Detection of the short-lived cation radical intermediate in the electrochemical oxidation of *N*,*N* -dimethylaniline (DMA) by scanning electrochemical microscopy (SECM)

Fahe Cao, Jiyeon Kim and Allen J. Bard*

Center for Electrochemistry, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, Texas 78712

Contents

1 Global Definitions

1.1 Parameters 1

Parameters

Name	Expression	Description
D	2.4*10^ - 5[cm^2/s]	diffusion coeff. m/s
cini	0.0004[mol/L]	initial Concentration
F	96485[C/mol]	Constant
n	1	
f	38.92[V^(-1)]	F/RT
EoDMA	0.98[V]	potential
ks	1[cm/s]	rate constant-DMA
al	0.5	transfer coefficient
Esub	0.76[V]	subtrate potential
Etip	1.3[V]	tip potential
tip_h	0.5[um]	

Name	Expression	Description
kc	10^8.4[l/(mol*s)]	second order chemical reaction
ksTMB	1[cm/s]	1st oxidation of TMB
ksTMB1	1[cm/s]	2nd oxidation of TMB
ETMB	0.59[V]	
ETMB1	0.74[V]	

1.2 Variables

1.2.1 Variables 1

Selection

Geometric entity level	Entire model

Name	Expression	Description
kft	ks*exp(-al*n*f*(Etip - EoDMA))	
kbt	ks*exp((1 - al)*n*f*(Etip - EoDMA))	
kfs	ks*exp(-al*n*f*(Esub - EoDMA))	
kbs	ks*exp((1 - al)*n*f*(Esub - EoDMA))	
kftTMB	ksTMB*exp(-al*n*f*(Etip - ETMB))	
kbtTMB	ksTMB*exp((1 - al)*n*f*(Etip - ETMB))	
kfsTMB	ksTMB*exp(-al*n*f*(Esub - ETMB))	
kbsTMB	ksTMB*exp((1 - al)*n*f*(Esub - ETMB))	
kftTMB1	ksTMB1*exp(-al*n*f*(Etip - ETMB1))	
kbtTMB1	ksTMB1*exp((1 - al)*n*f*(Etip - ETMB1))	
kfsTMB1	ksTMB1*exp(-al*n*f*(Esub - ETMB1))	
kbsTMB1	ksTMB1*exp((1 - al)*n*f*(Esub - ETMB1))	

2 Model 1 (mod1)

2.1 Definitions

2.1.1 Coordinate Systems

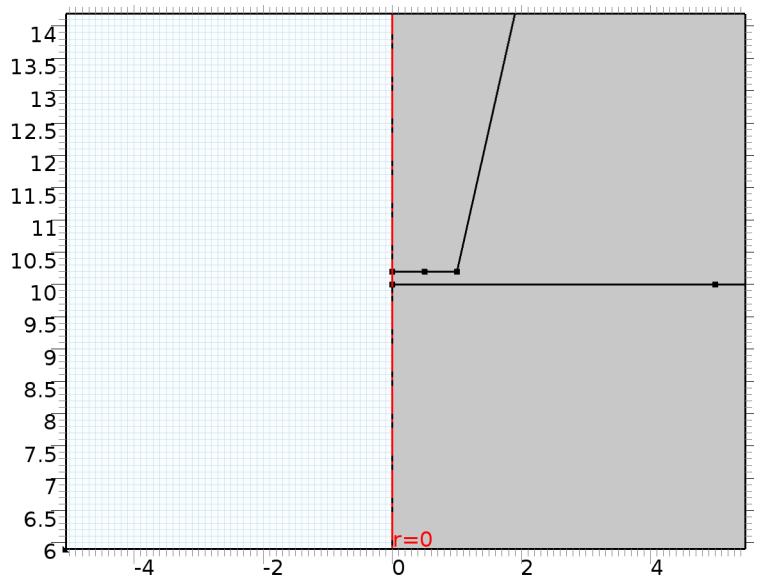
2.1.1.1 Boundary System 1

Coordinate system type	Boundary system
Identifier	sys1

Settings

Name	Value
Coordinate names	{t1, to, n}
Create first tangent direction from	Global Cartesian

2.2 Geometry 1



Geometry 1

Units

Length unit	µm
Angular unit	deg

Geometry statistics

Property	Value
Space dimension	2
Number of domains	3
Number of boundaries	14
Number of vertices	12

2.2.1 Rectangle 1 (r1)

Position

Name	Value
Position	{0, 0}
Width	50

Name	Value
Height	50
Size	{50, 50}

2.2.2 Bézier Polygon 1 (b1)

Polygon segments

Name	Value
Control points	{{0, 0.5}, {tip_h + 10, tip_h + 10}}
Degree	1
Weights	{1, 1}
Valid vertex coordinates	{{0, 10.5}, {0.5, 10.5}}

