Supplementary Information for: Mechanism of oxygen reduction by metallocene near liquid|liquid interfaces

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URL: http://lepa.epfl.ch/

Contents:

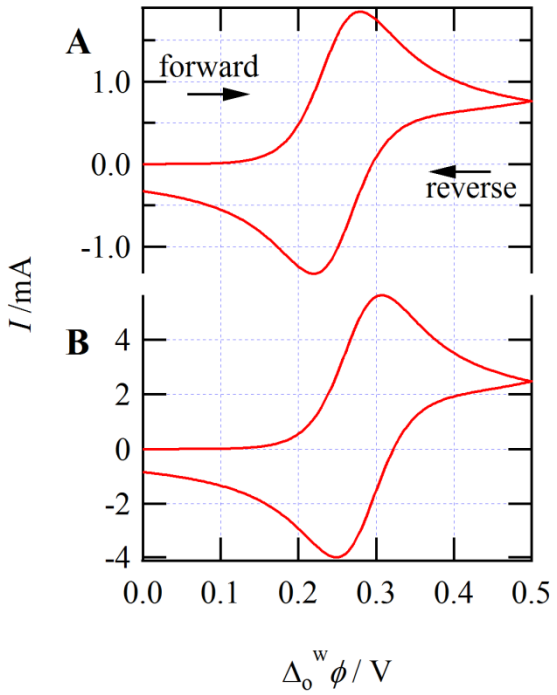


Figure S1: Simulated cyclic voltammograms of simple ion transfer of ion *i* of charge +1 transferring from w to o with initial concentrations $c_{i,\mathrm{w}}$ and $c_{i,\mathrm{o}}$ of 10 and 0 mol·m^{-3}, respectively; the scan rate, $\Delta_{\mathrm{o}}^{\mathrm{w}}\phi_i^{o'}$, k^o, and α were set equal to 0.020 V·s^{-1}, 0.250 V, 1 cm·s^{-1}, and 0.5, respectively. $D_{i,\mathrm{w}}$ and $D_{i,\mathrm{o}}$ were both equal to 1×10^{-5} cm^2·s^{-1} in **A**, while in **B**, $D_{i,\mathrm{w}}$ was changed to 9.3×10^{-5} cm^2·s^{-1} to better reflect proton mass transport.

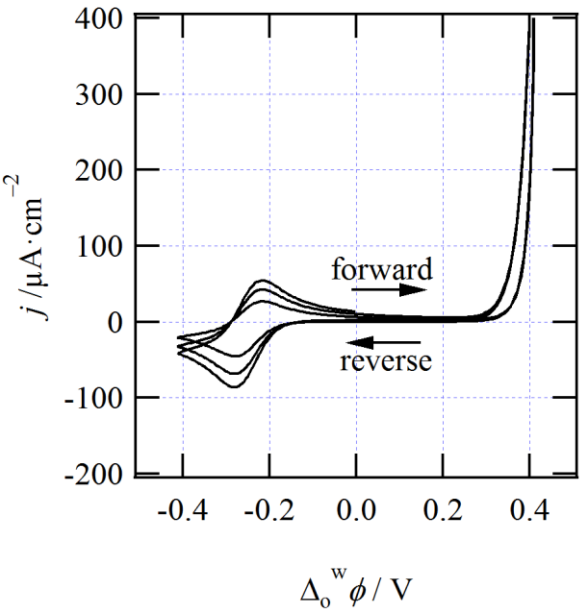


Figure S2: Simulated cyclic voltammogram obtained using the same simulation parameters described in Figure 6 of the main text except only $c_{H^+,w}$ equal to 1.000 mol·L^{-1} was utilized with a potential range of +/−0.413 V. Additionally the simulation run time was extended so that 3 forward/reverse sweeps were recorded.

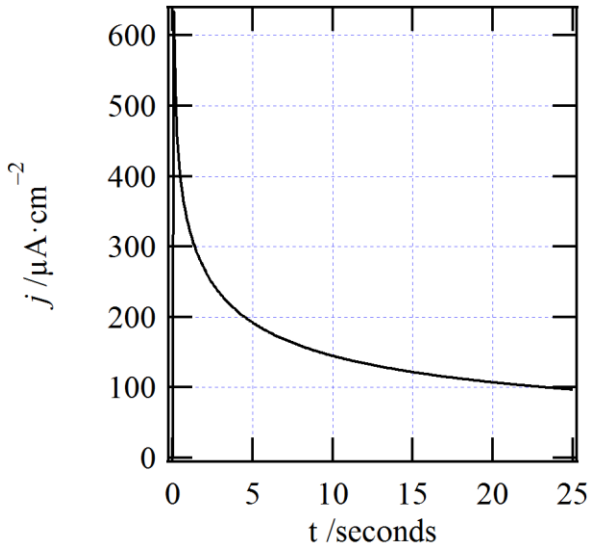


Figure S3: chronoamperometric curve generated using the simulation described in section 2 of the main text. Simulation parameters are the same as those described for Figure 7.

