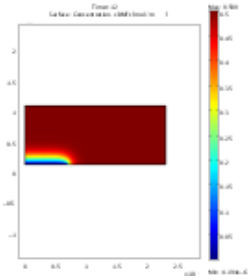
COMSOL Model Report



1. Table of Contents

2. Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Oct 4, 2012 5:34:52 PM
Creation date	Feb 27, 2012 6:15:26 PM
COMSOL version	COMSOL 3.5.0.603

File name: /home/dmitry/Desktop/Kathrin thin layer cell/Model for Kath/Nernst/1000um.mph

Application modes and modules used in this model:

- Geom1 (Axial symmetry (2D))
  - Diffusion

3. Constants

Name	Expression	Value	Description
Diff	1.86e-9[m^2/s]		Diffusion coefficient of DMFc
c0	0.5[mmol/L]		Bulk conc

F	96485[C/mol]		Faraday const
R	8.31[J/mol/K]		Gas const
T	298[K]		Temperature
SR	0.05[V/s]		scanrate
E0	0.0[V]		standard potential
Ei	-0.3[V]		initial voltage
Ef	0.3[V]		final voltage, reverse point

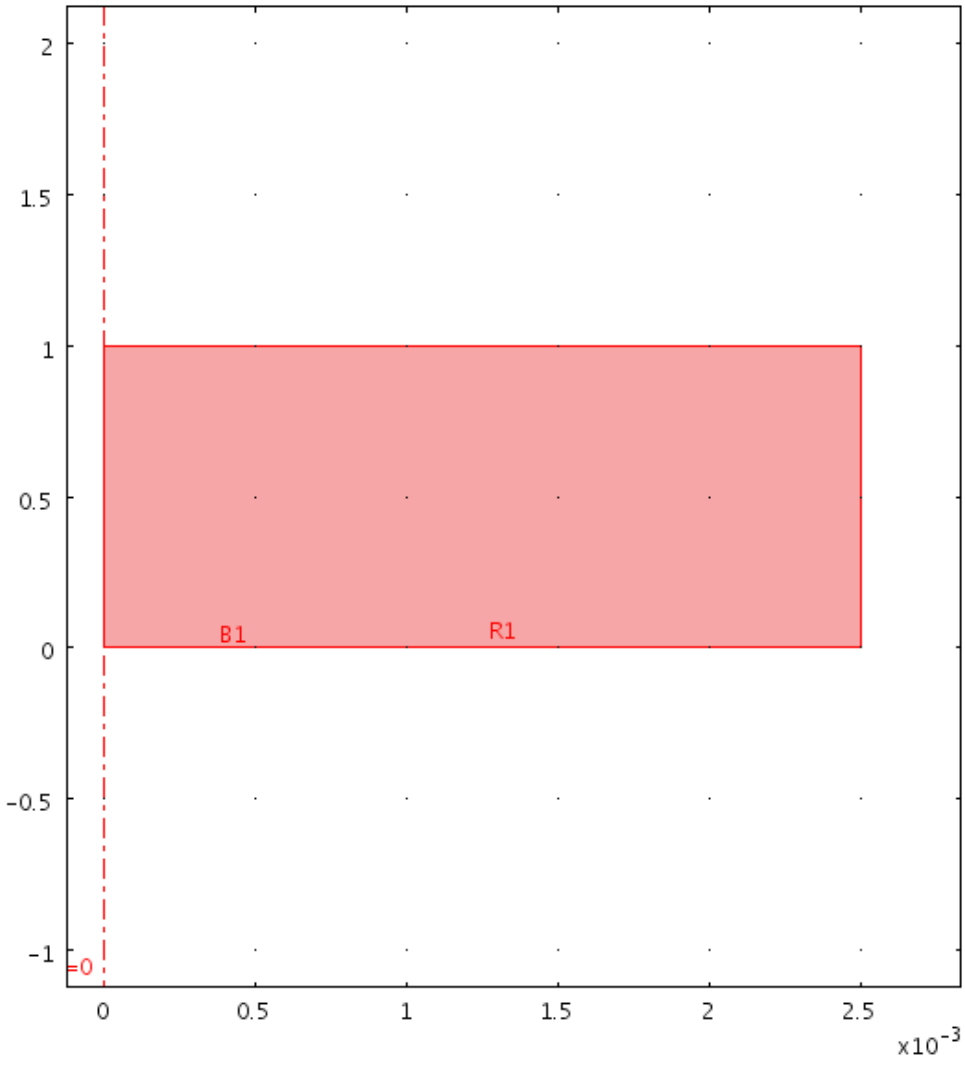
4. Global Expressions

Name	Expression	Unit	Description
cDMFcplus	(c0-cDMFc)	mol/m^3	concentration of DMFC+
celec	cDMFcplus*exp(F/(R*T)*(E0-Elin))	mol/m^3	concentration boundary condition at electrode according to Nernst equation
Elin	Ei+SR*t	V	linear sweep

