cdot \mathbf{N}_i = N_{0i}$$

Settings

Settings

Description	Value
Species Maq	On
Species OHaq	On
Species Fcplusaq	On
Species MOH	On
Inward flux	{-kb*Maq + kf*Mplus, -kb3*OHaq + kf3*OH, kf2*Fcplus - kb2*Fcplusaq, kmohf*MOHorg - kmohb*MOH}
Flux type	General inward flux

Used products

COMSOL Multiphysics

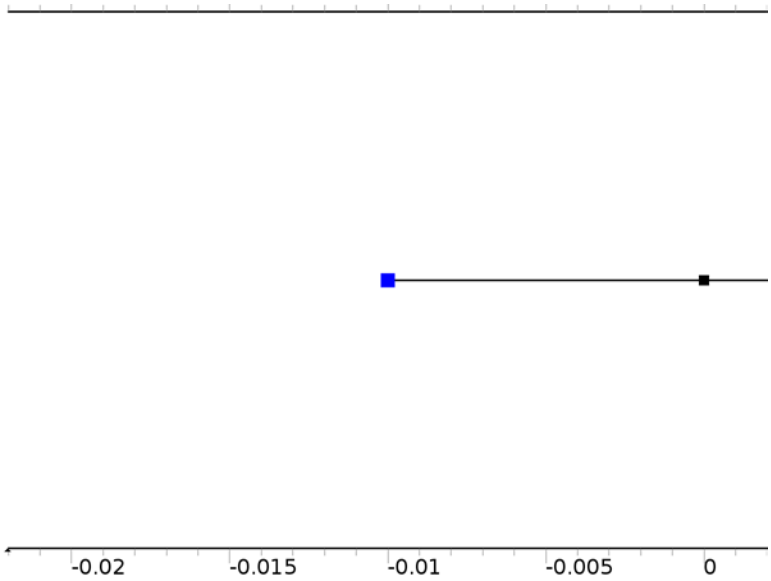
Variables

Name	Expression	Unit	Description	Selection
chds.cbf_Maq	Maq*(chds.u*chds.nxmesh+chds.v*chds.nymesh+chds.w*chds.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds.cbf_OHaq	OHaq*(chds.u*chds.nxmesh+chds.v*chds.nymesh+chds.w*chds.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds.cbf_Fcplusaq	Fcplusaq*(chds.u*chds.nxmesh+chds.v*chds.nymesh+chds.w*chds.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds.cbf_MOH	MOH*(chds.u*chds.nxmesh+chds.v*chds.nymesh+chds.w*chds.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2

Weak expressions

Weak expression	Integration frame	Selection
(-kb*Maq+kf*Mplus)*test(Maq)	Material	Boundary 2
(-kb3*OHaq+kf3*OH)*test(OHaq)	Material	Boundary 2
(kf2*Fcplus-kb2*Fcplusaq)*test(Fcplusaq)	Material	Boundary 2
(kmohf*MOHorg-kmohb*MOH)*test(MOH)	Material	Boundary 2

2.3.5 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 1

Equations

$$c_i = c_{0i}$$

Settings

Settings

Description	Value
Concentration	{cMaqi, cOHaqi, cDMFcplusaqi, cMOHi}
Species Maq	On
Species OHaq	On
Species Fcplusaq	On
Species MOH	On
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off

Used products

COMSOL Multiphysics

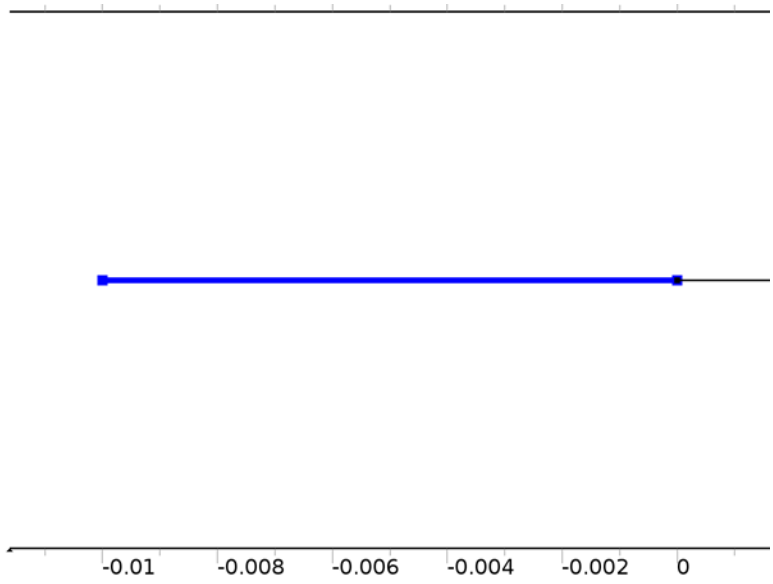
Variables

Name	Expression	Unit	Description	Selection
chds.c0_Maq	cMaqi	mol/m^3	Concentration	Boundary 1
chds.c0_OHaq	cOHaqi	mol/m^3	Concentration	Boundary 1
chds.c0_Fcplusaq	cDMFcplusaqi	mol/m^3	Concentration	Boundary 1
chds.c0_MOH	cMOHi	mol/m^3	Concentration	Boundary 1

Shape functions

Constraint	Constraint force	Shape function	Selection
-Maq+chds.c0_Maq	test(-Maq+chds.c0_Maq)	Lagrange (Linear)	Boundary 1
-OHaq+chds.c0_OHaq	test(-OHaq+chds.c0_OHaq)	Lagrange (Linear)	Boundary 1
-Fcplusaq+chds.c0_Fcplusaq	test(-Fcplusaq+chds.c0_Fcplusaq)	Lagrange (Linear)	Boundary 1
-MOH+chds.c0_MOH	test(-MOH+chds.c0_MOH)	Lagrange (Linear)	Boundary 1

2.3.6 Reactions 1



Reactions 1

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(-D_i \nabla c_i\right) + \mathbf{u} \cdot \nabla c_i = R_i$$

Settings

Settings

Description	Value
Total rate expression	{kmf*MOH - kmb*Maq*OHaq, kmf*MOH - kmb*Maq*OHaq, 0, -kmf*MOH + kmb*Maq*OHaq}

Used products

COMSOL Multiphysics

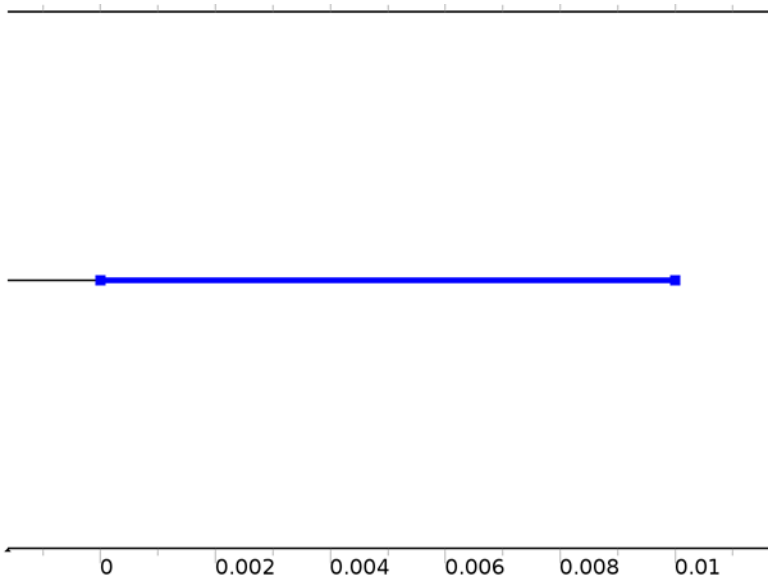
Variables

Name	Expression	Unit	Description	Selection
chds.R_Maq	kmf*MOH-kmb*Maq*OHaq	mol/(m^3*s)	Total rate expression	Domain 1
chds.R_OHaq	kmf*MOH-kmb*Maq*OHaq	mol/(m^3*s)	Total rate expression	Domain 1
chds.R_Fcplusaq	0	mol/(m^3*s)	Total rate expression	Domain 1
chds.R_MOH	-kmf*MOH+kmb*Maq*OHaq	mol/(m^3*s)	Total rate expression	Domain 1