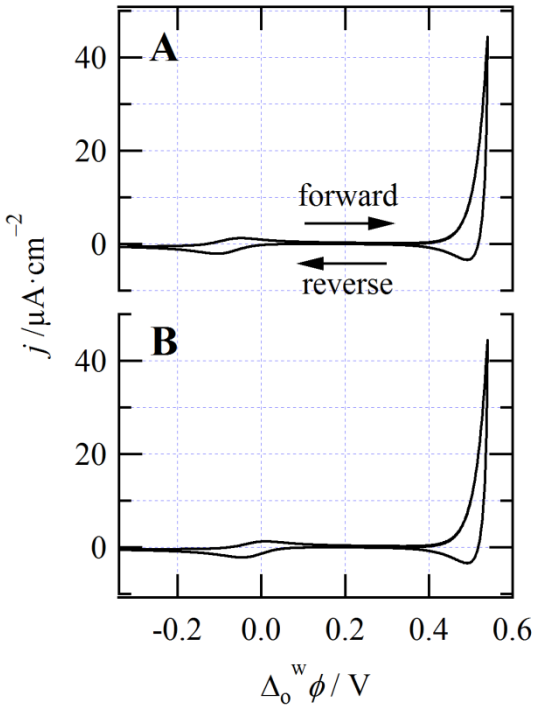


Figure S4: Simulated cyclic voltammograms of with the same simulation parameters a those listed for Figure 8 of the main text; however, with $\Delta_o^w\phi^{o'}_{DFc^+}$ and $\Delta_o^w\phi^{o'}_{DFc^+}$ equal to −0.078 and −0.016 V for **A** and **B**, respectively. k_{cf} and k_{chem}, were set equal to 1×10^2 and 5×10^2 L·mol^{-1}·s^{-1}, respectively, and the initial H^+ concentration was set equal to 0.001 mol·L^{-1}.

Table S1: Parameters used in the simulation including the diffusion coefficients in either phase ($D_{i,w}$/ $D_{i,o}$), the initial concentrations for either phase ($c^*_{i,w}$ / $c^*_{i,o}$), the formal ion transfer potentials ($\Delta^{w}_{o}\phi^{o'}_{iz}$), the partition coefficient ($P^{o'}_{i}$, from w to o), along with the final values of k_{cf} and k_{chem} for the associated electron donor species.

Species	$D_{i,w}$/ $D_{i,o}$ ($\times 10^{-5}$ cm^2·s^{-1})	$c^*_{i,w}$ / $c^*_{i,o}$ (mmol·L^{-1})	$\Delta^{w}_{o}\phi^{o'}_{iz}$ (V)	$P^{o'}_{i}$ (w to o)	k_{cf}	k_{chem}
					(L·mol^{-1}·s^{-1})	
H^+	9.3/1.0	*y* (Cell 1)/0	0.580	1.57×10^{-10}		
SO_4^-	NA	NA	−0.540	7.44×10^{-10}		
$DMFc^+$	0.7/0.7	0/0	−0.250	1.68×10^{4}	5×10^{2}	1×10^{4}
DFc^+	0.7/0.7	0/5	−0.078	21	1×10^{2}	5×10^{2}
Fc^+	0.7/0.7	0/5	−0.016	2	1×10^{2}	5×10^{2}
O_2	-/2.8	-/1	-	6		
BA	-	-	−0.699	6.55×10^{11}		
TB	-	-	0.718	1.37×10^{12}		

COMSOL Model Report

1. Table of Contents

2. Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Jan 13, 2014 11:27:32 AM
Creation date	Sep 9, 2013 11:57:51 AM
COMSOL version	COMSOL 3.5.0.603

File name: D:\documents\01~groupmeeting\manuscripts\manuscript_ORRsim\2013_1031_ORR\2013_1219_ORR.mph

Application modes and modules used in this model:

- Geom1 (Axial symmetry (2D))
  - Diffusion (Chemical Engineering Module)
  - Diffusion (Chemical Engineering Module)

3. Constants

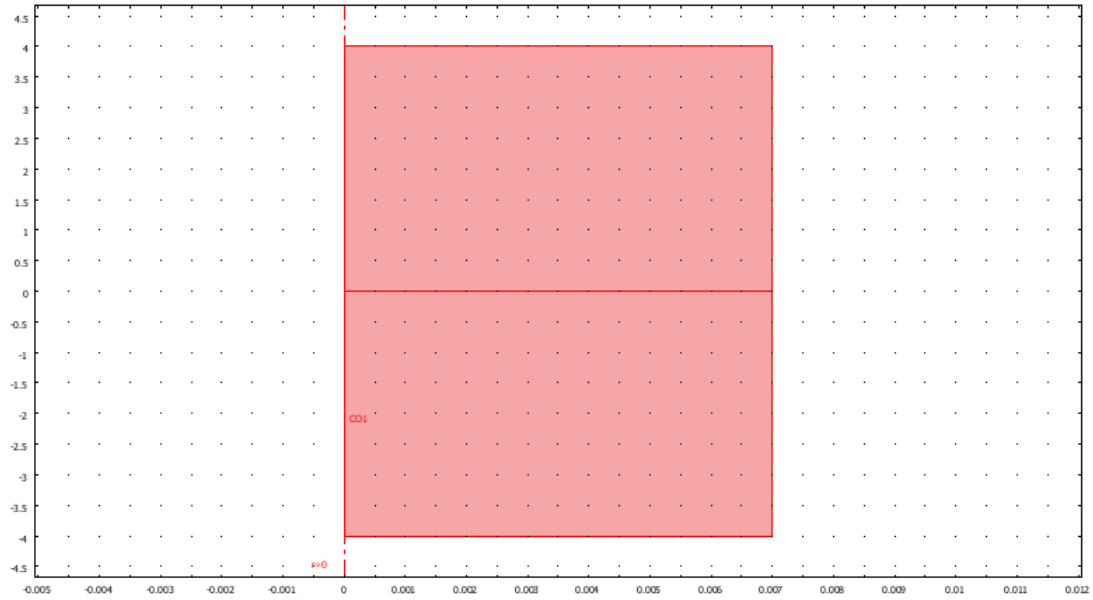
Name	Expression	Value	Description
F	96485 [C/mol]		
T	298.15 [K]		
R	8.314[J/mol/K]		
fara	F/(R*T)		

