Supporting Information for:

Evaluation of Gibbs Energy of dioxouranium transfer at an electrified liquid|liquid interface supported on a microhole

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1. Igor Curve fitting procedure
2. COMSOL microhole simulation report

1. Curve fitting Procedure use in Igor 6.12a software:

The following function was used to perform the curve fitting by using the cursor tools available with any graph generated in Igor. Two cursors were placed bracketing the desired portion of the wave. With the following function appearing in the Procedure window, the curve fitting option was selected from the Analysis drop down menu. A curve fitting window will appear. Under the Functions drop down menu the function “Oldham1” was selected and under the coefficients tab initial estimates for each coefficient were entered. Please note that under the Data Options tab the cursors option must be selected; curve fitting was then ready to perform.

Function Oldham1(E,I) : FitFunc

Wave E

Variable I

//CurveFitDialog/ These comments were created by the Curve Fitting dialog. Altering them will

//CurveFitDialog/ make the function less convenient to work with in the Curve Fitting dialog.

//CurveFitDialog/ Equation:

//CurveFitDialog/ $f(I) = E1/2 + RT/(zAF) * \ln((1 - zA/zB)(I/(I_{lim} - I) * (I_{lim}/(I_{lim} - I))^{(zA/zB)}))$

//CurveFitDialog/ End of Equation

//CurveFitDialog/ Independent Variables 1

```

//CurveFitDialog/ I
//CurveFitDialog/ Coefficients 4
//CurveFitDialog/ E[0] = lim
//CurveFitDialog/ E[1] = E1/2
//CurveFitDialog/ E[2] = fara
//CurveFitDialog/ E[3] = za

return E[1]+E[2]*ln((1+E[3])*(I/(E[0]-I))*(E[0]/(E[0]-I))^(E[3]))
End

```

2. Simulation Code

The following is the Model Report as generated internally by COMSOL software for the microhole simulation.

COMSOL Model Report

1. Table of Contents

- Title - COMSOL Model Report
- Table of Contents
- Model Properties
- Constants
- Geometry
- Geom1
- Materials/Coefficients Library
- Integration Coupling Variables
- Solver Settings
- Postprocessing
- Variables

2. Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Jun 28, 2011 5:27:07 PM
Creation date	Jun 30, 2005 8:09:00 PM
COMSOL version	COMSOL 3.5.0.603

File name: D:\LL_EC1_UO2\Comsol35\micro-ITIES\2011\061411_microhole\061411_microhole.mph

Application modes and modules used in this model:

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

3. Constants

Name	Expression	Value	Description
R	8.314		
T	298.15		

F	96485.33		
fara	$F/(R \cdot T)$		
nu	0.02		scan rate
Ei	0		
Ef	0.5		
Daq	2.5e-9		
Dorg	2.5e-9		
Caq	0		
Corg	0		
n1	1		UO2
n2	1		TMA
n3	-1		TB
E0	0.250		UO2
E02	0.500		TMA
E03	0.9405		TB
alpha	0.5		
k0	1e-5		
Ci1	0		[UO2]org
Ci2	1.0		[UO2]aq
Ci3	0		[TMA]org
Ci4	0		[TMA]aq
Ci5	0		{TB} org
Ci6	0		{TB} aq

Daq1	1e-9		UO2 (aq)
Daq2	2.6e-9		TMA (aq)
Daq3	1.4e-9		TB (aq)
Dorg1	Daq1		UO2 (org)
Dorg2	Daq2		TMA (org)
Dorg3	Daq3		TB (org)
k01	1e-4		UO2
k02	1e-5		TMA
k03	1e-5		TB

4. Geometry

Number of geometries: 1

4.1. Geom1

4.1.1. Point mode

4.1.2. Boundary mode

5. Geom1

Space dimensions: Axial symmetry (2D)