Weak expressions

Weak expression	Integration frame	Selection
(kmf*MOH-kmb*Maq*OHaq)*test(Maq)	Material	Domain 1
(kmf*MOH-kmb*Maq*OHaq)*test(OHaq)	Material	Domain 1
(-kmf*MOH+kmb*Maq*OHaq)*test(MOH)	Material	Domain 1

2.4 Transport of Diluted Species 2 (chds2)



Transport of Diluted Species 2

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(-D_i \nabla c_i\right) + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\mathbf{N}_i = -D_i \nabla c_i + \mathbf{u} c_i$$

Settings

Description	Value
Concentration	Linear
Compute boundary fluxes	On
Apply smoothing to boundary fluxes	On
Value type when using splitting of complex variables	Real
Migration in electric field	0
Convection	1
Convective term	Non - conservative form
Equation residual	Approximate residual
Enable space-dependent physics interfaces	0

Description	Value
Synchronize with COMSOL Multiphysics	

Used products

COMSOL Multiphysics
Chemical Reaction Engineering Module

Variables

Name	Expression	Unit	Description	Selection
chds2.nx	unx		Normal vector, x component	Boundary 2
chds2.ny	0		Normal vector, y component	Boundary 2
chds2.nz	0		Normal vector, z component	Boundary 2
chds2.nx	dnx		Normal vector, x component	Boundary 3
chds2.ny	0		Normal vector, y component	Boundary 3
chds2.nz	0		Normal vector, z component	Boundary 3
chds2.nxmesh	root.unxmesh		Normal vector (mesh), x component	Boundary 2

Name	Expression	Unit	Description	Selection
chds2.nymesh	0		Normal vector (mesh), y component	Boundary 2
chds2.nzmesh	0		Normal vector (mesh), z component	Boundary 2
chds2.nxmesh	root.dnxmesh		Normal vector (mesh), x component	Boundary 3
chds2.nymesh	0		Normal vector (mesh), y component	Boundary 3
chds2.nzmesh	0		Normal vector (mesh), z component	Boundary 3
chds2.R_Mplus	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_OH	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_Fc	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_FcH	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_Fcplus	0	mol/(m^3*s)	Total rate expression	Domain 2

Name	Expression	Unit	Description	Selection
chds2.R_MOHorg	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_O2	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_HO2	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_HO2minus	0	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_H2O2	0	mol/(m^3*s)	Total rate expression	Domain 2
domflux.Mplusx	chds2.dfluxx_Mplus	mol/(m^2*s)	Domain flux	Domain 2
domflux.OHx	chds2.dfluxx_OH	mol/(m^2*s)	Domain flux	Domain 2
domflux.Fcx	chds2.dfluxx_Fc	mol/(m^2*s)	Domain flux	Domain 2
domflux.FcHx	chds2.dfluxx_FcH	mol/(m^2*s)	Domain flux	Domain 2
domflux.Fcplusx	chds2.dfluxx_Fcplus	mol/(m^2*s)	Domain flux	Domain 2
domflux.MOHorgx	chds2.dfluxx_MOHorg	mol/(m^2*s)	Domain flux	Domain 2
domflux.O2x	chds2.dfluxx_O2	mol/(m^2*s)	Domain flux	Domain 2
domflux.HO2x	chds2.dfluxx_HO2	mol/(m^2*s)	Domain flux	Domain 2
domflux.HO2minusx	chds2.dfluxx_HO2minus	mol/(m^2*s)	Domain flux	Domain 2
domflux.H2O2x	chds2.dfluxx_H2O2	mol/(m^2*s)	Domain flux	Domain 2
chds2.bndFlux_Mplus	-uflux_spatial(Mplus)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_Mplus	-dflux_spatial(Mplus)	mol/(m^2*s)	Boundary flux	Boundary 3
chds2.ntflux_Mplus	chds2.bndFlux_Mplus+chds2.cfluxx_Mplus*chds2.nx+chds2.cflu	mol/(m^2*s)	Normal total flux	Boundaries 2–3

Name	Expression	Unit	Description	Selection
	xy_Mplus*chds2.ny+chds2.cfluxz_Mplus*chds2.nz			
chds2.ndflux_Mplus	chds2.bndFlux_Mplus	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_Mplus	chds2.cfluxx_Mplus*chds2.nx+chds2.cfluxy_Mplus*chds2.ny+chds2.cfluxz_Mplus*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_OH	-uflux_spatial(OH)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_OH	-dflux_spatial(OH)	mol/(m^2*s)	Boundary flux	Boundary 3
chds2.ntflux_OH	chds2.bndFlux_OH+chds2.cfluxx_OH*chds2.nx+chds2.cfluxy_OH*chds2.ny+chds2.cfluxz_OH*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_OH	chds2.bndFlux_OH	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_OH	chds2.cfluxx_OH*chds2.nx+chds2.cfluxy_OH*chds2.ny+chds2.cfluxz_OH*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_Fc	-uflux_spatial(Fc)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_Fc	-dflux_spatial(Fc)	mol/(m^2*s)	Boundary flux	Boundary 3

Name	Expression	Unit	Description	Selection
chds2.ntflux_Fc	chds2.bndFlux_Fc+chds2.cfluxx_Fc*chds2.nx+chds2.cfluxy_Fc*chds2.ny+chds2.cfluxz_Fc*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_Fc	chds2.bndFlux_Fc	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_Fc	chds2.cfluxx_Fc*chds2.nx+chds2.cfluxy_Fc*chds2.ny+chds2.cfluxz_Fc*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_FcH	-uflux_spatial(FcH)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_FcH	-dflux_spatial(FcH)	mol/(m^2*s)	Boundary flux	Boundary 3
chds2.ntflux_FcH	chds2.bndFlux_FcH+chds2.cfluxx_FcH*chds2.nx+chds2.cfluxy_FcH*chds2.ny+chds2.cfluxz_FcH*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_FcH	chds2.bndFlux_FcH	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_FcH	chds2.cfluxx_FcH*chds2.nx+chds2.cfluxy_FcH*chds2.ny+chds2.cfluxz_FcH*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_Fcplus	-uflux_spatial(Fcplus)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_Fcplus	-dflux_spatial(Fcplus)	mol/(m^2*s)	Boundary flux	Boundary 3