cHaqi	10[mmol/L]		
cHorgi	0[mmol/L]		
cH2i	0[mmol/L]		
cFcHi	0[mmol/L]		
cO2i	1.3[mmol/L]		
cO2Hi	0[mmol/L]		
cDMFci	0[mmol/L]		
cDMFcplusi	0[mmol/L]		
cDMFcplusaqi	0[mmol/L]		
D_H	9.3e-9[m^2/s]		
D_DMFc	0.726e-9[m^2/s]		
D_DMFcplus	7.26e-6[cm^2/s]		from Haiqiangs data
D_O2	2.76e-9[m^2/s]		
D_Horg	0.5e-9[m^2/s]		
Ei	0.0[V]		
Ef	0.452[V]		
E0	0.580[V]		H+ IT
E02	-0.250[V]		DMFc+ IT
nu	0.02[V/s]		scan rate
alpha	0.5		
test1	R*T/F		
n1	1		number of electrons
k0	1[cm/s]		standard rate constant
kcf	5e+2[L/mol/s]		
kcb	1[1/s]		
K	kcf/kcb		
kchem	1e+10[L/mol/s]		
kf_jane	1[m/s]		

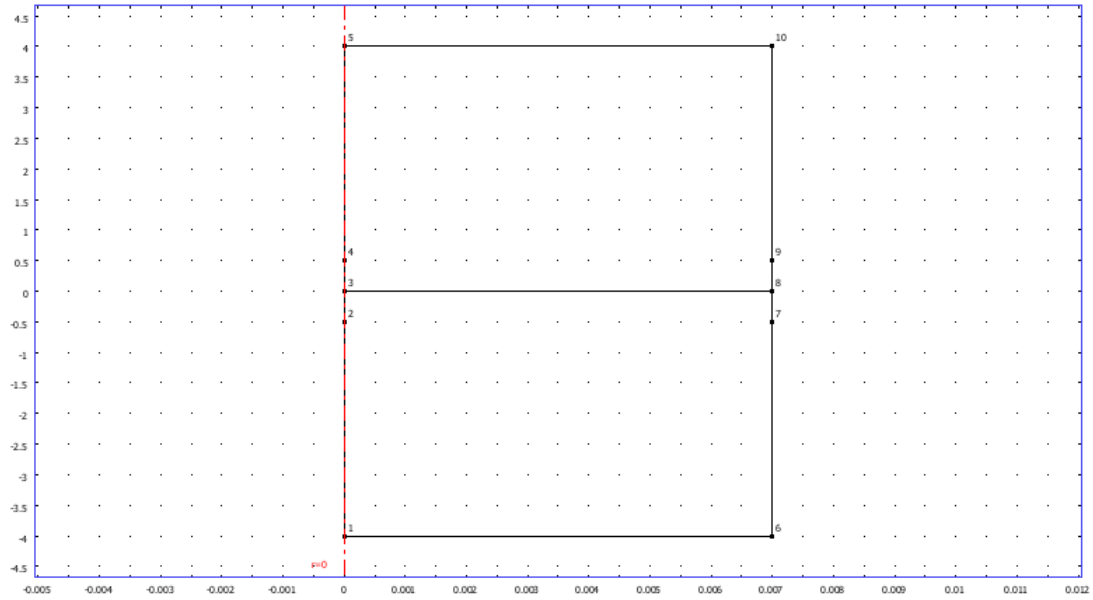
4. Geometry

Number of geometries: 1

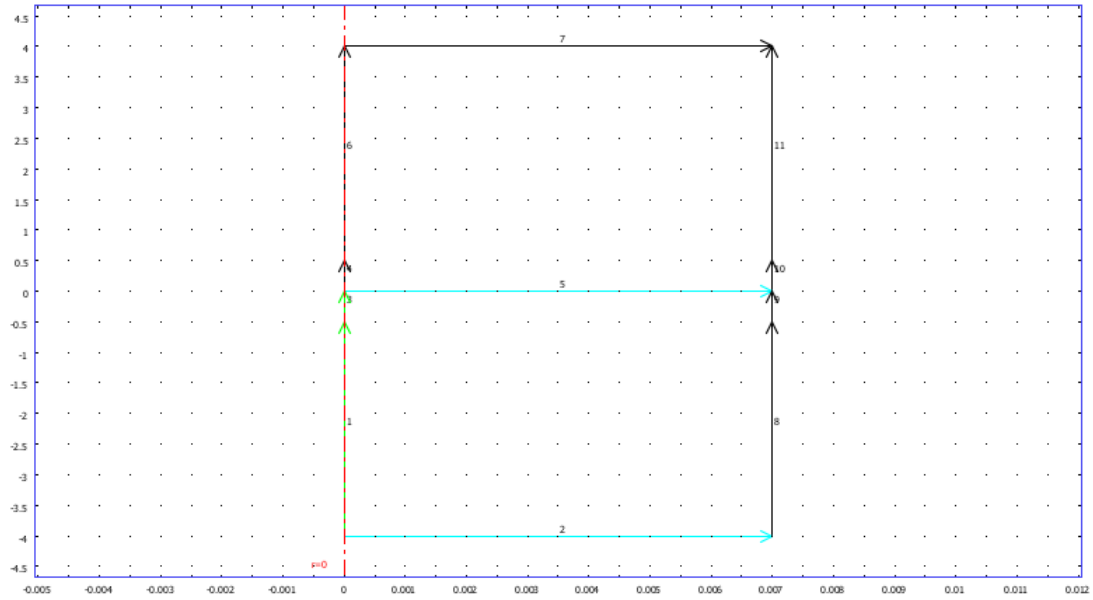
4.1. Geom1


CO1
r=0
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-0.005
-0.004
-0.003
-0.002
-0.001
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
0.01
0.011
0.012