2.2.3 Bézier Polygon 2 (b2)

Polygon segments

Name	Value
Control points	{{0.5, 1}, {tip_h + 10, tip_h + 10}}
Degree	1
Weights	{1, 1}
Valid vertex coordinates	{{0.5, 10.5}, {1, 10.5}}

2.2.4 Bézier Polygon 3 (b3)

Polygon segments

Name	Value
Control points	{{1, 10}, {tip_h + 10, 50}}
Degree	1
Weights	{1, 1}
Valid vertex coordinates	{{1, 10.5}, {10, 50}}

2.2.5 Bézier Polygon 4 (b4)

Polygon segments

Name	Value
Control points	{{0, 5}, {10, 10}}
Degree	1
Weights	{1, 1}
Valid vertex coordinates	{{0, 10}, {5, 10}}

2.2.6 Bézier Polygon 5 (b5)

Polygon segments

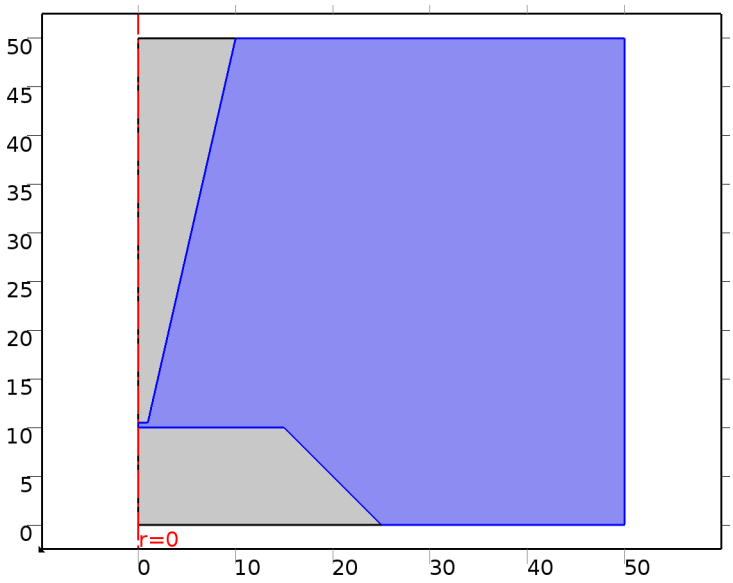
Name	Value
Control points	{{5, 15}, {10, 10}}
Degree	1
Weights	{1, 1}
Valid vertex coordinates	{{5, 10}, {15, 10}}

2.2.7 Bézier Polygon 6 (b6)

Polygon segments

Name	Value
Control points	{{15, 25}, {10, 0}}
Degree	1
Weights	{1, 1}
Valid vertex coordinates	{{15, 10}, {25, 0}}

2.3 Transport of Diluted Species (chds)



Transport of Diluted Species

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\nabla \cdot \left(-D_i \nabla c_i\right) = R_i$$
$$\mathbf{N}_i = -D_i \nabla c_i$$

Settings

Description	Value
Concentration	Linear
Value type when using splitting of complex variables	Complex
Compute boundary fluxes	Off
Migration in electric field	0
Convection	0
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

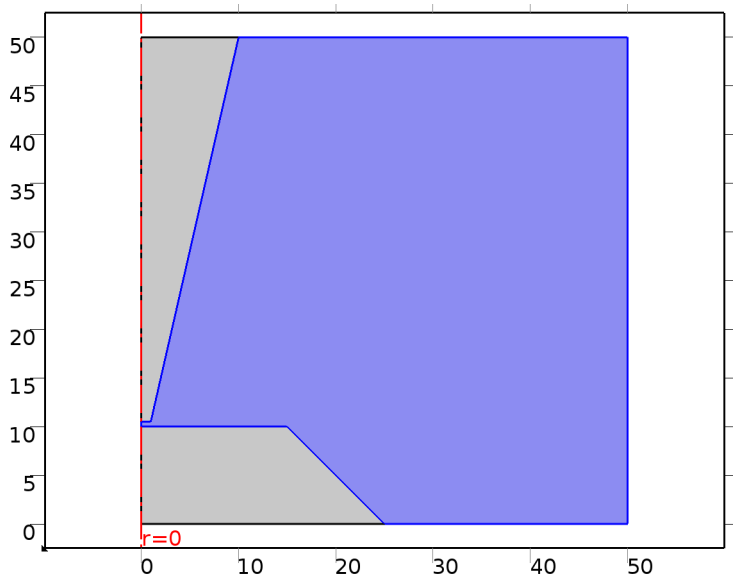
Name	Expression	Unit	Description	Selection
chds.nr	unr		Normal vector, r component	Boundaries 4, 10, 12
chds.nphi	0		Normal vector, phi component	Boundaries 4, 10, 12
chds.nz	unz		Normal vector, z component	Boundaries 4, 10, 12
chds.nr	dnr		Normal vector, r component	Boundaries 3, 6, 8–9, 11, 13–14
chds.nphi	0		Normal vector, phi component	Boundaries 3, 6, 8–9, 11, 13–14
chds.nz	dnz		Normal vector, z component	Boundaries 3, 6, 8–9, 11, 13–14