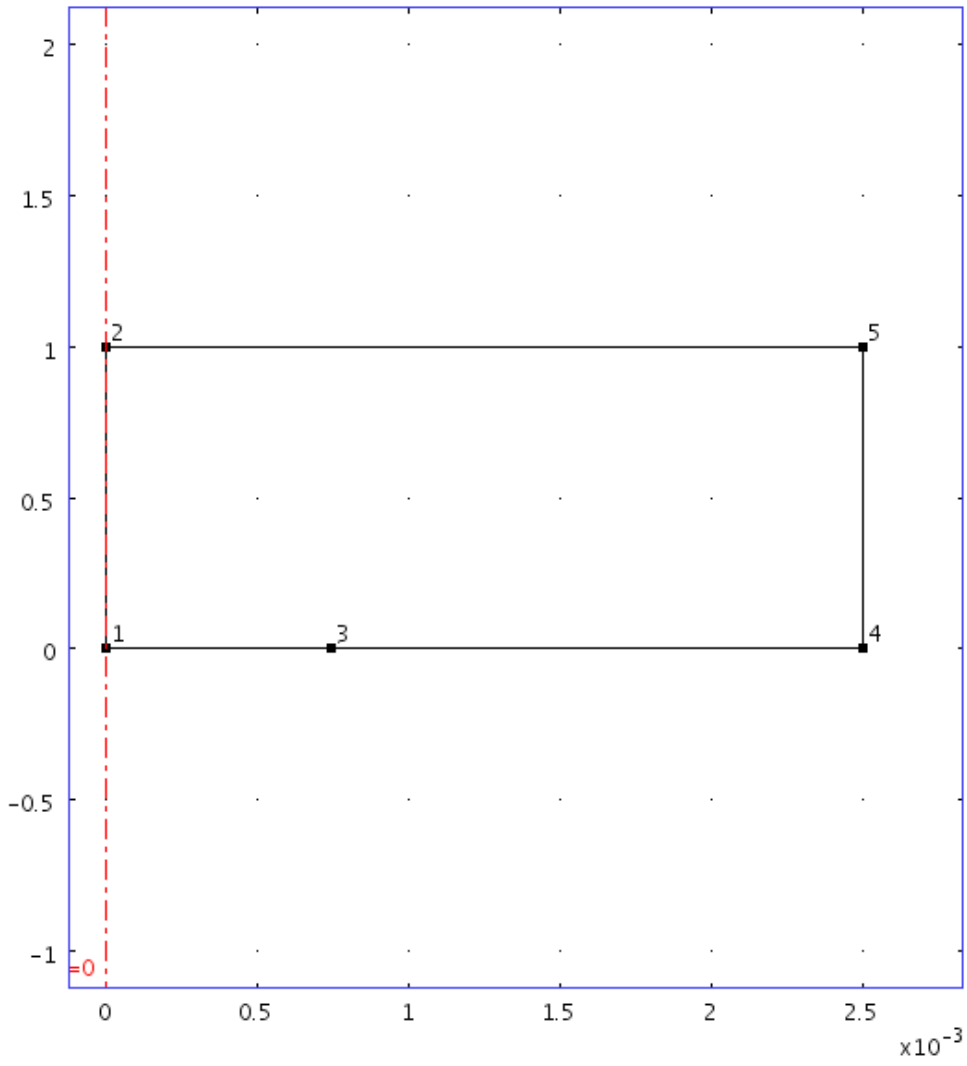
5. Geometry

Number of geometries: 1

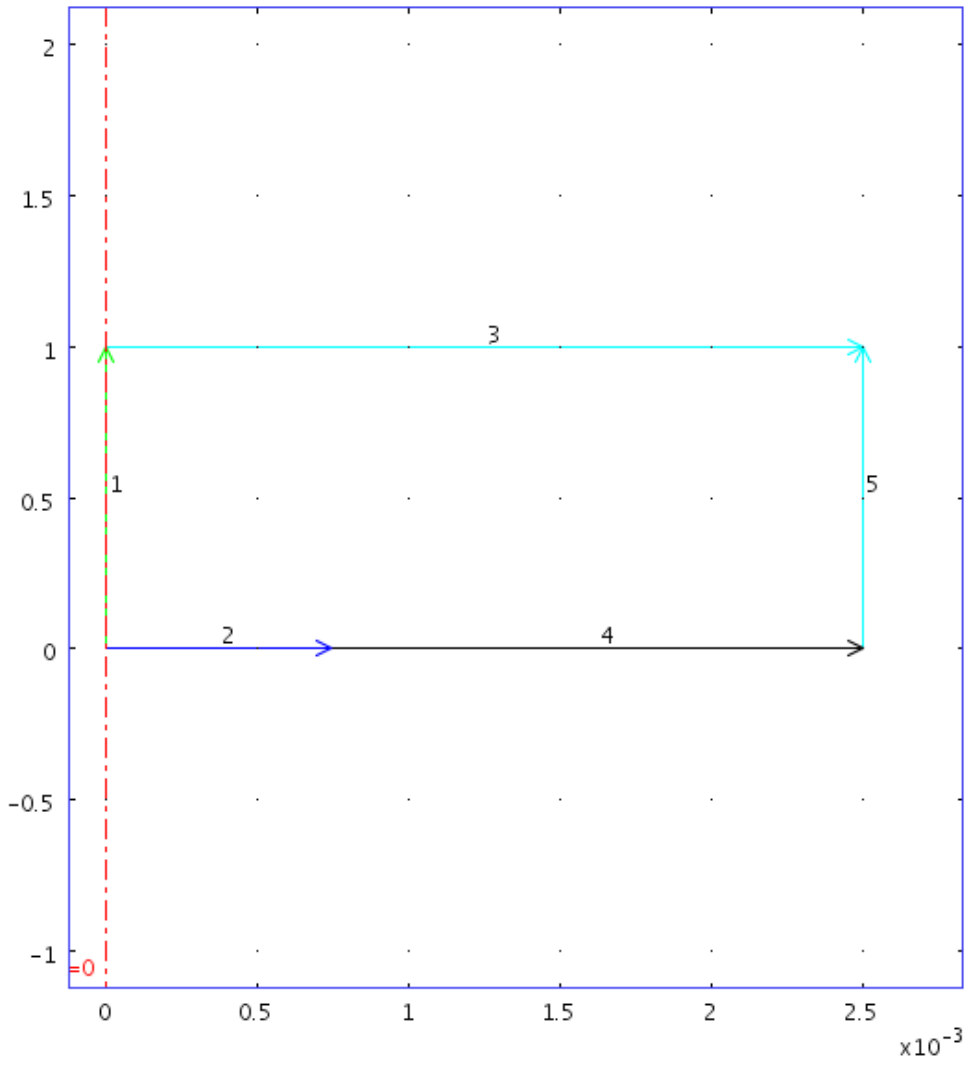
5.1. Geom1



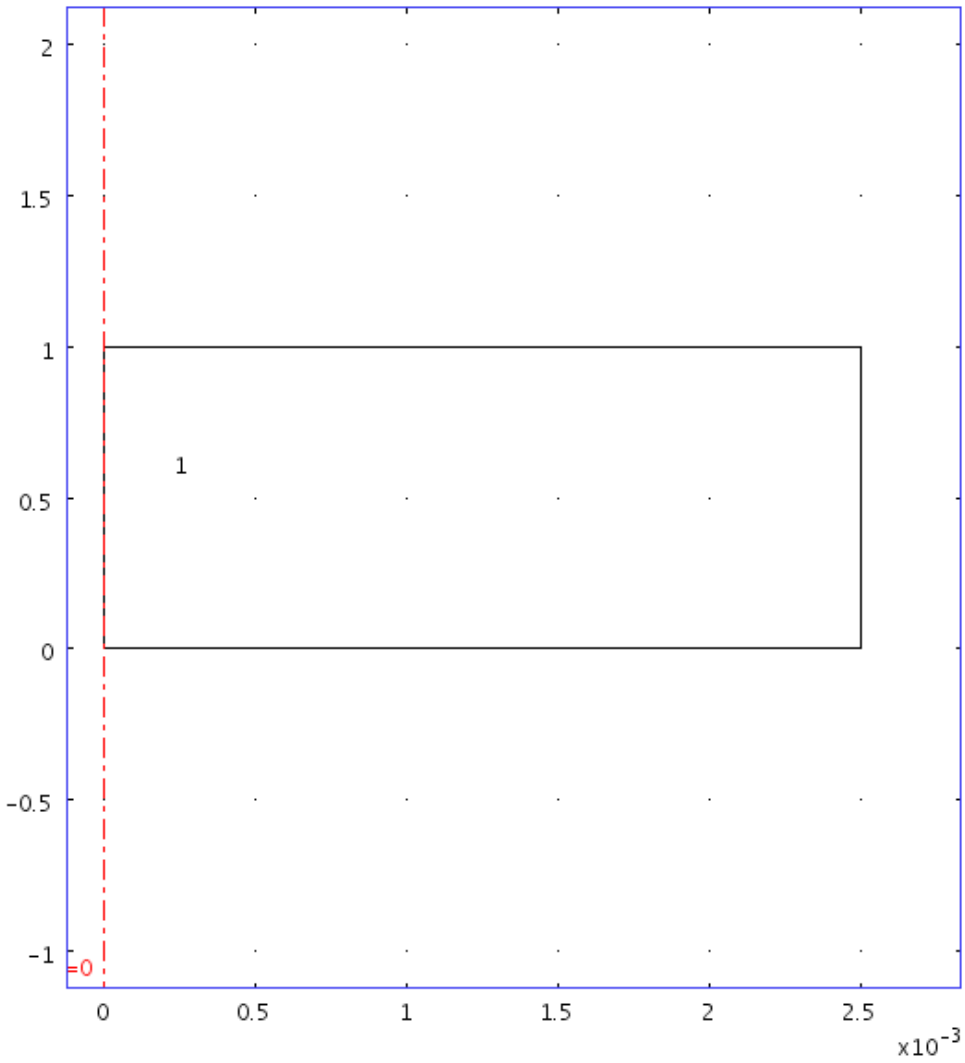
5.1.1. Point mode



5.1.2. Boundary mode



5.1.3. Subdomain mode



6. Geom1

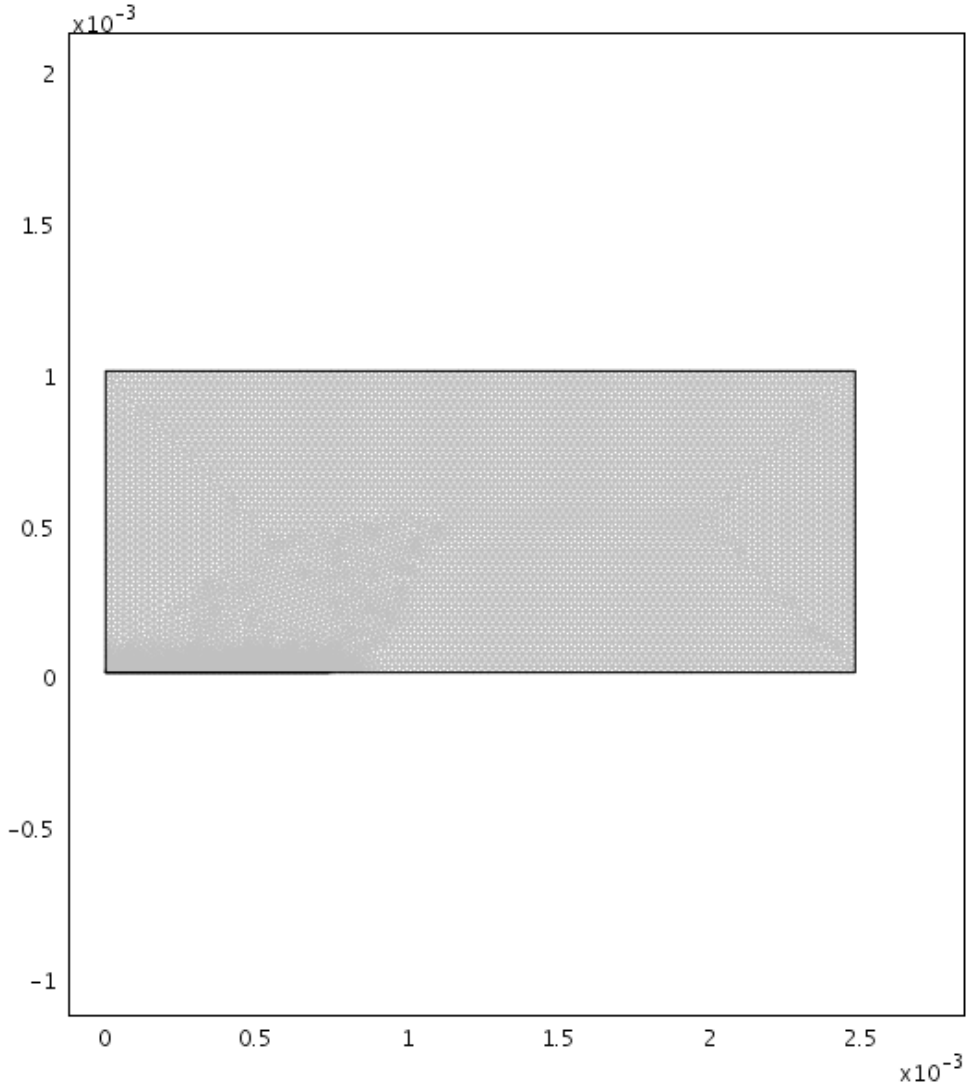
Space dimensions: Axial symmetry (2D)

Independent variables: r, phi, z

6.1. Mesh

6.1.1. Mesh Statistics

Number of degrees of freedom	81424
Number of mesh points	20800
Number of elements	39825
Triangular	39825
Quadrilateral	0
Number of boundary elements	1773
Number of vertex elements	5
Minimum element quality	0.751
Element area ratio	0



6.2. Application Mode: Diffusion (di)

Application mode type: Diffusion

Application mode name: di

6.2.1. Application Mode Properties

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

6.2.2. Variables

Dependent variables: cDMFc

Shape functions: shlag(2,'cDMFc')

Interior boundaries not active

6.2.3. Boundary Settings

Boundary		1	2	3, 5
Type		Axial symmetry	Concentration	Concentration
Concentration (c0)	mol/m3	0	**celec**	**c0**

Boundary		4
Type		Insulation/Symmetry
Concentration (c0)	mol/m3	0

6.2.4. Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m2/s	**Diff**

Subdomain initial value		1
Concentration, cDMFc (cDMFc)	mol/m3	c0

7. Integration Coupling Variables

7.1. Geom1

7.1.1. Source Boundary: 2

Name	**Value**
Variable name	I
Expression	2*pi*r*F*ndflux_cDMFc_di
Order	4
Global	Yes