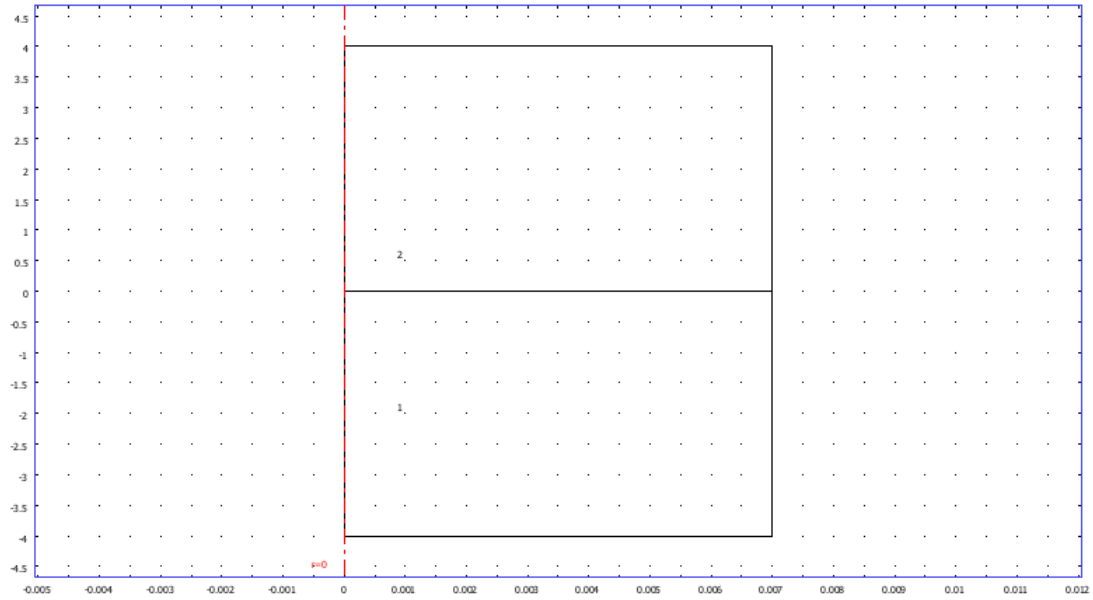
4.1.1. Point mode



4.1.2. Boundary mode



4.1.3. Subdomain mode



5. Geom1

Space dimensions: Axial symmetry (2D)

Independent variables: r, phi, z

5.1. Scalar Expressions

Name	Expression	Unit	Description
E_swp	Ei+(2*(Ef-Ei))/pi*asin(sin((pi*nu*t)/(2*(Ef-Ei))))	V	
kf	k0*exp(-alpha*fara*n1*(E_swp-E0))	m/s	H+ IT
kb	k0*exp((1-alpha)*fara*n1*(E_swp-E0))	m/s	
kf2	k0*exp(-alpha*fara*n1*(E_swp-E02))	m/s	DMFc+ IT
kb2	k0*exp((1-alpha)*fara*n1*(E_swp-E02))	m/s	
E_swp2	(Ei)*(t<25)+(Ef)*(t>=25)	V	

5.2. Expressions

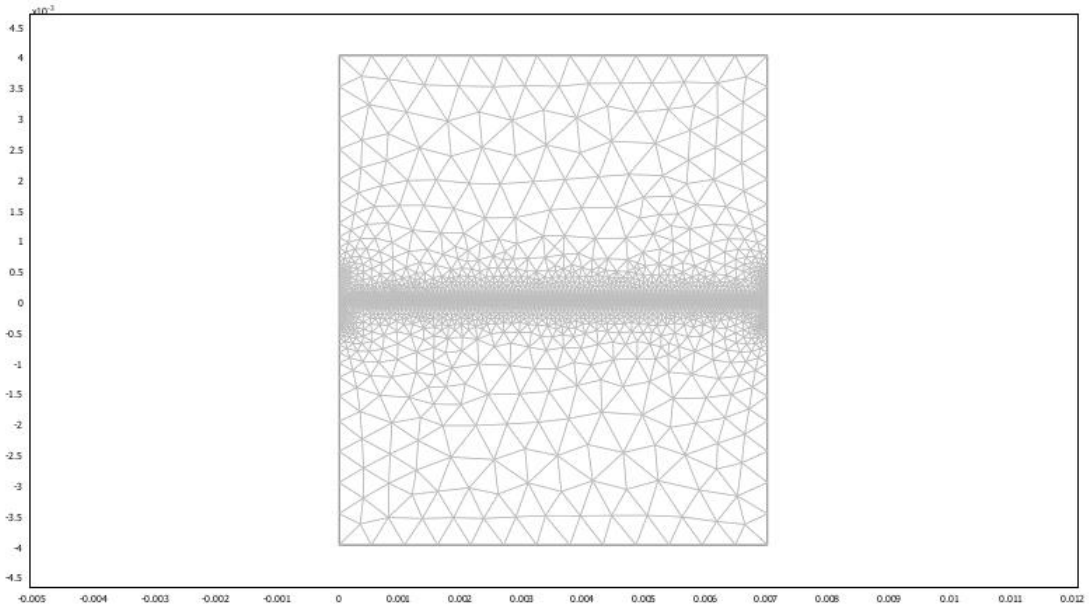
5.2.1. Subdomain Expressions

Subdomain		1	2
cH	mol/m^3	Horg	Haq

5.3. Mesh

5.3.1. Mesh Statistics

Number of degrees of freedom	44856
Number of mesh points	2738
Number of elements	5356
Triangular	5356
Quadrilateral	0
Number of boundary elements	318
Number of vertex elements	10
Minimum element quality	0.797
Element area ratio	0.002