Name	Expression	Unit	Description	Selection
chds.nrmesh	root.unrmesh		Normal vector (mesh), r component	Boundaries 4, 10, 12
chds.nphimesh	0		Normal vector (mesh), phi component	Boundaries 4, 10, 12
chds.nzmesh	root.unzmesh		Normal vector (mesh), z component	Boundaries 4, 10, 12
chds.nrmesh	root.dnrmesh		Normal vector (mesh), r component	Boundaries 3, 6, 8–9, 11, 13–14
chds.nphimesh	0		Normal vector (mesh), phi component	Boundaries 3, 6, 8–9, 11, 13–14
chds.nzmesh	root.dnzmesh		Normal vector (mesh), z component	Boundaries 3, 6, 8–9, 11, 13–14
chds.R_cDMA	0	mol/(m^3*s)	Total rate expression	Domain 2
chds.R_cDMARadic	0	mol/(m^3*s)	Total rate expression	Domain 2
chds.R_cTMB	0	mol/(m^3*s)	Total rate expression	Domain 2
chds.R_cTMB1	0	mol/(m^3*s)	Total rate expression	Domain 2
chds.R_cTMB2	0	mol/(m^3*s)	Total rate expression	Domain 2
domflux.cDMAr	chds.dfluxr_cDMA	mol/(m^2*s)	Domain flux	Domain 2
domflux.cDMAz	chds.dfluxphi_cDMA	mol/(m^2*s)	Domain flux	Domain 2
domflux.cDMARadicr	chds.dfluxr_cDMARadic	mol/(m^2*s)	Domain flux	Domain 2
domflux.cDMARadicz	chds.dfluxphi_cDMARadic	mol/(m^2*s)	Domain flux	Domain 2

Name	Expression	Unit	Description	Selection
domflux.cTMBr	chds.dfluxr_cTMB	mol/(m^2*s)	Domain flux	Domain 2
domflux.cTMBz	chds.dfluxphi_cTMB	mol/(m^2*s)	Domain flux	Domain 2
domflux.cTMB1r	chds.dfluxr_cTMB1	mol/(m^2*s)	Domain flux	Domain 2
domflux.cTMB1z	chds.dfluxphi_cTMB1	mol/(m^2*s)	Domain flux	Domain 2
domflux.cTMB2r	chds.dfluxr_cTMB2	mol/(m^2*s)	Domain flux	Domain 2
domflux.cTMB2z	chds.dfluxphi_cTMB2	mol/(m^2*s)	Domain flux	Domain 2
chds.nrc	root.nrc/sqrt(root.nrc^2 +root.nzc^2+eps)		Normal vector, r component	Boundaries 3–4, 6, 8–14
chds.nphic	0		Normal vector, phi component	Boundaries 3–4, 6, 8–14
chds.nzc	root.nzc/sqrt(root.nrc^2 +root.nzc^2+eps)		Normal vector, z component	Boundaries 3–4, 6, 8–14
chds.bndFlux_cDMA	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*uflux_spatial(cDMA)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 4, 10, 12
chds.bndFlux_cDMA	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cDMA)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 6, 8–9, 11, 13–14
chds.ntflux_cDMA	chds.bndFlux_cDMA	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 8–14
chds.ndflux_cDMA	chds.bndFlux_cDMA	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 8–14
chds.bndFlux_cDMARadic	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*uflux_spatial(cDMARadic)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 4, 10, 12
chds.bndFlux_cDMARadic	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cDMARadic)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 6, 8–9, 11, 13–14
chds.ntflux_cDMARadic	chds.bndFlux_cDMARadic	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 8–14
chds.ndflux_cDMARadic	chds.bndFlux_cDMARadic	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 8–14