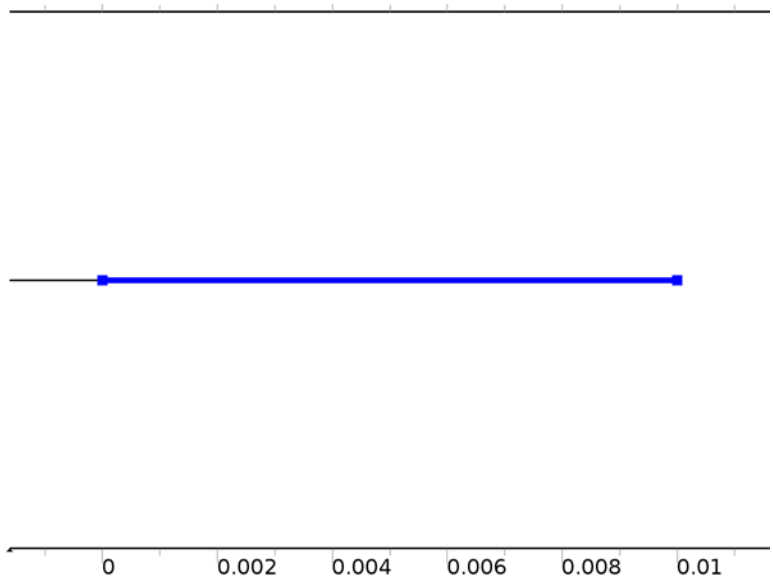
Name	Expression	Unit	Description	Selection
chds2.ntflux_Fcplus	chds2.bndFlux_Fcplus+chds2.cfluxx_Fcplus*chds2.nx+chds2.cfluxy_Fcplus*chds2.ny+chds2.cfluxz_Fcplus*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_Fcplus	chds2.bndFlux_Fcplus	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_Fcplus	chds2.cfluxx_Fcplus*chds2.nx+chds2.cfluxy_Fcplus*chds2.ny+chds2.cfluxz_Fcplus*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_MOHorg	-uflux_spatial(MOHorg)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_MOHorg	-dflux_spatial(MOHorg)	mol/(m^2*s)	Boundary flux	Boundary 3
chds2.ntflux_MOHorg	chds2.bndFlux_MOHorg+chds2.cfluxx_MOHorg*chds2.nx+chds2.cfluxy_MOHorg*chds2.ny+chds2.cfluxz_MOHorg*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_MOHorg	chds2.bndFlux_MOHorg	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_MOHorg	chds2.cfluxx_MOHorg*chds2.nx+chds2.cfluxy_MOHorg*chds2.	mol/(m^2*s)	Normal convective flux	Boundaries 2–3

Name	Expression	Unit	Description	Selection
	ny+chds2.cfluxz_MOHorg*chds2.nz			
chds2.bndFlux_O2	-uflux_spatial(O2)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_O2	-dflux_spatial(O2)	mol/(m^2*s)	Boundary flux	Boundary 3
chds2.ntflux_O2	chds2.bndFlux_O2+chds2.cfluxx_O2*chds2.nx+chds2.cfluxy_O2*chds2.ny+chds2.cfluxz_O2*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_O2	chds2.bndFlux_O2	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_O2	chds2.cfluxx_O2*chds2.nx+chds2.cfluxy_O2*chds2.ny+chds2.cfluxz_O2*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_HO2	-uflux_spatial(HO2)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_HO2	-dflux_spatial(HO2)	mol/(m^2*s)	Boundary flux	Boundary 3
chds2.ntflux_HO2	chds2.bndFlux_HO2+chds2.cfluxx_HO2*chds2.nx+chds2.cfluxy_HO2*chds2.ny+chds2.cfluxz_HO2*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_HO2	chds2.bndFlux_HO2	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3

Name	Expression	Unit	Description	Selection
chds2.ncflux_HO2	chds2.cfluxx_HO2*chds2.nx+chds2.cfluxy_HO2*chds2.ny+chds2.cfluxz_HO2*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_HO2minus	-uflux_spatial(HO2minus)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_HO2minus	-dflux_spatial(HO2minus)	mol/(m^2*s)	Boundary flux	Boundary 3
chds2.ntflux_HO2minus	chds2.bndFlux_HO2minus+chds2.cfluxx_HO2minus*chds2.nx+chds2.cfluxy_HO2minus*chds2.ny+chds2.cfluxz_HO2minus*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_HO2minus	chds2.bndFlux_HO2minus	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_HO2minus	chds2.cfluxx_HO2minus*chds2.nx+chds2.cfluxy_HO2minus*chds2.ny+chds2.cfluxz_HO2minus*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3
chds2.bndFlux_H2O2	-uflux_spatial(H2O2)	mol/(m^2*s)	Boundary flux	Boundary 2
chds2.bndFlux_H2O2	-dflux_spatial(H2O2)	mol/(m^2*s)	Boundary flux	Boundary 3

Name	Expression	Unit	Description	Selection
chds2.ntflux_H2O2	chds2.bndFlux_H2O2+chds2.cfluxx_H2O2*chds2.nx+chds2.cfluxy_H2O2*chds2.ny+chds2.cfluxz_H2O2*chds2.nz	mol/(m^2*s)	Normal total flux	Boundaries 2–3
chds2.ndflux_H2O2	chds2.bndFlux_H2O2	mol/(m^2*s)	Normal diffusive flux	Boundaries 2–3
chds2.ncflux_H2O2	chds2.cfluxx_H2O2*chds2.nx+chds2.cfluxy_H2O2*chds2.ny+chds2.cfluxz_H2O2*chds2.nz	mol/(m^2*s)	Normal convective flux	Boundaries 2–3

2.4.1 Convection and Diffusion 1



Convection and Diffusion 1

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(-D_i \nabla c_i\right) + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\mathbf{N}_i = -D_i \nabla c_i + \mathbf{u} c_i$$

Settings

Settings

Description	Value
Velocity field	User defined
Velocity field	{0, 0, 0}
Electric potential	User defined
Electric potential	0
Diffusion coefficient	User defined
Diffusion coefficient	{{D_M, 0, 0}, {0, D_M, 0}, {0, 0, D_M}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_Cl, 0, 0}, {0, D_Cl, 0}, {0, 0, D_Cl}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_DMFc, 0, 0}, {0, D_DMFc, 0}, {0, 0, D_DMFc}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_DMFcplus, 0, 0}, {0, D_DMFcplus, 0}, {0, 0, D_DMFcplus}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_DMFcplus, 0, 0}, {0, D_DMFcplus, 0}, {0, 0, D_DMFcplus}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_M, 0, 0}, {0, D_M, 0}, {0, 0, D_M}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_O2, 0, 0}, {0, D_O2, 0}, {0, 0, D_O2}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D_OH, 0, 0}, {0, D_OH, 0}, {0, 0, D_OH}}
Bulk material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{D_OH, 0, 0}, {0, D_OH, 0}, {0, 0, D_OH}}
Diffusion coefficient	User defined

Description	Value
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}

Used products

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
chds2.cbf_Mplus	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_OH	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_Fc	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_FcH	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_Fcplus	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_MOHorg	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_O2	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_HO2	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_HO2minus	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.cbf_H2O2	0	mol/(m^2*s)	Convective boundary flux	Boundaries 2–3
chds2.Dxx_Mplus	D_M	m^2/s	Diffusion coefficient, xx component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dyx_Mplus	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_Mplus	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_Mplus	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_Mplus	D_M	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_Mplus	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_Mplus	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_Mplus	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_Mplus	D_M	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_Mplus	chds2.Dxx_Mplus	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_Mplus	-chds2.Dxx_Mplus*Mplusx+chds2.cfluxx_Mplus	mol/(m^2*s)	Total flux, x component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.tfluxy_Mplus	-chds2.Dyx_Mplus*Mplusx+chds2.cfluxy_Mplus	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_Mplus	-chds2.Dzx_Mplus*Mplusx+chds2.cfluxz_Mplus	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_Mplus	-chds2.Dxx_Mplus*Mplusx	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_Mplus	-chds2.Dyx_Mplus*Mplusx	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_Mplus	-chds2.Dzx_Mplus*Mplusx	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_Mplus	Mplusx	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_Mplus	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_Mplus	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_Mplus	sqrt(chds2.dfluxx_Mplus^2+chds2.dfluxy_Mplus^2+chds2.dfluxz_Mplus^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_Mplus	sqrt(chds2.tfluxx_Mplus^2+chds2.tfluxy_Mplus^2+chds2.tfluxz_Mplus^2)	mol/(m^2*s)	Total flux magnitude	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dxx_OH	D_Cl	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_OH	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_OH	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_OH	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_OH	D_Cl	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_OH	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_OH	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_OH	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_OH	D_Cl	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_OH	chds2.Dxx_OH	m^2/s	Average diffusion coefficient	Domain 2