5.4. Application Mode: Diffusion (chdi2)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: chdi2

5.4.1. Application Mode Properties

Property	**Value**

Default element type	Lagrange - Quadratic
Analysis type	Transient
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

5.4.2. Variables

Dependent variables: Horg, Fc, Fcplus, FcH, O2, O2H

Shape functions: shlag(2,'Horg'), shlag(2,'Fc'), shlag(2,'Fcplus'), shlag(2,'FcH'), shlag(2,'O2'), shlag(2,'O2H')

Interior boundaries not active

5.4.3. Boundary Settings

Boundary		1, 3	2	5
Type		Axial symmetry	Concentration	Flux
Inward flux (N)	mol/(m^2·s)	{0;0;0;0;0;0}	{0;0;0;0;0;0}	**{kb*Haq-kf*Horg;0;-kf2*Fcplus+kb2*Fcplusaq;0;0;0}**
Concentration (c0)	mol/m^3	{0;0;0;0;0;0}	**{cHorgi;cDMFci;cDMFcplusi;cFcHi;cO2i;cO2Hi}**	{0;0;0;0;0;0}

Boundary		8-9
Type		Insulation/Symmetry
Inward flux (N)	mol/(m^2·s)	{0;0;0;0;0;0}
Concentration (c0)	mol/m^3	{0;0;0;0;0;0}

5.4.4. Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m^2/s	**{D_Horg;D_DMFc;D_DMFcplus;D_DMFc;D_O2;D_O2}**
Reaction rate (R)	mol/(m^3·s)	**{-kcf*Horg*Fc+kcb*FcH;-kcf*Horg*Fc+kcb*FcH;kchem2*FcH*O2;kcf*Horg*Fc-kcb*FcH-kchem2*FcH*O2;-kchem2*FcH*O2;kchem2*FcH*O2}**

Subdomain initial value		1
Concentration, Horg (Horg)	mol/m^3	cHorgi
Concentration, Fc (Fc)	mol/m^3	cDMFci
Concentration, Fcplus (Fcplus)	mol/m^3	cDMFcplusi
Concentration, FcH (FcH)	mol/m^3	cFcHi
Concentration, O2 (O2)	mol/m^3	cO2i
Concentration, O2H (O2H)	mol/m^3	cO2Hi

5.5. Application Mode: Diffusion (chdi)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: chdi

5.5.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic
Analysis type	Transient
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

5.5.2. Variables

Dependent variables: Haq, Fcplusaq

Shape functions: shlag(2,'Haq'), shlag(2,'Fcplusaq')

Interior boundaries not active

5.5.3. Boundary Settings

Boundary		10-11	4, 6	7
Type		Insulation/Symmetry	Axial symmetry	Concentration
Inward flux (N)	mol/(m^2·s)	{0;0}	{0;0}	{0;0}
Concentration (c0)	mol/m^3	{0;0}	{0;0}	**{cHaqi;cDMFcplusaqi}**

Boundary		5
Type		Flux
Inward flux (N)	mol/(m^2·s)	**{(-kb*Haq+kf*Horg);kf2*Fcplus-kb2*Fcplusaq}**
Concentration (c0)	mol/m^3	{0;0}

5.5.4. Subdomain Settings

Subdomain		2
Diffusion coefficient (D)	m^2/s	**{D_H;D_DMFcplus}**

Subdomain initial value		2
Concentration, Haq (Haq)	mol/m^3	cHaqi
Concentration, Fcplusaq (Fcplusaq)	mol/m^3	cDMFcplusaqi

6. Integration Coupling Variables

6.1. Geom1

6.1.1. Source Boundary: 5

Name	Value
Variable name	Ibar
Expression	2*pi*r*F*(ndflux_Haq_chdi+ndflux_Fcplusaq_chdi)
Order	4
Global	Yes

7. Solver Settings

Solve using a script: off

Analysis type	Transient
Auto select solver	On
Solver	Time dependent
Solution form	Automatic
Symmetric	auto
Adaptive mesh refinement	Off
Optimization/Sensitivity	Off
Plot while solving	Off

7.1. Direct (UMFPACK)

Solver type: Linear system solver

Parameter	Value
Pivot threshold	0.1
Memory allocation factor	0.7

7.2. Time Stepping

Parameter	Value
Times	range(0,0.1,45.2)
Relative tolerance	1e-7
Absolute tolerance	1e-7
Times to store in output	Specified times
Time steps taken by solver	Free
Maximum BDF order	5
Singular mass matrix	Maybe
Consistent initialization of DAE systems	Backward Euler
Error estimation strategy	Include algebraic
Allow complex numbers	Off

7.3. Advanced

Parameter	Value
Constraint handling method	Elimination
Null-space function	Automatic
Automatic assembly block size	On
Assembly block size	1000
Use Hermitian transpose of constraint matrix and in symmetry detection	Off
Use complex functions with real input	Off
Stop if error due to undefined operation	On
Store solution on file	Off
Type of scaling	Automatic
Manual scaling	
Row equilibration	On
Manual control of reassembly	Off
Load constant	On
Constraint constant	On
Mass constant	On
Damping (mass) constant	On
Jacobian constant	On
Constraint Jacobian constant	On