Independent variables: r, phi, z

5.1. Scalar Expressions

Name	Expression	Description
theta	$\exp(-1 \cdot \text{fara} \cdot E_0)$	
st	$\exp(\text{fara} \cdot E_{\text{swp}})$	
E_swp	$E_i + 2 \cdot ((E_f - E_i) / \pi) \cdot \text{asin}(\sin((\pi \cdot \text{nu} \cdot t) / (2 \cdot (E_f - E_i))))$	
nernst1	$\exp(n_1 \cdot \text{fara} \cdot (E_{\text{swp}} - E_0))$	

nernst2	$\exp(n2 \cdot \text{fara} \cdot (E_{\text{swp}} - E02))$	
nernst3	$\exp(n3 \cdot \text{fara} \cdot (E_{\text{swp}} - E03))$	
kf1	$k01 \cdot \exp(-1 \cdot \alpha \cdot (n1 \cdot \text{fara} \cdot (E_{\text{swp}} - E0)))$	
kb1	$k01 \cdot \exp((1 - \alpha) \cdot (n1 \cdot \text{fara} \cdot (E_{\text{swp}} - E0)))$	
kf2	$k02 \cdot \exp(-1 \cdot \alpha \cdot (n2 \cdot \text{fara} \cdot (E_{\text{swp}} - E02)))$	
kb2	$k02 \cdot \exp((1 - \alpha) \cdot (n2 \cdot \text{fara} \cdot (E_{\text{swp}} - E02)))$	
kf3	$k03 \cdot \exp(-1 \cdot \alpha \cdot (n3 \cdot \text{fara} \cdot (E_{\text{swp}} - E03)))$	
kb3	$k03 \cdot \exp((1 - \alpha) \cdot (n3 \cdot \text{fara} \cdot (E_{\text{swp}} - E03)))$	

5.2. Mesh

5.2.1. Mesh Statistics

Number of degrees of freedom	35719
Number of mesh points	3025
Number of elements	5713
Triangular	5713
Quadrilateral	0
Number of boundary elements	395
Number of vertex elements	17
Minimum element quality	0.855
Element area ratio	0

5.3. Application Mode: Diffusion (di2)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: di2

5.3.1. Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Analysis type	Transient
Equilibrium assumption	Off
Frame	Frame (rz)
Weak constraints	Off

Constraint type	Ideal
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5.3.2. Variables

Dependent variables: c2

Shape functions: shlag(2,'c2')

Interior boundaries not active

5.3.3. Boundary Settings

Boundary	4, 6-7	5	9, 11, 13
Type	Axial symmetry	Flux	Insulation/Symmetry
Mass transfer coefficient (kc)	0	kb1	0
Bulk concentration (cb)	0	c1/nernst1	0
Concentration (c0)	0	c1/nernst	0
Boundary	8, 18		
Type	Concentration		
Mass transfer coefficient (kc)	0		
Bulk concentration (cb)	0		
Concentration (c0)	Ci2		

5.3.4. Subdomain Settings

Subdomain	2
Diffusion coefficient (D)	Daq1
Subdomain initial value	2
Concentration, c2 (c2)	Ci2

5.4. Application Mode: Diffusion (di)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: di

5.4.1. Application Mode Properties

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

5.4.2. Variables

Dependent variables: c1

Shape functions: shlag(2,'lm1'), shlag(2,'c1')

Interior boundaries not active

5.4.3. Boundary Settings

Boundary	1, 3	2, 16-17	5
Type	Axial symmetry	Concentration	Flux
Mass transfer coefficient (kc)	0	0	kf1
Bulk concentration (cb)	0	0	c2*nernst1
Concentration (c0)	0	Ci1	c2*nernst

Boundary	10	12, 14	15
Type	Insulation/Symmetry	Insulation/Symmetry	Insulation/Symmetry
Mass transfer coefficient (kc)	kf1	0	0
Bulk concentration (cb)	c2*nernst1	0	0
Concentration (c0)	c2*nernst	0	Corg

5.4.4. Subdomain Settings

Subdomain	1
Shape functions (shape)	shlag(2,'lm1') shlag(2,'c1')
Diffusion coefficient (D)	Dorg1
Subdomain initial value	1
Concentration, c1 (c1)	Ci1

5.5. Application Mode: Diffusion (di3)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: di3

5.5.1. Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Analysis type	Transient
Equilibrium assumption	Off
Frame	Frame (rz)

Weak constraints	Off
Constraint type	Ideal

5.5.2. Variables

Dependent variables: c_3

Shape functions: $\text{shlag}(2, 'c_3')$

Interior boundaries not active

5.5.3. Boundary Settings

Boundary	1, 3	2, 16-17	5
Type	Axial symmetry	Concentration	Flux
Mass transfer coefficient (k_c)	0	0	k_f^2
Bulk concentration (c_b)	0	0	$c_4 \cdot \text{nernst}^2$
Concentration (c_0)	0	C_i^3	c_4 / nernst^2
Boundary	10	12, 14	15
Type	Insulation/Symmetry	Insulation/Symmetry	Insulation/Symmetry
Mass transfer coefficient (k_c)	k_b^2	0	0
Bulk concentration (c_b)	c_4 / nernst^2	0	0
Concentration (c_0)	c_4 / nernst^2	0	C_{org}