Name	Expression	Unit	Description	Selection
chds2.tfluxx_OH	-chds2.Dxx_OH*OHx+chds2.cfluxx_OH	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_OH	-chds2.Dyx_OH*OHx+chds2.cfluxy_OH	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_OH	-chds2.Dzx_OH*OHx+chds2.cfluxz_OH	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_OH	-chds2.Dxx_OH*OHx	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_OH	-chds2.Dyx_OH*OHx	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_OH	-chds2.Dzx_OH*OHx	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_OH	OHx	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_OH	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_OH	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_OH	sqrt(chds2.dfluxx_OH^2+chds2.dfluxy_OH^2+chds2.dfluxz_OH^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2

Name	Expression	Unit	Description	Selection
chds2.tfluxMag_OH	sqrt(chds2.tfluxx_OH^2+chds2.tfluxy_OH^2+chds2.tfluxz_OH^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_Fc	D_DMFc	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_Fc	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_Fc	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_Fc	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_Fc	D_DMFc	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_Fc	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_Fc	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_Fc	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_Fc	D_DMFc	m^2/s	Diffusion coefficient, zz component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dav_Fc	chds2.Dxx_Fc	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_Fc	-chds2.Dxx_Fc*Fcx+chds2.cfluxx_Fc	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_Fc	-chds2.Dyx_Fc*Fcx+chds2.cfluxy_Fc	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_Fc	-chds2.Dzx_Fc*Fcx+chds2.cfluxz_Fc	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_Fc	-chds2.Dxx_Fc*Fcx	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_Fc	-chds2.Dyx_Fc*Fcx	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_Fc	-chds2.Dzx_Fc*Fcx	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_Fc	Fcx	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_Fc	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_Fc	0	mol/m^4	Concentration gradient, z component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.dfluxMag_Fc	sqrt(chds2.dfluxx_Fc^2+chds2.dfluxy_Fc^2+chds2.dfluxz_Fc^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_Fc	sqrt(chds2.tfluxx_Fc^2+chds2.tfluxy_Fc^2+chds2.tfluxz_Fc^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_FcH	D_DMFcplus	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_FcH	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_FcH	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_FcH	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_FcH	D_DMFcplus	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_FcH	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_FcH	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_FcH	0	m^2/s	Diffusion coefficient, yz component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dzz_FcH	D_DMFcplus	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_FcH	chds2.Dxx_FcH	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_FcH	-chds2.Dxx_FcH*FcHx+chds2.cfluxx_FcH	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_FcH	-chds2.Dyx_FcH*FcHx+chds2.cfluxy_FcH	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_FcH	-chds2.Dzx_FcH*FcHx+chds2.cfluxz_FcH	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_FcH	-chds2.Dxx_FcH*FcHx	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_FcH	-chds2.Dyx_FcH*FcHx	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_FcH	-chds2.Dzx_FcH*FcHx	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_FcH	FcHx	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_FcH	0	mol/m^4	Concentration gradient, y component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.gradz_FcH	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_FcH	sqrt(chds2.dfluxx_FcH^2+chds2.dfluxy_FcH^2+chds2.dfluxz_FcH^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_FcH	sqrt(chds2.tfluxx_FcH^2+chds2.tfluxy_FcH^2+chds2.tfluxz_FcH^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_Fcplus	D_DMFcplus	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_Fcplus	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_Fcplus	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_Fcplus	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_Fcplus	D_DMFcplus	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_Fcplus	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_Fcplus	0	m^2/s	Diffusion coefficient, xz component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dyz_Fcplus	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_Fcplus	D_DMFcplus	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_Fcplus	chds2.Dxx_Fcplus	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_Fcplus	-chds2.Dxx_Fcplus*Fcplusx+chds2.cfluxx_Fcplus	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_Fcplus	-chds2.Dyx_Fcplus*Fcplusx+chds2.cfluxy_Fcplus	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_Fcplus	-chds2.Dzx_Fcplus*Fcplusx+chds2.cfluxz_Fcplus	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_Fcplus	-chds2.Dxx_Fcplus*Fcplusx	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_Fcplus	-chds2.Dyx_Fcplus*Fcplusx	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_Fcplus	-chds2.Dzx_Fcplus*Fcplusx	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_Fcplus	Fcplusx	mol/m^4	Concentration gradient, x component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.grady_Fcplus	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_Fcplus	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_Fcplus	sqrt(chds2.dfluxx_Fcplus^2+chds2.dfluxy_Fcplus^2+chds2.dfluxz_Fcplus^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_Fcplus	sqrt(chds2.tfluxx_Fcplus^2+chds2.tfluxy_Fcplus^2+chds2.tfluxz_Fcplus^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_MOHorg	D_M	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_MOHorg	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_MOHorg	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_MOHorg	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_MOHorg	D_M	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_MOHorg	0	m^2/s	Diffusion coefficient, zy component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dxz_MOHorg	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_MOHorg	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_MOHorg	D_M	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_MOHorg	chds2.Dxx_MOHorg	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_MOHorg	-chds2.Dxx_MOHorg*MOHorgx+chds2.cfluxx_MOHorg	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_MOHorg	-chds2.Dyx_MOHorg*MOHorgx+chds2.cfluxy_MOHorg	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_MOHorg	-chds2.Dzx_MOHorg*MOHorgx+chds2.cfluxz_MOHorg	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_MOHorg	-chds2.Dxx_MOHorg*MOHorgx	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_MOHorg	-chds2.Dyx_MOHorg*MOHorgx	mol/(m^2*s)	Diffusive flux, y component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.dfluxz_MOHorg	-chds2.Dzx_MOHorg*MOHorgx	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_MOHorg	MOHorgx	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_MOHorg	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_MOHorg	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_MOHorg	sqrt(chds2.dfluxx_MOHorg^2+chds2.dfluxy_MOHorg^2+chds2.dfluxz_MOHorg^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_MOHorg	sqrt(chds2.tfluxx_MOHorg^2+chds2.tfluxy_MOHorg^2+chds2.tfluxz_MOHorg^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_O2	D_O2	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_O2	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_O2	0	m^2/s	Diffusion coefficient, zx component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dxy_O2	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_O2	D_O2	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_O2	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_O2	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_O2	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_O2	D_O2	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_O2	chds2.Dxx_O2	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_O2	-chds2.Dxx_O2*O2x+chds2.cfluxx_O2	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_O2	-chds2.Dyx_O2*O2x+chds2.cfluxy_O2	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_O2	-chds2.Dzx_O2*O2x+chds2.cfluxz_O2	mol/(m^2*s)	Total flux, z component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.dfluxx_O2	-chds2.Dxx_O2*O2x	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_O2	-chds2.Dyx_O2*O2x	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_O2	-chds2.Dzx_O2*O2x	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_O2	O2x	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_O2	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_O2	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_O2	sqrt(chds2.dfluxx_O2^2+chds2.dfluxy_O2^2+chds2.dfluxz_O2^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_O2	sqrt(chds2.tfluxx_O2^2+chds2.tfluxy_O2^2+chds2.tfluxz_O2^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_HO2	D_OH	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_HO2	0	m^2/s	Diffusion coefficient, yx component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dzx_HO2	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_HO2	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_HO2	D_OH	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_HO2	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_HO2	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_HO2	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_HO2	D_OH	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_HO2	chds2.Dxx_HO2	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_HO2	-chds2.Dxx_HO2*HO2x+chds2.cfluxx_HO2	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_HO2	-chds2.Dyx_HO2*HO2x+chds2.cfluxy_HO2	mol/(m^2*s)	Total flux, y component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.tfluxz_HO2	-chds2.Dzx_HO2*HO2x+chds2.cfluxz_HO2	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_HO2	-chds2.Dxx_HO2*HO2x	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_HO2	-chds2.Dyx_HO2*HO2x	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_HO2	-chds2.Dzx_HO2*HO2x	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_HO2	HO2x	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_HO2	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_HO2	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_HO2	sqrt(chds2.dfluxx_HO2^2+chds2.dfluxy_HO2^2+chds2.dfluxz_HO2^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_HO2	sqrt(chds2.tfluxx_HO2^2+chds2.tfluxy_HO2^2+chds2.tfluxz_HO2^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_HO2minus	D_OH	m^2/s	Diffusion coefficient, xx component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dyx_HO2minus	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_HO2minus	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_HO2minus	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_HO2minus	D_OH	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_HO2minus	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_HO2minus	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_HO2minus	0	m^2/s	Diffusion coefficient, yz component	Domain 2
chds2.Dzz_HO2minus	D_OH	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_HO2minus	chds2.Dxx_HO2minus	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_HO2minus	-chds2.Dxx_HO2minus*H	mol/(m^2*s)	Total flux, x component	Domain 2