8. Variables

8.1. Boundary

8.1.1. Boundary 1-3, 8-9

Name	Description	Unit	Expression
ndflux_Horg_chdi2	Normal diffusive flux, Horg	mol/(m^2*s)	nr_chdi2 * dflux_Horg_r_chdi2+nz_chdi2 * dflux_Horg_z_chdi2
ndflux_Fc_chdi2	Normal diffusive flux, Fc	mol/(m^2*s)	nr_chdi2 * dflux_Fc_r_chdi2+nz_chdi2 * dflux_Fc_z_chdi2
ndflux_Fcplus_chdi2	Normal diffusive flux, Fcplus	mol/(m^2*s)	nr_chdi2 * dflux_Fcplus_r_chdi2+nz_chdi2 * dflux_Fcplus_z_chdi2
ndflux_FcH_chdi2	Normal diffusive flux, FcH	mol/(m^2*s)	nr_chdi2 * dflux_FcH_r_chdi2+nz_chdi2 * dflux_FcH_z_chdi2
ndflux_O2_chdi2	Normal diffusive flux, O2	mol/(m^2*s)	nr_chdi2 * dflux_O2_r_chdi2+nz_chdi2 * dflux_O2_z_chdi2
ndflux_O2H_chdi2	Normal diffusive flux, O2H	mol/(m^2*s)	nr_chdi2 * dflux_O2H_r_chdi2+nz_chdi2 * dflux_O2H_z_chdi2
ndflux_Haq_chdi	Normal diffusive flux, Haq	mol/(m^2*s)	
ndflux_Fcplusaq_chdi	Normal diffusive flux, Fcplusaq	mol/(m^2*s)	

8.1.2. Boundary 4, 6-7, 10-11

Name	Description	Unit	Expression
ndflux_Horg_chdi2	Normal diffusive flux, Horg	mol/(m^2*s)	
ndflux_Fc_chdi2	Normal diffusive flux, Fc	mol/(m^2*s)	

ndflux_Fcplus_chdi2	Normal diffusive flux, Fcplus	mol/(m^2*s)	
ndflux_FcH_chdi2	Normal diffusive flux, FcH	mol/(m^2*s)	
ndflux_O2_chdi2	Normal diffusive flux, O2	mol/(m^2*s)	
ndflux_O2H_chdi2	Normal diffusive flux, O2H	mol/(m^2*s)	
ndflux_Haq_chdi	Normal diffusive flux, Haq	mol/(m^2*s)	nr_chdi * dflux_Haq_r_chdi+nz_chdi * dflux_Haq_z_chdi
ndflux_Fcplusaq_chdi	Normal diffusive flux, Fcplusaq	mol/(m^2*s)	nr_chdi * dflux_Fcplusaq_r_chdi+nz_chdi * dflux_Fcplusaq_z_chdi

8.1.3. Boundary 5

Name	Description	Unit	Expression
ndflux_Horg_chdi2	Normal diffusive flux, Horg	mol/(m^2*s)	nr_chdi2 * dflux_Horg_r_chdi2+nz_chdi2 * dflux_Horg_z_chdi2
ndflux_Fc_chdi2	Normal diffusive flux, Fc	mol/(m^2*s)	nr_chdi2 * dflux_Fc_r_chdi2+nz_chdi2 * dflux_Fc_z_chdi2
ndflux_Fcplus_chdi2	Normal diffusive flux, Fcplus	mol/(m^2*s)	nr_chdi2 * dflux_Fcplus_r_chdi2+nz_chdi2 * dflux_Fcplus_z_chdi2
ndflux_FcH_chdi2	Normal diffusive flux, FcH	mol/(m^2*s)	nr_chdi2 * dflux_FcH_r_chdi2+nz_chdi2 * dflux_FcH_z_chdi2
ndflux_O2_chdi2	Normal diffusive flux, O2	mol/(m^2*s)	nr_chdi2 * dflux_O2_r_chdi2+nz_chdi2 * dflux_O2_z_chdi2
ndflux_O2H_chdi2	Normal diffusive flux, O2H	mol/(m^2*s)	nr_chdi2 * dflux_O2H_r_chdi2+nz_chdi2 * dflux_O2H_z_chdi2
ndflux_Haq_chdi	Normal diffusive flux, Haq	mol/(m^2*s)	nr_chdi * dflux_Haq_r_chdi+nz_chdi * dflux_Haq_z_chdi
ndflux_Fcplusaq_chdi	Normal diffusive flux, Fcplusaq	mol/(m^2*s)	nr_chdi * dflux_Fcplusaq_r_chdi+nz_chdi * dflux_Fcplusaq_z_chdi

8.2. Subdomain

8.2.1. Subdomain 1

Name	Description	Unit	Expression
grad_Horg_r_chdi2	Concentration gradient, Horg, r component	mol/m^4	Horgr
dflux_Horg_r_chdi2	Diffusive flux, Horg, r component	mol/(m^2*s)	-Drr_Horg_chdi2 * Horgr-Drz_Horg_chdi2 * Horgz
grad_Horg_z_chdi2	Concentration gradient, Horg, z component	mol/m^4	Horgz
dflux_Horg_z_chdi2	Diffusive flux, Horg, z component	mol/(m^2*s)	-Dzr_Horg_chdi2 * Horgr-Dzz_Horg_chdi2 * Horgz
grad_Horg_chdi2	Concentration gradient, Horg	mol/m^4	sqrt(grad_Horg_r_chdi2^2+grad_Horg_z_chdi2^2)
dflux_Horg_chdi2	Diffusive flux, Horg	mol/(m^2*s)	sqrt(dflux_Horg_r_chdi2^2+dflux_Horg_z_chdi2^2)
grad_Fc_r_chdi2	Concentration gradient, Fc, r component	mol/m^4	Fcr
dflux_Fc_r_chdi2	Diffusive flux, Fc, r component	mol/(m^2*s)	-Drr_Fc_chdi2 * Fcr-Drz_Fc_chdi2 * Fcz
grad_Fc_z_chdi2	Concentration gradient, Fc, z component	mol/m^4	Fcz
dflux_Fc_z_chdi2	Diffusive flux, Fc, z component	mol/(m^2*s)	-Dzr_Fc_chdi2 * Fcr-Dzz_Fc_chdi2 * Fcz
grad_Fc_chdi2	Concentration gradient, Fc	mol/m^4	sqrt(grad_Fc_r_chdi2^2+grad_Fc_z_chdi2^2)
dflux_Fc_chdi2	Diffusive flux, Fc	mol/(m^2*s)	sqrt(dflux_Fc_r_chdi2^2+dflux_Fc_z_chdi2^2)