Name	Expression	Unit	Description	Selection
chds.bndFlux_cTMB	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*uflux_spatial(cTMB)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 4, 10, 12
chds.bndFlux_cTMB	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cTMB)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 6, 8–9, 11, 13–14
chds.ntflux_cTMB	chds.bndFlux_cTMB	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 8–14
chds.ndflux_cTMB	chds.bndFlux_cTMB	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 8–14
chds.bndFlux_cTMB1	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*uflux_spatial(cTMB1)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 4, 10, 12
chds.bndFlux_cTMB1	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cTMB1)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 6, 8–9, 11, 13–14
chds.ntflux_cTMB1	chds.bndFlux_cTMB1	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 8–14
chds.ndflux_cTMB1	chds.bndFlux_cTMB1	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 8–14
chds.bndFlux_cTMB2	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*uflux_spatial(cTMB2)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 4, 10, 12
chds.bndFlux_cTMB2	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cTMB2)/(r*pi),NaN)	mol/(m^2*s)	Boundary flux	Boundaries 3, 6, 8–9, 11, 13–14
chds.ntflux_cTMB2	chds.bndFlux_cTMB2	mol/(m^2*s)	Normal total flux	Boundaries 3–4, 6, 8–14
chds.ndflux_cTMB2	chds.bndFlux_cTMB2	mol/(m^2*s)	Normal diffusive flux	Boundaries 3–4, 6, 8–14

2.3.1 Diffusion



Diffusion

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\nabla \cdot \left(-D_i \nabla c_i\right) = R_i$$

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

2.3.1.1 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, 0, 0}, {0, D, 0}, {0, 0, D}}
Bulk material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{D, 0, 0}, {0, D, 0}, {0, 0, D}}
Diffusion coefficient	User defined

Description	Value
Diffusion coefficient	{{D, 0, 0}, {0, D, 0}, {0, 0, D}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D, 0, 0}, {0, D, 0}, {0, 0, D}}
Diffusion coefficient	User defined
Diffusion coefficient	{{D, 0, 0}, {0, D, 0}, {0, 0, D}}
Mobility	User defined

2.3.1.2 Used products

COMSOL Multiphysics

2.3.1.3 Variables

Name	Expression	Unit	Description	Selection
chds.Drr_cDMA	D	m^2/s	Diffusion coefficient, rr component	Domain 2
chds.Dphir_cDMA	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chds.Dzr_cDMA	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chds.Drphi_cDMA	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chds.Dphiphi_cDMA	D	m^2/s	Diffusion coefficient, phiphi component	Domain 2
chds.Dzphi_cDMA	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chds.Drz_cDMA	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chds.Dphiz_cDMA	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chds.Dzz_cDMA	D	m^2/s	Diffusion coefficient, zz	Domain 2

Name	Expression	Unit	Description	Selection
			component	
chds.Dav_cDMA	0.5*(chds.Drr_cDMA+chds.Dzz_cDMA)	m^2/s	Average diffusion coefficient	Domain 2
chds.tfluxr_cDMA	-chds.Drr_cDMA*cDMAr-chds.Drz_cDMA*cDMAz	mol/(m^2*s)	Total flux, r component	Domain 2
chds.tfluxphi_cDMA	-chds.Dphir_cDMA*cDMAr-chds.Dphiz_cDMA*cDMAz	mol/(m^2*s)	Total flux, phi component	Domain 2
chds.tfluxz_cDMA	-chds.Dzr_cDMA*cDMAr-chds.Dzz_cDMA*cDMAz	mol/(m^2*s)	Total flux, z component	Domain 2
chds.dfluxr_cDMA	-chds.Drr_cDMA*cDMAr-chds.Drz_cDMA*cDMAz	mol/(m^2*s)	Diffusive flux, r component	Domain 2
chds.dfluxphi_cDMA	-chds.Dphir_cDMA*cDMAr-chds.Dphiz_cDMA*cDMAz	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chds.dfluxz_cDMA	-chds.Dzr_cDMA*cDMAr-chds.Dzz_cDMA*cDMAz	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds.gradr_cDMA	cDMAr	mol/m^4	Concentration gradient, r component	Domain 2
chds.gradphi_cDMA	0	mol/m^4	Concentration gradient, phi component	Domain 2
chds.gradz_cDMA	cDMAz	mol/m^4	Concentration gradient, z component	Domain 2
chds.dfluxMag_cDMA	sqrt(chds.dfluxr_cDMA^2+chds.dfluxphi_cDMA^2+chds.dfluxz_cDMA^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds.tfluxMag_cDMA	sqrt(chds.tfluxr_cDMA^2+chds.tfluxphi_cDMA^2+chds.tfluxz_cDMA^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds.Drr_cDMARadic	D	m^2/s	Diffusion coefficient, rr component	Domain 2
chds.Dphir_cDMARadic	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chds.Dzr_cDMARadic	0	m^2/s	Diffusion coefficient, zr	Domain 2