8. 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

8.1. Direct (UMFPACK)

Solver type: Linear system solver

Parameter	**Value**
Pivot threshold	0.1
Memory allocation factor	0.7

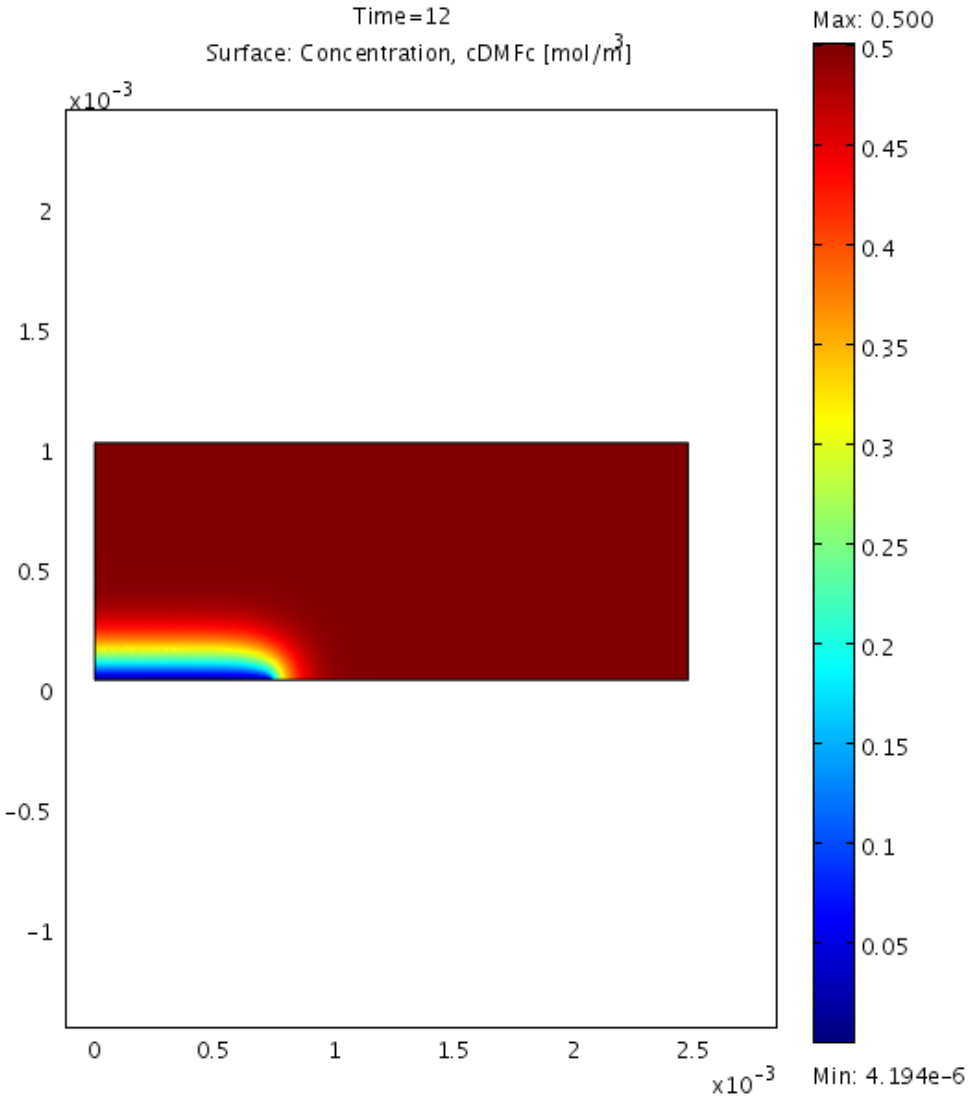
8.2. Time Stepping

Parameter	Value
Times	range(0,1,12)
Relative tolerance	1e-5
Absolute tolerance	1e-6
Times to store in output	Time steps from solver
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	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

9. Postprocessing



10. Variables

10.1. Boundary

Name	Description	Unit	Expression
ndflux_cDMFc_di	Normal diffusive flux, cDMFc	mol/(m^2*s)	nr_di * dflux_cDMFc_r_di+nz_di * dflux_cDMFc_z_di

10.2. Subdomain

Name	Description	Unit	Expression
grad_cDMFc_r_di	Concentration gradient, cDMFc, r component	mol/m^4	cDMFcr
dflux_cDMFc_r_di	Diffusive flux, cDMFc, r component	mol/(m^2*s)	-Drr_cDMFc_di * cDMFcr-Drz_cDMFc_di * cDMFcz
grad_cDMFc_z_di	Concentration gradient, cDMFc, z component	mol/m^4	cDMFcz
dflux_cDMFc_z_di	Diffusive flux, cDMFc, z component	mol/(m^2*s)	-Dzr_cDMFc_di * cDMFcr-Dzz_cDMFc_di * cDMFcz
grad_cDMFc_di	Concentration gradient, cDMFc	mol/m^4	sqrt(grad_cDMFc_r_di^2+grad_cDMFc_z_di^2)
dflux_cDMFc_di	Diffusive flux, cDMFc	mol/(m^2*s)	sqrt(dflux_cDMFc_r_di^2+dflux_cDMFc_z_di^2)