5.5.4. Subdomain Settings

Subdomain	1
Diffusion coefficient (D)	D_{org}^2
Subdomain initial value	1

Concentration, c3 (c3)	Ci3
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5.6. Application Mode: Diffusion (di4)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: di4

5.6.1. Application Mode Properties

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

5.6.2. Variables

Dependent variables: c4

Shape functions: shlag(2,'c4')

Interior boundaries not active

5.6.3. Boundary Settings

Boundary	4, 6-7	5	9, 11, 13
Type	Axial symmetry	Flux	Insulation/Symmetry
Mass transfer coefficient (kc)	0	kb2	0
Bulk concentration (cb)	0	c3/nernst2	0

Concentration (c0)	0	c3/ernst2	0
Boundary	8, 18		
Type	Concentration		
Mass transfer coefficient (kc)	0		
Bulk concentration (cb)	0		
Concentration (c0)	Ci4		

5.6.4. Subdomain Settings

Subdomain	2
Diffusion coefficient (D)	Daq2
Subdomain initial value	2
Concentration, c4 (c4)	Ci4

5.7. Application Mode: Diffusion (di5)

Application mode type: Diffusion

Application mode name: di5

5.7.1. Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Analysis type	Transient
Frame	Frame (rz)
Weak constraints	On
Constraint type	Ideal

5.7.2. Variables

Dependent variables: c5

Shape functions: shlag(2,'lm5'), shlag(2,'c5')

Interior boundaries not active

5.7.3. Boundary Settings

Boundary	1, 3	2, 16-17	5
Type	Axial symmetry	Concentration	Flux
Mass transfer coefficient (kc)	0	0	kf3
Bulk concentration (cb)	0	0	c6*nernst3
Concentration (c0)	0	Ci5	c6*nernst3

Boundary	10	12, 14	15
Type	Insulation/Symmetry	Insulation/Symmetry	Insulation/Symmetry
Mass transfer coefficient (kc)	kf3	0	0
Bulk concentration (cb)	c6*nernst3	0	0
Concentration (c0)	c6*nernst3	0	Corg

5.7.4. Subdomain Settings

Subdomain	1
Shape functions (shape)	shlag(2,'lm5') shlag(2,'c5')
Integration order (gporder)	4
Diffusion coefficient (D)	Dorg3
Subdomain initial value	1

Concentration, c5 (c5)	Ci5
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5.8. Application Mode: Diffusion (di6)

Application mode type: Diffusion

Application mode name: di6

5.8.1. Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Analysis type	Transient
Frame	Frame (rz)
Weak constraints	Off
Constraint type	Ideal

5.8.2. Variables

Dependent variables: c6

Shape functions: shlag(2,'c6')

Interior boundaries not active

5.8.3. Boundary Settings

Boundary	4, 6-7	5	9, 11, 13
Type	Axial symmetry	Flux	Insulation/Symmetry
Mass transfer coefficient (kc)	0	kb3	0
Bulk concentration (cb)	0	c5/nernst3	0
Concentration (c0)	0	c5*nernst3	0

Boundary	8, 18
Type	Concentration
Mass transfer coefficient (kc)	0
Bulk concentration (cb)	0
Concentration (c0)	Ci6

5.8.4. Subdomain Settings

Subdomain	2
Diffusion coefficient (D)	Daq3
Subdomain initial value	2
Concentration, c6 (c6)	Ci6

6. Materials/Coefficients Library

6.1. Water

Parameter	Value
Heat capacity at constant pressure (C)	$C_p(T[1/K])[J/(kg \cdot K)]$
Speed of sound (cs)	$cs(T[1/K])[m/s]$
Dynamic viscosity (eta)	$eta(T[1/K])[Pa \cdot s]$
Ratio of specific heats (gamma)	1.0
Thermal conductivity (k)	$k(T[1/K])[W/(m \cdot K)]$
Kinematic viscosity (nu0)	$nu_0(T[1/K])[m^2/s]$
Density (rho)	$rho(T[1/K])[kg/m^3]$
Electric conductivity (sigma)	5.5e-6[S/m]