Name	Expression	Unit	Description	Selection
	O2minusx+chds2.cfluxx_HO2minus			
chds2.tfluxy_HO2minus	-chds2.Dyx_HO2minus*HO2minusx+chds2.cfluxy_HO2minus	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_HO2minus	-chds2.Dzx_HO2minus*HO2minusx+chds2.cfluxz_HO2minus	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_HO2minus	-chds2.Dxx_HO2minus*HO2minusx	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_HO2minus	-chds2.Dyx_HO2minus*HO2minusx	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_HO2minus	-chds2.Dzx_HO2minus*HO2minusx	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_HO2minus	HO2minusx	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_HO2minus	0	mol/m^4	Concentration gradient, y component	Domain 2
chds2.gradz_HO2minus	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_HO2minus	sqrt(chds2.dfluxx_HO2minus^2+chds2.dfluxy_HO2	mol/(m^2*s)	Diffusive flux magnitude	Domain 2

Name	Expression	Unit	Description	Selection
	minus^2+chds2.dfluxz_HO2minus^2)			
chds2.tfluxMag_HO2minus	sqrt(chds2.tfluxx_HO2minus^2+chds2.tfluxy_HO2minus^2+chds2.tfluxz_HO2minus^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.Dxx_H2O2	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, xx component	Domain 2
chds2.Dyx_H2O2	0	m^2/s	Diffusion coefficient, yx component	Domain 2
chds2.Dzx_H2O2	0	m^2/s	Diffusion coefficient, zx component	Domain 2
chds2.Dxy_H2O2	0	m^2/s	Diffusion coefficient, xy component	Domain 2
chds2.Dyy_H2O2	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, yy component	Domain 2
chds2.Dzy_H2O2	0	m^2/s	Diffusion coefficient, zy component	Domain 2
chds2.Dxz_H2O2	0	m^2/s	Diffusion coefficient, xz component	Domain 2
chds2.Dyz_H2O2	0	m^2/s	Diffusion coefficient, yz component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Dzz_H2O2	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, zz component	Domain 2
chds2.Dav_H2O2	chds2.Dxx_H2O2	m^2/s	Average diffusion coefficient	Domain 2
chds2.tfluxx_H2O2	-chds2.Dxx_H2O2*H2O2x+chds2.cfluxx_H2O2	mol/(m^2*s)	Total flux, x component	Domain 2
chds2.tfluxy_H2O2	-chds2.Dyx_H2O2*H2O2x+chds2.cfluxy_H2O2	mol/(m^2*s)	Total flux, y component	Domain 2
chds2.tfluxz_H2O2	-chds2.Dzx_H2O2*H2O2x+chds2.cfluxz_H2O2	mol/(m^2*s)	Total flux, z component	Domain 2
chds2.dfluxx_H2O2	-chds2.Dxx_H2O2*H2O2x	mol/(m^2*s)	Diffusive flux, x component	Domain 2
chds2.dfluxy_H2O2	-chds2.Dyx_H2O2*H2O2x	mol/(m^2*s)	Diffusive flux, y component	Domain 2
chds2.dfluxz_H2O2	-chds2.Dzx_H2O2*H2O2x	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds2.gradx_H2O2	H2O2x	mol/m^4	Concentration gradient, x component	Domain 2
chds2.grady_H2O2	0	mol/m^4	Concentration gradient, y component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.gradz_H2O2	0	mol/m^4	Concentration gradient, z component	Domain 2
chds2.dfluxMag_H2O2	sqrt(chds2.dfluxx_H2O2^2+chds2.dfluxy_H2O2^2+chds2.dfluxz_H2O2^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds2.tfluxMag_H2O2	sqrt(chds2.tfluxx_H2O2^2+chds2.tfluxy_H2O2^2+chds2.tfluxz_H2O2^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds2.u	model.input.u1	m/s	Velocity field, x component	Domain 2
chds2.v	model.input.u2	m/s	Velocity field, y component	Domain 2
chds2.w	model.input.u3	m/s	Velocity field, z component	Domain 2
chds2.cfluxx_Mplus	Mplus*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_Mplus	Mplus*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_Mplus	Mplus*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_Mplus	sqrt(chds2.cfluxx_Mplus^2+chds2.cfluxy_Mplus^2+chds2.cfluxz_Mplus^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2

Name	Expression	Unit	Description	Selection
chds2.cfluxx_OH	OH*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_OH	OH*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_OH	OH*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_OH	sqrt(chds2.cfluxx_OH^2+chds2.cfluxy_OH^2+chds2.cfluxz_OH^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.cfluxx_Fc	Fc*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_Fc	Fc*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_Fc	Fc*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_Fc	sqrt(chds2.cfluxx_Fc^2+chds2.cfluxy_Fc^2+chds2.cfluxz_Fc^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.cfluxx_FcH	FcH*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_FcH	FcH*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.cfluxz_FcH	FcH*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_FcH	sqrt(chds2.cfluxx_FcH^2+chds2.cfluxy_FcH^2+chds2.cfluxz_FcH^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.cfluxx_Fcplus	Fcplus*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_Fcplus	Fcplus*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_Fcplus	Fcplus*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_Fcplus	sqrt(chds2.cfluxx_Fcplus^2+chds2.cfluxy_Fcplus^2+chds2.cfluxz_Fcplus^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.cfluxx_MOHorg	MOHorg*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_MOHorg	MOHorg*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_MOHorg	MOHorg*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_MOHorg	sqrt(chds2.cfluxx_MOHorg^2+chds2.cfluxy_MOHo	mol/(m^2*s)	Convective flux magnitude	Domain 2

Name	Expression	Unit	Description	Selection
	rg^2+chds2.cfluxz_MOHorg^2)			
chds2.cfluxx_O2	O2*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_O2	O2*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_O2	O2*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_O2	sqrt(chds2.cfluxx_O2^2+chds2.cfluxy_O2^2+chds2.cfluxz_O2^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.cfluxx_HO2	HO2*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_HO2	HO2*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_HO2	HO2*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_HO2	sqrt(chds2.cfluxx_HO2^2+chds2.cfluxy_HO2^2+chds2.cfluxz_HO2^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.cfluxx_HO2minus	HO2minus*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2

Name	Expression	Unit	Description	Selection
chds2.cfluxy_HO2minus	HO2minus*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_HO2minus	HO2minus*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_HO2minus	sqrt(chds2.cfluxx_HO2minus^2+chds2.cfluxy_HO2minus^2+chds2.cfluxz_HO2minus^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.cfluxx_H2O2	H2O2*model.input.u1	mol/(m^2*s)	Convective flux, x component	Domain 2
chds2.cfluxy_H2O2	H2O2*model.input.u2	mol/(m^2*s)	Convective flux, y component	Domain 2
chds2.cfluxz_H2O2	H2O2*model.input.u3	mol/(m^2*s)	Convective flux, z component	Domain 2
chds2.cfluxMag_H2O2	sqrt(chds2.cfluxx_H2O2^2+chds2.cfluxy_H2O2^2+chds2.cfluxz_H2O2^2)	mol/(m^2*s)	Convective flux magnitude	Domain 2
chds2.helem	h	m	Element size	Domain 2
chds2.Res_Mplus	chds2.u*Mplusx-chds2.R_Mplus	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_OH	chds2.u*OHx-chds2.R_OH	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_Fc	chds2.u*Fcx-chds2.R_Fc	mol/(m^3*s)	Equation residual	Domain 2