grad_Fcplus_r_chdi2	Concentration gradient, Fcplus, r component	mol/m^4	Fcplusr
dflux_Fcplus_r_chdi2	Diffusive flux, Fcplus, r component	mol/(m^2*s)	-Drr_Fcplus_chdi2 * Fcplusr-Drz_Fcplus_chdi2 * Fcplusz
grad_Fcplus_z_chdi2	Concentration gradient, Fcplus, z component	mol/m^4	Fcplusz
dflux_Fcplus_z_chdi2	Diffusive flux, Fcplus, z component	mol/(m^2*s)	-Dzr_Fcplus_chdi2 * Fcplusr-Dzz_Fcplus_chdi2 * Fcplusz
grad_Fcplus_chdi2	Concentration gradient, Fcplus	mol/m^4	sqrt(grad_Fcplus_r_chdi2^2+grad_Fcplus_z_chdi2^2)
dflux_Fcplus_chdi2	Diffusive flux, Fcplus	mol/(m^2*s)	sqrt(dflux_Fcplus_r_chdi2^2+dflux_Fcplus_z_chdi2^2)
grad_FcH_r_chdi2	Concentration gradient, FcH, r component	mol/m^4	FcHr
dflux_FcH_r_chdi2	Diffusive flux, FcH, r component	mol/(m^2*s)	-Drr_FcH_chdi2 * FcHr-Drz_FcH_chdi2 * FcHz
grad_FcH_z_chdi2	Concentration gradient, FcH, z component	mol/m^4	FcHz
dflux_FcH_z_chdi2	Diffusive flux, FcH, z component	mol/(m^2*s)	-Dzr_FcH_chdi2 * FcHr-Dzz_FcH_chdi2 * FcHz
grad_FcH_chdi2	Concentration gradient, FcH	mol/m^4	sqrt(grad_FcH_r_chdi2^2+grad_FcH_z_chdi2^2)
dflux_FcH_chdi2	Diffusive flux, FcH	mol/(m^2*s)	sqrt(dflux_FcH_r_chdi2^2+dflux_FcH_z_chdi2^2)
grad_O2_r_chdi2	Concentration gradient, O2, r component	mol/m^4	O2r
dflux_O2_r_chdi2	Diffusive flux, O2, r component	mol/(m^2*s)	-Drr_O2_chdi2 * O2r-Drz_O2_chdi2 * O2z
grad_O2_z_chdi2	Concentration gradient, O2, z component	mol/m^4	O2z
dflux_O2_z_chdi2	Diffusive flux, O2, z component	mol/(m^2*s)	-Dzr_O2_chdi2 * O2r-Dzz_O2_chdi2 * O2z
grad_O2_chdi2	Concentration gradient, O2	mol/m^4	sqrt(grad_O2_r_chdi2^2+grad_O2_z_chdi2^2)
dflux_O2_chdi2	Diffusive flux, O2	mol/(m^2*s)	sqrt(dflux_O2_r_chdi2^2+dflux_O2_z_chdi2^2)
grad_O2H_r_chdi2	Concentration gradient, O2H, r component	mol/m^4	O2Hr
dflux_O2H_r_chdi2	Diffusive flux, O2H, r component	mol/(m^2*s)	-Drr_O2H_chdi2 * O2Hr-Drz_O2H_chdi2 * O2Hz
grad_O2H_z_chdi2	Concentration gradient, O2H, z component	mol/m^4	O2Hz
dflux_O2H_z_chdi2	Diffusive flux, O2H, z component	mol/(m^2*s)	-Dzr_O2H_chdi2 * O2Hr-Dzz_O2H_chdi2 * O2Hz
grad_O2H_chdi2	Concentration gradient, O2H	mol/m^4	sqrt(grad_O2H_r_chdi2^2+grad_O2H_z_chdi2^2)
dflux_O2H_chdi2	Diffusive flux, O2H	mol/(m^2*s)	sqrt(dflux_O2H_r_chdi2^2+dflux_O2H_z_chdi2^2)
grad_Haq_r_chdi	Concentration gradient, Haq, r component	mol/m^4	
dflux_Haq_r_chdi	Diffusive flux, Haq, r component	mol/(m^2*s)	
grad_Haq_z_chdi	Concentration gradient, Haq, z component	mol/m^4	
dflux_Haq_z_chdi	Diffusive flux, Haq, z component	mol/(m^2*s)	
grad_Haq_chdi	Concentration gradient, Haq	mol/m^4	
dflux_Haq_chdi	Diffusive flux, Haq	mol/(m^2*s)	

grad_Fcplusaq_r_chdi	Concentration gradient, Fcplusaq, r component	mol/m^4	
dflux_Fcplusaq_r_chdi	Diffusive flux, Fcplusaq, r component	mol/(m^2*s)	
grad_Fcplusaq_z_chdi	Concentration gradient, Fcplusaq, z component	mol/m^4	
dflux_Fcplusaq_z_chdi	Diffusive flux, Fcplusaq, z component	mol/(m^2*s)	
grad_Fcplusaq_chdi	Concentration gradient, Fcplusaq	mol/m^4	
dflux_Fcplusaq_chdi	Diffusive flux, Fcplusaq	mol/(m^2*s)	