6.1.1. Piecewise Analytic Functions

6.1.1.1. Function: rho(T)

Type: Polynomial

x_{start}	x_{end}	$f(x)$
273.15	553.75	0 8.38466135E+02 1 1.40050603E+00 2 -3.01123760E-03 3 3.71822313E-07

6.1.1.2. Function: Cp(T)

Type: Polynomial

x_{start}	x_{end}	$f(x)$
273.15	553.75	0 1.20101471E+04 1 -8.04072879E+01 2 3.09866854E-01 3 -5.38186884E-04 4 3.62536437E-07

6.1.1.3. Function: eta(T)

Type: Polynomial

x_{start}	x_{end}	$f(x)$
273.15	413.15	0 1.3799566804E+00 1 -2.1224019151E-02 2 1.3604562827E-04 3 -4.6454090319E-07 4 8.9042735735E-10 5 -9.0790692686E-13 6 3.8457331488E-16
413.15	553.75	0 4.01235783E-03 1 -2.10746715E-05 2 3.85772275E-08 3 -2.39730284E-11

6.1.1.4. Function: nu0(T)

Type: Polynomial

x_{start}	x_{end}	$f(x)$
273.15	413.15	0 1.3903230155E-03 1 -2.1392545737E-05 2 1.3717187260E-07 3 -4.6851166702E-10 4 8.9823339887E-13 5 -9.1602964729E-16 6

		3.8807189536E-19
413.15	553.75	0 1.36222834E-06 1 -4.45388688E-09 2 4.04364450E-12

6.1.1.5. Function: k(T)

Type: Polynomial

x _{start}	x _{end}	f(x)
273.15	553.75	0 -8.69083936E-01 1 8.94880345E-03 2 -1.58366345E-05 3 7.97543259E-09

6.1.2. Interpolation Functions

6.1.2.1. Interpolation Function: cs

Interpolation method: Piecewise Cubic

Data source type: Table

x	f(x)
273	1403
278	1427
283	1447
293	1481
303	1507
313	1526
323	1541
333	1552
343	1555
353	1555

363	1550
373	1543

7. Integration Coupling Variables

7.1. Geom1

7.1.1. Source Boundary: 5

Name	Value
Variable name	c6_flux
Expression	$\text{ndflux_c6_di6} * 2 * \pi * r * n^3 * F$
Order	4
Global	Yes

7.1.2. Source Boundary: 5

Name	Value
Variable name	c5_flux
Expression	$-\text{ndflux_c5_di5} * 2 * \pi * r * n^3 * F$
Order	4
Global	Yes

7.1.3. Source Boundary: 5

Name	Value
Variable name	ct_flux
Expression	$2 * \pi * r * F * (n1 * \text{ndflux_c2_di2} + n2 * \text{ndflux_c4_di4} + n3 * \text{ndflux_c6_di6})$

Order	4
Global	Yes

8. Solver Settings

Solve using a script: off

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

8.1. Direct (UMFPACK)

Solver type: Linear system solver

Parameter	Value
Pivot threshold	0.1
Memory allocation factor	0.7

8.2. Time Stepping

Parameter	Value
Times	range(0,1.0,25)

Relative tolerance	1e-5
Absolute tolerance	1e-5
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

8.3. Advanced

Parameter	Value
Constraint handling method	Elimination
Null-space function	Automatic
Automatic assembly block size	On
Assembly block size	5000
Use Hermitian transpose of constraint matrix and in symmetry detection	On
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

9. Postprocessing

10. Variables

10.1. Boundary

10.1.1. Boundary 1-3, 10, 12, 14-17

Name	Description	Expression
ndflux_c2_di2	Normal diffusive flux, c2	
ndflux_c1_di	Normal diffusive flux, c1	$nr_di * dflux_c1_r_di + nz_di * dflux_c1_z_di$
ndflux_c3_di3	Normal diffusive flux, c3	$nr_di3 * dflux_c3_r_di3 + nz_di3 * dflux_c3_z_di3$
ndflux_c4_di4	Normal diffusive flux, c4	
ndflux_c5_di5	Normal diffusive flux, c5	$nr_di5 * dflux_c5_r_di5 + nz_di5 * dflux_c5_z_di5$
ndflux_c6_di6	Normal diffusive flux, c6	