Name	Expression	Unit	Description	Selection
chds2.Res_FcH	chds2.u*FcHx-chds2.R_FcH	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_Fcplus	chds2.u*Fcplusx-chds2.R_Fcplus	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_MOHorg	chds2.u*MOHorgx-chds2.R_MOHorg	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_O2	chds2.u*O2x-chds2.R_O2	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_HO2	chds2.u*HO2x-chds2.R_HO2	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_HO2minus	chds2.u*HO2minusx-chds2.R_HO2minus	mol/(m^3*s)	Equation residual	Domain 2
chds2.Res_H2O2	chds2.u*H2O2x-chds2.R_H2O2	mol/(m^3*s)	Equation residual	Domain 2

Shape functions

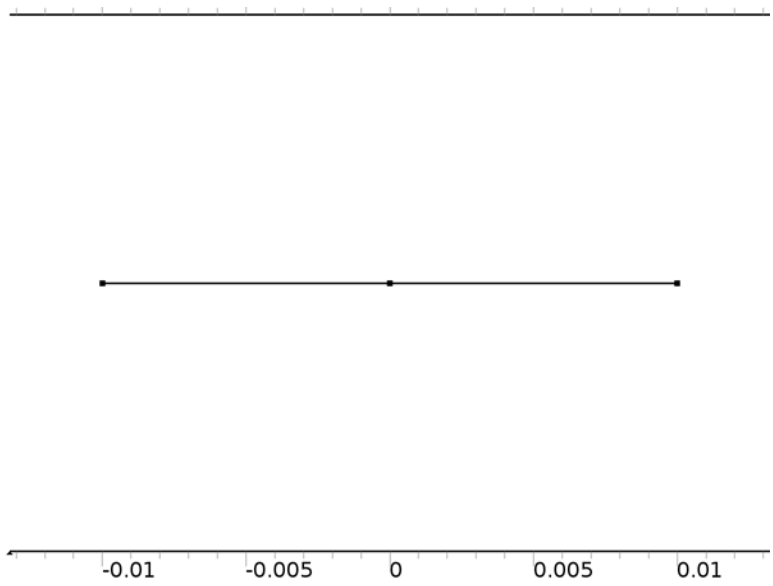
Name	Shape function	Unit	Description	Shape frame	Selection
Mplus	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
OH	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
Fc	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
FcH	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
Fcplus	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
MOHorg	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
O2	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
HO2	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
HO2minus	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
H2O2	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2

Weak expressions

Weak expression	Integration frame	Selection
-d(Mplus,t)*test(Mplus)-chds2.Dxx_Mplus*Mplusx*test(Mplusx)	Material	Domain 2
-d(OH,t)*test(OH)-chds2.Dxx_OH*OHx*test(OHx)	Material	Domain 2
-d(Fc,t)*test(Fc)-chds2.Dxx_Fc*Fcx*test(Fcx)	Material	Domain 2
-d(FcH,t)*test(FcH)-chds2.Dxx_FcH*FcHx*test(FcHx)	Material	Domain 2
-d(Fcplus,t)*test(Fcplus)-chds2.Dxx_Fcplus*Fcplusx*test(Fcplusx)	Material	Domain 2
-d(MOHorg,t)*test(MOHorg)-chds2.Dxx_MOHorg*MOHorgx*test(MOHorgx)	Material	Domain 2
-d(O2,t)*test(O2)-chds2.Dxx_O2*O2x*test(O2x)	Material	Domain 2
-d(HO2,t)*test(HO2)-chds2.Dxx_HO2*HO2x*test(HO2x)	Material	Domain 2
-d(HO2minus,t)*test(HO2minus)-chds2.Dxx_HO2minus*HO2minusx*test(HO2minusx)	Material	Domain 2
-d(H2O2,t)*test(H2O2)-chds2.Dxx_H2O2*H2O2x*test(H2O2x)	Material	Domain 2
-chds2.u*Mplusx*test(Mplus)	Material	Domain 2
chds2.cbf_Mplus*test(Mplus)	Material	Boundaries 2–3
-chds2.u*OHx*test(OH)	Material	Domain 2
chds2.cbf_OH*test(OH)	Material	Boundaries 2–3
-chds2.u*Fcx*test(Fc)	Material	Domain 2
chds2.cbf_Fc*test(Fc)	Material	Boundaries 2–3
-chds2.u*FcHx*test(FcH)	Material	Domain 2
chds2.cbf_FcH*test(FcH)	Material	Boundaries 2–3
-chds2.u*Fcplusx*test(Fcplus)	Material	Domain 2

Weak expression	Integration frame	Selection
chds2.cbf_Fcplus*test(Fcplus)	Material	Boundaries 2–3
-chds2.u*MOHorgx*test(MOHorg)	Material	Domain 2
chds2.cbf_MOHorg*test(MOHorg)	Material	Boundaries 2–3
-chds2.u*O2x*test(O2)	Material	Domain 2
chds2.cbf_O2*test(O2)	Material	Boundaries 2–3
-chds2.u*HO2x*test(HO2)	Material	Domain 2
chds2.cbf_HO2*test(HO2)	Material	Boundaries 2–3
-chds2.u*HO2minusx*test(HO2minus)	Material	Domain 2
chds2.cbf_HO2minus*test(HO2minus)	Material	Boundaries 2–3
-chds2.u*H2O2x*test(H2O2)	Material	Domain 2
chds2.cbf_H2O2*test(H2O2)	Material	Boundaries 2–3
chds2.streamline	Material	Domain 2
chds2.crosswind	Material	Domain 2