8.2.2. Subdomain 2

Name	**Description**	**Unit**	**Expression**
grad_Horg_r_chdi2	Concentration gradient, Horg, r component	mol/m^4	
dflux_Horg_r_chdi2	Diffusive flux, Horg, r component	mol/(m^2*s)	
grad_Horg_z_chdi2	Concentration gradient, Horg, z component	mol/m^4	
dflux_Horg_z_chdi2	Diffusive flux, Horg, z component	mol/(m^2*s)	
grad_Horg_chdi2	Concentration gradient, Horg	mol/m^4	
dflux_Horg_chdi2	Diffusive flux, Horg	mol/(m^2*s)	
grad_Fc_r_chdi2	Concentration gradient, Fc, r component	mol/m^4	
dflux_Fc_r_chdi2	Diffusive flux, Fc, r component	mol/(m^2*s)	
grad_Fc_z_chdi2	Concentration gradient, Fc, z component	mol/m^4	
dflux_Fc_z_chdi2	Diffusive flux, Fc, z component	mol/(m^2*s)	
grad_Fc_chdi2	Concentration gradient, Fc	mol/m^4	
dflux_Fc_chdi2	Diffusive flux, Fc	mol/(m^2*s)	
grad_Fcplus_r_chdi2	Concentration gradient, Fcplus, r component	mol/m^4	
dflux_Fcplus_r_chdi2	Diffusive flux, Fcplus, r component	mol/(m^2*s)	
grad_Fcplus_z_chdi2	Concentration gradient, Fcplus, z component	mol/m^4	
dflux_Fcplus_z_chdi2	Diffusive flux, Fcplus, z component	mol/(m^2*s)	
grad_Fcplus_chdi2	Concentration gradient, Fcplus	mol/m^4	
dflux_Fcplus_chdi2	Diffusive flux, Fcplus	mol/(m^2*s)	
grad_FcH_r_chdi2	Concentration gradient, FcH, r component	mol/m^4	
dflux_FcH_r_chdi2	Diffusive flux, FcH, r component	mol/(m^2*s)	

grad_FcH_z_chdi2	Concentration gradient, FcH, z component	mol/m^4	
dflux_FcH_z_chdi2	Diffusive flux, FcH, z component	mol/(m^2*s)	
grad_FcH_chdi2	Concentration gradient, FcH	mol/m^4	
dflux_FcH_chdi2	Diffusive flux, FcH	mol/(m^2*s)	
grad_O2_r_chdi2	Concentration gradient, O2, r component	mol/m^4	
dflux_O2_r_chdi2	Diffusive flux, O2, r component	mol/(m^2*s)	
grad_O2_z_chdi2	Concentration gradient, O2, z component	mol/m^4	
dflux_O2_z_chdi2	Diffusive flux, O2, z component	mol/(m^2*s)	
grad_O2_chdi2	Concentration gradient, O2	mol/m^4	
dflux_O2_chdi2	Diffusive flux, O2	mol/(m^2*s)	
grad_O2H_r_chdi2	Concentration gradient, O2H, r component	mol/m^4	
dflux_O2H_r_chdi2	Diffusive flux, O2H, r component	mol/(m^2*s)	
grad_O2H_z_chdi2	Concentration gradient, O2H, z component	mol/m^4	
dflux_O2H_z_chdi2	Diffusive flux, O2H, z component	mol/(m^2*s)	
grad_O2H_chdi2	Concentration gradient, O2H	mol/m^4	
dflux_O2H_chdi2	Diffusive flux, O2H	mol/(m^2*s)	
grad_Haq_r_chdi	Concentration gradient, Haq, r component	mol/m^4	Haqr
dflux_Haq_r_chdi	Diffusive flux, Haq, r component	mol/(m^2*s)	-Drr_Haq_chdi * Haqr-Drz_Haq_chdi * Haqz
grad_Haq_z_chdi	Concentration gradient, Haq, z component	mol/m^4	Haqz
dflux_Haq_z_chdi	Diffusive flux, Haq, z component	mol/(m^2*s)	-Dzr_Haq_chdi * Haqr-Dzz_Haq_chdi * Haqz
grad_Haq_chdi	Concentration gradient, Haq	mol/m^4	sqrt(grad_Haq_r_chdi^2+grad_Haq_z_chdi^2)
dflux_Haq_chdi	Diffusive flux, Haq	mol/(m^2*s)	sqrt(dflux_Haq_r_chdi^2+dflux_Haq_z_chdi^2)
grad_Fcplusaq_r_chdi	Concentration gradient, Fcplusaq, r component	mol/m^4	Fcplusaqr
dflux_Fcplusaq_r_chdi	Diffusive flux, Fcplusaq, r component	mol/(m^2*s)	-Drr_Fcplusaq_chdi * Fcplusaqr-Drz_Fcplusaq_chdi * Fcplusaqz
grad_Fcplusaq_z_chdi	Concentration gradient, Fcplusaq, z component	mol/m^4	Fcplusaqz
dflux_Fcplusaq_z_chdi	Diffusive flux, Fcplusaq, z component	mol/(m^2*s)	-Dzr_Fcplusaq_chdi * Fcplusaqr-Dzz_Fcplusaq_chdi * Fcplusaqz
grad_Fcplusaq_chdi	Concentration gradient, Fcplusaq	mol/m^4	sqrt(grad_Fcplusaq_r_chdi^2+grad_Fcplusaq_z_chdi^2)
dflux_Fcplusaq_chdi	Diffusive flux, Fcplusaq	mol/(m^2*s)	sqrt(dflux_Fcplusaq_r_chdi^2+dflux_Fcplusaq_z_chdi^2)