10.1.2. Boundary 4, 6-9, 11, 13, 18

Name	Description	Expression
ndflux_c2_di2	Normal diffusive flux, c2	$nr_di2 * dflux_c2_r_di2 + nz_di2 * dflux_c2_z_di2$
ndflux_c1_di	Normal diffusive flux, c1	
ndflux_c3_di3	Normal diffusive flux, c3	
ndflux_c4_di4	Normal diffusive flux, c4	$nr_di4 * dflux_c4_r_di4 + nz_di4 * dflux_c4_z_di4$
ndflux_c5_di5	Normal diffusive flux, c5	
ndflux_c6_di6	Normal diffusive flux, c6	$nr_di6 * dflux_c6_r_di6 + nz_di6 * dflux_c6_z_di6$

10.1.3. Boundary 5

Name	Description	Expression
ndflux_c2_di2	Normal diffusive flux, c2	$nr_di2 * dflux_c2_r_di2 + nz_di2 * dflux_c2_z_di2$
ndflux_c1_di	Normal diffusive flux, c1	$nr_di * dflux_c1_r_di + nz_di * dflux_c1_z_di$

ndflux_c3_di3	Normal diffusive flux, c3	$nr_di3 * dflux_c3_r_di3 + nz_di3 * dflux_c3_z_di3$
ndflux_c4_di4	Normal diffusive flux, c4	$nr_di4 * dflux_c4_r_di4 + nz_di4 * dflux_c4_z_di4$
ndflux_c5_di5	Normal diffusive flux, c5	$nr_di5 * dflux_c5_r_di5 + nz_di5 * dflux_c5_z_di5$
ndflux_c6_di6	Normal diffusive flux, c6	$nr_di6 * dflux_c6_r_di6 + nz_di6 * dflux_c6_z_di6$

10.2. Subdomain

10.2.1. Subdomain 1

Name	Description	Expression
grad_c2_r_di2	Concentration gradient, c2, r component	
dflux_c2_r_di2	Diffusive flux, c2, r component	
grad_c2_z_di2	Concentration gradient, c2, z component	
dflux_c2_z_di2	Diffusive flux, c2, z component	
grad_c2_di2	Concentration gradient, c2	
dflux_c2_di2	Diffusive flux, c2	
grad_c1_r_di	Concentration gradient, c1, r component	c1r
dflux_c1_r_di	Diffusive flux, c1, r component	$-Drr_c1_di * c1r - Drz_c1_di * c1z$
grad_c1_z_di	Concentration gradient, c1, z component	c1z
dflux_c1_z_di	Diffusive flux, c1, z component	$-Dzr_c1_di * c1r - Dzz_c1_di * c1z$
grad_c1_di	Concentration gradient, c1	$\sqrt{grad_c1_r_di^2 + grad_c1_z_di^2}$

dflux_c1_di	Diffusive flux, c1	$\text{sqrt}(\text{dflux_c1_r_di}^2 + \text{dflux_c1_z_di}^2)$
grad_c3_r_di3	Concentration gradient, c3, r component	c3r
dflux_c3_r_di3	Diffusive flux, c3, r component	$-\text{Drr_c3_di3} * \text{c3r} - \text{Drz_c3_di3} * \text{c3z}$
grad_c3_z_di3	Concentration gradient, c3, z component	c3z
dflux_c3_z_di3	Diffusive flux, c3, z component	$-\text{Dzr_c3_di3} * \text{c3r} - \text{Dzz_c3_di3} * \text{c3z}$
grad_c3_di3	Concentration gradient, c3	$\text{sqrt}(\text{grad_c3_r_di3}^2 + \text{grad_c3_z_di3}^2)$
dflux_c3_di3	Diffusive flux, c3	$\text{sqrt}(\text{dflux_c3_r_di3}^2 + \text{dflux_c3_z_di3}^2)$
grad_c4_r_di4	Concentration gradient, c4, r component	
dflux_c4_r_di4	Diffusive flux, c4, r component	
grad_c4_z_di4	Concentration gradient, c4, z component	
dflux_c4_z_di4	Diffusive flux, c4, z component	
grad_c4_di4	Concentration gradient, c4	
dflux_c4_di4	Diffusive flux, c4	
grad_c5_r_di5	Concentration gradient, c5, r component	c5r
dflux_c5_r_di5	Diffusive flux, c5, r component	$-\text{Drr_c5_di5} * \text{c5r} - \text{Drz_c5_di5} * \text{c5z}$
grad_c5_z_di5	Concentration gradient, c5, z component	c5z
dflux_c5_z_di5	Diffusive flux, c5, z component	$-\text{Dzr_c5_di5} * \text{c5r} - \text{Dzz_c5_di5} * \text{c5z}$