2.4.2 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	No boundaries

Equations

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

Settings

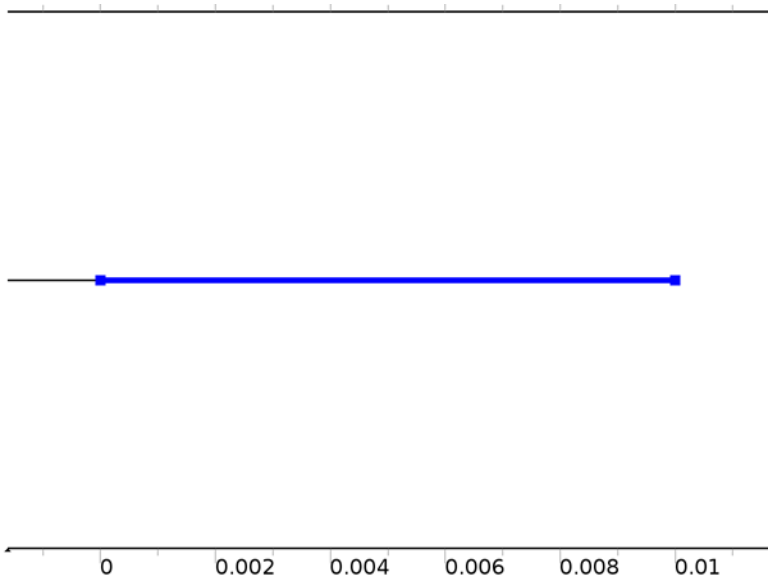
Settings

Description	Value
Apply for all species	Apply for all species

Used products

COMSOL Multiphysics

2.4.3 Initial Values 1



Initial Values 1

Selection

Geometric entity level	Domain
Selection	Domain 2

Settings

Settings

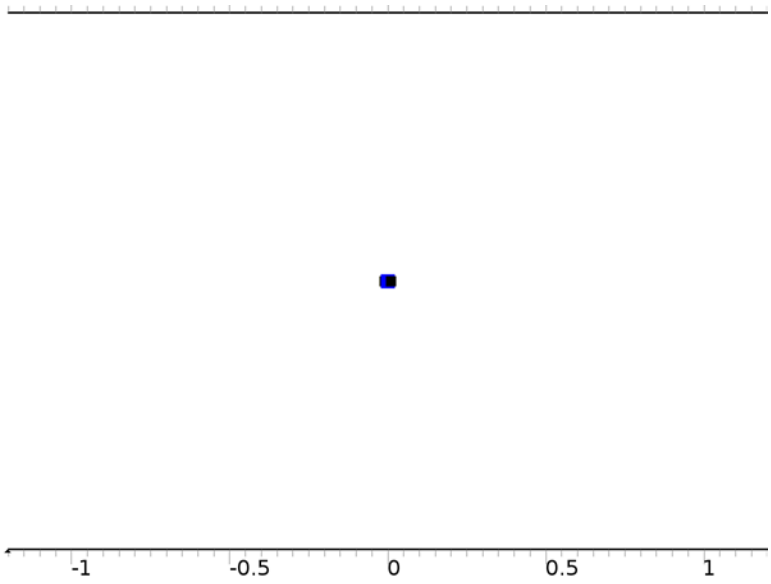
Description	Value
Concentration	cMorgi
Concentration	cOHorgi

Description	Value
Concentration	cDMFci
Concentration	cFcHi
Concentration	cDMFcplusi
Concentration	cMOHi
Concentration	cO2i
Concentration	cHO2i
Concentration	0
Concentration	0

Used products

COMSOL Multiphysics

2.4.4 Flux 1



Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundary 2

Equations

$$-\mathbf{n}\cdot\mathbf{N}_i = N_{0,i}$$

Settings

Settings

Description	Value
Species Mplus	On
Species OH	On
Species Fc	Off
Species FcH	Off
Species Fcplus	On
Species MOHorg	On
Species O2	Off
Species HO2	Off
Species HO2minus	Off
Species H2O2	Off
Inward flux	{kb*Maq - kf*Mplus, kb3*OHaq - kf3*OH, 0, 0, -kf2*Fcplus + kb2*Fcplusaq, -kmohf*MOHorg + kmohb*MOH, 0, 0, 0, 0}
Flux type	General inward flux

Used products

COMSOL Multiphysics

Variables

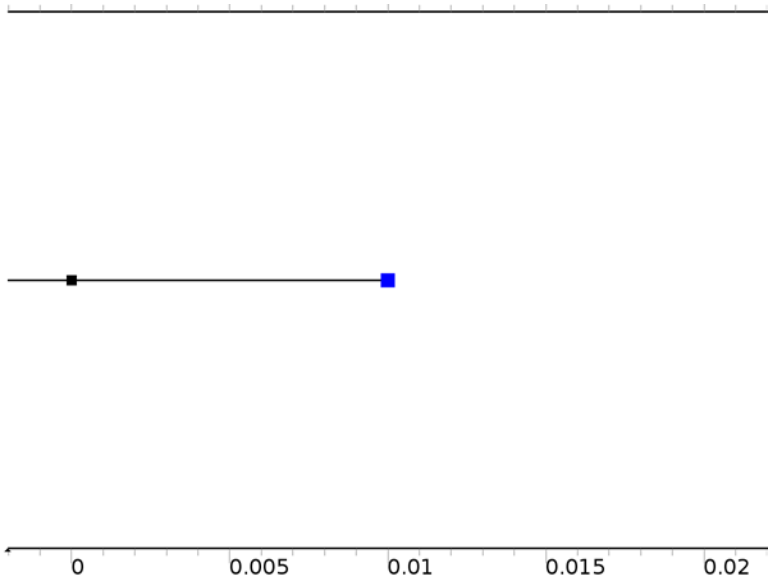
Name	Expression	Unit	Description	Selection
chds2.cbf_Mplus	Mplus*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_OH	OH*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_Fc	Fc*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2

Name	Expression	Unit	Description	Selection
chds2.cbf_FcH	FcH*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_Fcplus	Fcplus*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_MOHorg	MOHorg*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_O2	O2*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_HO2	HO2*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_HO2minus	HO2minus*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2
chds2.cbf_H2O2	H2O2*(chds2.u*chds2.nxmesh+chds2.v*chds2.nymesh+chds2.w*chds2.nzmesh)	mol/(m^2*s)	Convective boundary flux	Boundary 2

Weak expressions

Weak expression	Integration frame	Selection
(kb*Maq-kf*Mplus)*test(Mplus)	Material	Boundary 2
(kb3*OHaq-kf3*OH)*test(OH)	Material	Boundary 2
(-kf2*Fcplus+kb2*Fcplusaq)*test(Fcplus)	Material	Boundary 2
(-kmohf*MOHorg+kmohb*MOH)*test(MOHorg)	Material	Boundary 2

2.4.5 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 3

Equations

$$c_i = c_{0i}$$

Settings

Settings

Description	Value
Concentration	{cMorgi, cOHorgi, cDMFci, cFcHi, cDMFcplusi, cMOHi, cO2i, cHO2i, 0, 0}
Species Mplus	On
Species OH	On
Species Fc	On
Species FcH	On
Species Fcplus	On
Species MOHorg	On
Species O2	On

Description	Value
Species HO2	On
Species HO2minus	On
Species H2O2	On
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off

Used products

COMSOL Multiphysics

Variables

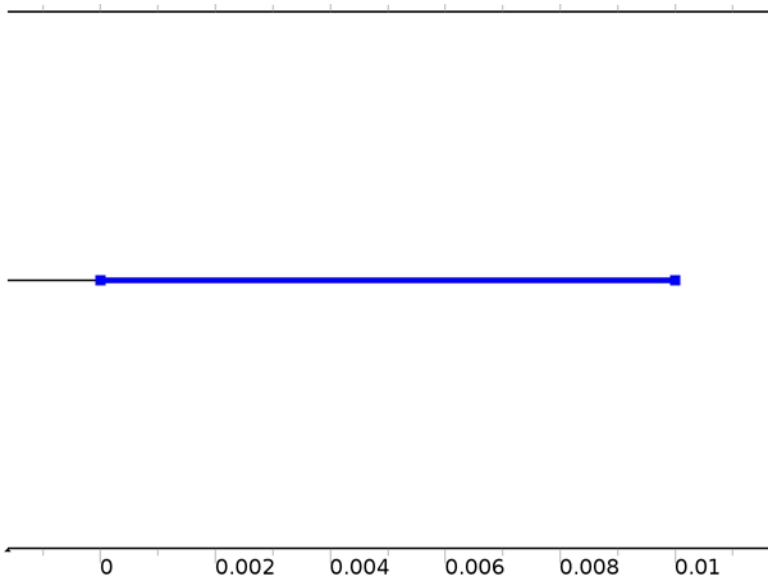
Name	Expression	Unit	Description	Selection
chds2.c0_Mplus	cMorgi	mol/m^3	Concentration	Boundary 3
chds2.c0_OH	cOHorgi	mol/m^3	Concentration	Boundary 3
chds2.c0_Fc	cDMFci	mol/m^3	Concentration	Boundary 3
chds2.c0_FcH	cFcHi	mol/m^3	Concentration	Boundary 3
chds2.c0_Fcplus	cDMFcplusi	mol/m^3	Concentration	Boundary 3
chds2.c0_MOHorg	cMOHi	mol/m^3	Concentration	Boundary 3
chds2.c0_O2	cO2i	mol/m^3	Concentration	Boundary 3
chds2.c0_HO2	cHO2i	mol/m^3	Concentration	Boundary 3
chds2.c0_HO2minus	0	mol/m^3	Concentration	Boundary 3
chds2.c0_H2O2	0	mol/m^3	Concentration	Boundary 3

Shape functions

Constraint	Constraint force	Shape function	Selection
-Mplus+chds2.c0_Mplus	test(-Mplus+chds2.c0_Mplus)	Lagrange (Linear)	Boundary 3
-OH+chds2.c0_OH	test(-OH+chds2.c0_OH)	Lagrange (Linear)	Boundary 3
-Fc+chds2.c0_Fc	test(-Fc+chds2.c0_Fc)	Lagrange (Linear)	Boundary 3
-FcH+chds2.c0_FcH	test(-FcH+chds2.c0_FcH)	Lagrange (Linear)	Boundary 3

Constraint	Constraint force	Shape function	Selection
-Fcplus+chds2.c0_Fcplus	test(-Fcplus+chds2.c0_Fcplus)	Lagrange (Linear)	Boundary 3
-MOHorg+chds2.c0_MOHorg	test(-MOHorg+chds2.c0_MOHorg)	Lagrange (Linear)	Boundary 3
-O2+chds2.c0_O2	test(-O2+chds2.c0_O2)	Lagrange (Linear)	Boundary 3
-HO2+chds2.c0_HO2	test(-HO2+chds2.c0_HO2)	Lagrange (Linear)	Boundary 3
-HO2minus+chds2.c0_HO2minus	test(-HO2minus+chds2.c0_HO2minus)	Lagrange (Linear)	Boundary 3
-H2O2+chds2.c0_H2O2	test(-H2O2+chds2.c0_H2O2)	Lagrange (Linear)	Boundary 3

2.4.6 Reactions 1



Reactions 1

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i$$

Settings

Settings

Description	Value
Total rate expression	{-kcf2*Mplus*OH + kcb2*MOHorg - kcf*Mplus*Fc + kcb*FcH*MOHorg - kchem4*HO2minus*Mplus, -kcf2*Mplus*OH + kcb2*MOHorg + kchem3*HO2minus^2, -kcf*Mplus*Fc + kcb*FcH*MOHorg - kchem2*Fc*HO2, kcf*Mplus*Fc - kcb*FcH*MOHorg - kchem1*FcH*O2, kchem1*FcH*O2 + kchem2*Fc*HO2, kcf2*Mplus*OH - kcb2*MOHorg + kcf*Mplus*Fc - kcb*FcH*MOHorg + kchem4*HO2minus*Mplus, -kchem1*FcH*O2 + kchem3*HO2minus^2, kchem1*FcH*O2 - kchem2*Fc*HO2, kchem2*Fc*HO2 - kchem3*HO2minus^2 - kchem4*HO2minus*Mplus, kchem4*HO2minus*Mplus}

Used products

COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
chds2.R_Mplus	-kcf2*Mplus*OH+kcb2*MOHorg-kcf*Mplus*Fc+kcb*FcH*MOHorg-kchem4*HO2minus*Mplus	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_OH	-kcf2*Mplus*OH+kcb2*MOHorg+kchem3*HO2minus^2	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_Fc	-kcf*Mplus*Fc+kcb*FcH*MOHorg-kchem2*Fc*HO2	mol/(m^3*s)	Total rate expression	Domain 2

Name	Expression	Unit	Description	Selection
chds2.R_FcH	kcf*Mplus*Fc-kcb*FcH*MOHorg-kchem1*FcH*O2	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_Fcplus	kchem1*FcH*O2+kchem2*Fc*HO2	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_MOHorg	kcf2*Mplus*OH-kcb2*MOHorg+kcf*Mplus*Fc-kcb*FcH*MOHorg+kchem4*HO2minus*Mplus	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_O2	-kchem1*FcH*O2+kchem3*HO2minus^2	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_HO2	kchem1*FcH*O2-kchem2*Fc*HO2	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_HO2minus	kchem2*Fc*HO2-kchem3*HO2minus^2-kchem4*HO2minus*Mplus	mol/(m^3*s)	Total rate expression	Domain 2
chds2.R_H2O2	kchem4*HO2minus*Mplus	mol/(m^3*s)	Total rate expression	Domain 2

Weak expressions

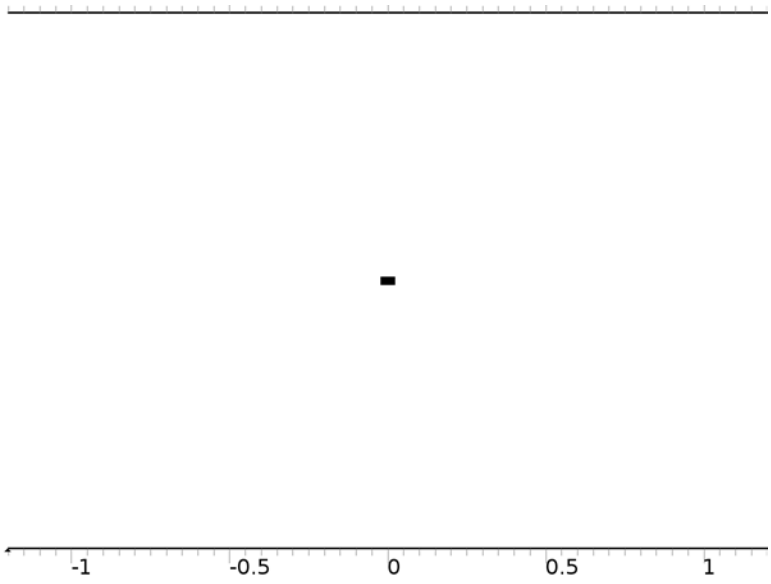
Weak expression	Integration frame	Selection
(-kcf2*Mplus*OH+kcb2*MOHorg-kcf*Mplus*Fc+kcb*FcH*MOHorg-kchem4*HO2minus*Mplus)*test(Mplus)	Material	Domain 2
(-kcf2*Mplus*OH+kcb2*MOHorg+kchem3*HO2minus^2)*test(OH)	Material	Domain 2
(-kcf*Mplus*Fc+kcb*FcH*MOHorg-kchem2*Fc*HO2)*test(Fc)	Material	Domain 2

Weak expression	Integration frame	Selection
(kcf*Mplus*Fc-kcb*FcH*MOHorg-kchem1*FcH*O2)*test(FcH)	Material	Domain 2
(kchem1*FcH*O2+kchem2*Fc*HO2)*test(Fcplus)	Material	Domain 2
(kcf2*Mplus*OH-kcb2*MOHorg+kcf*Mplus*Fc-kcb*FcH*MOHorg+kchem4*HO2minus*Mplus)*test(MOHorg)	Material	Domain 2
(-kchem1*FcH*O2+kchem3*HO2minus^2)*test(O2)	Material	Domain 2
(kchem1*FcH*O2-kchem2*Fc*HO2)*test(HO2)	Material	Domain 2
(kchem2*Fc*HO2-kchem3*HO2minus^2-kchem4*HO2minus*Mplus)*test(HO2minus)	Material	Domain 2
kchem4*HO2minus*Mplus*test(H2O2)	Material	Domain 2

2.5 Mesh 1

Mesh statistics

Property	Value
Minimum element quality	1.0
Average element quality	1.0
Edge elements	4000
Vertex elements	3



Mesh 1

2.5.1 Size (size)

Settings

Name	Value
Maximum element size	5e-6
Minimum element size	6.0E-6
Curvature factor	0.3
Maximum element growth rate	1.3
Custom element size	Custom

2.5.2 Edge 1 (edg1)

Selection

Geometric entity level	Remaining