grad_c5_di5	Concentration gradient, c5	$\text{sqrt}(\text{grad_c5_r_di5}^2 + \text{grad_c5_z_di5}^2)$
dflux_c5_di5	Diffusive flux, c5	$\text{sqrt}(\text{dflux_c5_r_di5}^2 + \text{dflux_c5_z_di5}^2)$
grad_c6_r_di6	Concentration gradient, c6, r component	
dflux_c6_r_di6	Diffusive flux, c6, r component	
grad_c6_z_di6	Concentration gradient, c6, z component	
dflux_c6_z_di6	Diffusive flux, c6, z component	
grad_c6_di6	Concentration gradient, c6	
dflux_c6_di6	Diffusive flux, c6	

10.2.2. Subdomain 2

Name	Description	Expression
grad_c2_r_di2	Concentration gradient, c2, r component	c2r
dflux_c2_r_di2	Diffusive flux, c2, r component	$-\text{Drr_c2_di2} * \text{c2r} - \text{Drz_c2_di2} * \text{c2z}$
grad_c2_z_di2	Concentration gradient, c2, z component	c2z
dflux_c2_z_di2	Diffusive flux, c2, z component	$-\text{Dzr_c2_di2} * \text{c2r} - \text{Dzz_c2_di2} * \text{c2z}$
grad_c2_di2	Concentration gradient, c2	$\text{sqrt}(\text{grad_c2_r_di2}^2 + \text{grad_c2_z_di2}^2)$
dflux_c2_di2	Diffusive flux, c2	$\text{sqrt}(\text{dflux_c2_r_di2}^2 + \text{dflux_c2_z_di2}^2)$
grad_c1_r_di	Concentration gradient, c1, r component	
dflux_c1_r_di	Diffusive flux, c1, r component	

grad_c1_z_di	Concentration gradient, c1, z component	
dflux_c1_z_di	Diffusive flux, c1, z component	
grad_c1_di	Concentration gradient, c1	
dflux_c1_di	Diffusive flux, c1	
grad_c3_r_di3	Concentration gradient, c3, r component	
dflux_c3_r_di3	Diffusive flux, c3, r component	
grad_c3_z_di3	Concentration gradient, c3, z component	
dflux_c3_z_di3	Diffusive flux, c3, z component	
grad_c3_di3	Concentration gradient, c3	
dflux_c3_di3	Diffusive flux, c3	
grad_c4_r_di4	Concentration gradient, c4, r component	c4r
dflux_c4_r_di4	Diffusive flux, c4, r component	-Drr_c4_di4 * c4r-Drz_c4_di4 * c4z
grad_c4_z_di4	Concentration gradient, c4, z component	c4z
dflux_c4_z_di4	Diffusive flux, c4, z component	-Dzr_c4_di4 * c4r-Dzz_c4_di4 * c4z
grad_c4_di4	Concentration gradient, c4	$\sqrt{\text{grad_c4_r_di4}^2 + \text{grad_c4_z_di4}^2}$
dflux_c4_di4	Diffusive flux, c4	$\sqrt{\text{dflux_c4_r_di4}^2 + \text{dflux_c4_z_di4}^2}$
grad_c5_r_di5	Concentration gradient, c5, r component	

dflux_c5_r_di5	Diffusive flux, c5, r component	
grad_c5_z_di5	Concentration gradient, c5, z component	
dflux_c5_z_di5	Diffusive flux, c5, z component	
grad_c5_di5	Concentration gradient, c5	
dflux_c5_di5	Diffusive flux, c5	
grad_c6_r_di6	Concentration gradient, c6, r component	c6r
dflux_c6_r_di6	Diffusive flux, c6, r component	-Drr_c6_di6 * c6r-Drz_c6_di6 * c6z
grad_c6_z_di6	Concentration gradient, c6, z component	c6z
dflux_c6_z_di6	Diffusive flux, c6, z component	-Dzr_c6_di6 * c6r-Dzz_c6_di6 * c6z
grad_c6_di6	Concentration gradient, c6	$\sqrt{\text{grad_c6_r_di6}^2 + \text{grad_c6_z_di6}^2}$
dflux_c6_di6	Diffusive flux, c6	$\sqrt{\text{dflux_c6_r_di6}^2 + \text{dflux_c6_z_di6}^2}$