Name	Expression	Unit	Description	Selection
			component	
chds.Drphi_cDMARadic	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chds.Dphiphi_cDMARadic	D	m^2/s	Diffusion coefficient, phiphi component	Domain 2
chds.Dzphi_cDMARadic	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chds.Drz_cDMARadic	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chds.Dphiz_cDMARadic	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chds.Dzz_cDMARadic	D	m^2/s	Diffusion coefficient, zz component	Domain 2
chds.Dav_cDMARadic	0.5*(chds.Drr_cDMARadic+chds.Dzz_cDMARadic)	m^2/s	Average diffusion coefficient	Domain 2
chds.tfluxr_cDMARadic	-chds.Drr_cDMARadic*cDMARadicr-chds.Drz_cDMARadic*cDMARadicz	mol/(m^2*s)	Total flux, r component	Domain 2
chds.tfluxphi_cDMARadic	-chds.Dphir_cDMARadic*cDMARadicr-chds.Dphiz_cDMARadic*cDMARadicz	mol/(m^2*s)	Total flux, phi component	Domain 2
chds.tfluxz_cDMARadic	-chds.Dzr_cDMARadic*cDMARadicr-chds.Dzz_cDMARadic*cDMARadicz	mol/(m^2*s)	Total flux, z component	Domain 2
chds.dfluxr_cDMARadic	-chds.Drr_cDMARadic*cDMARadicr-chds.Drz_cDMARadic*cDMA	mol/(m^2*s)	Diffusive flux, r component	Domain 2

Name	Expression	Unit	Description	Selection
	Radicz			
chds.dfluxphi_cDMARadic	-chds.Dphir_cDMARadic*cDMARadicr-chds.Dphiz_cDMARadic*cDMARadicz	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chds.dfluxz_cDMARadic	-chds.Dzr_cDMARadic*cDMARadicr-chds.Dzz_cDMARadic*cDMARadicz	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds.gradr_cDMARadic	cDMARadicr	mol/m^4	Concentration gradient, r component	Domain 2
chds.gradphi_cDMARadic	0	mol/m^4	Concentration gradient, phi component	Domain 2
chds.gradz_cDMARadic	cDMARadicz	mol/m^4	Concentration gradient, z component	Domain 2
chds.dfluxMag_cDMARadic	sqrt(chds.dfluxr_cDMARadic^2+chds.dfluxphi_cDMARadic^2+chds.dfluxz_cDMARadic^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds.tfluxMag_cDMARadic	sqrt(chds.tfluxr_cDMARadic^2+chds.tfluxphi_cDMARadic^2+chds.tfluxz_cDMARadic^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds.Drr_cTMB	D	m^2/s	Diffusion coefficient, rr component	Domain 2
chds.Dphir_cTMB	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chds.Dzr_cTMB	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chds.Drphi_cTMB	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chds.Dphiphi_c	D	m^2/s	Diffusion	Domain 2

Name	Expression	Unit	Description	Selection
TMB			coefficient, phiphi component	
chds.Dzphi_cTMB	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chds.Drz_cTMB	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chds.Dphiz_cTMB	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chds.Dzz_cTMB	D	m^2/s	Diffusion coefficient, zz component	Domain 2
chds.Dav_cTMB	0.5*(chds.Drr_cTMB+chds.Dzz_cTMB)	m^2/s	Average diffusion coefficient	Domain 2
chds.tfluxr_cTMB	-chds.Drr_cTMB*cTMBr-chds.Drz_cTMB*cTMBz	mol/(m^2*s)	Total flux, r component	Domain 2
chds.tfluxphi_cTMB	-chds.Dphir_cTMB*cTMBr-chds.Dphiz_cTMB*cTMBz	mol/(m^2*s)	Total flux, phi component	Domain 2
chds.tfluxz_cTMB	-chds.Dzr_cTMB*cTMBr-chds.Dzz_cTMB*cTMBz	mol/(m^2*s)	Total flux, z component	Domain 2
chds.dfluxr_cTMB	-chds.Drr_cTMB*cTMBr-chds.Drz_cTMB*cTMBz	mol/(m^2*s)	Diffusive flux, r component	Domain 2
chds.dfluxphi_cTMB	-chds.Dphir_cTMB*cTMBr-chds.Dphiz_cTMB*cTMBz	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chds.dfluxz_cTMB	-chds.Dzr_cTMB*cTMBr-chds.Dzz_cTMB*cTMBz	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds.gradr_cTMB	cTMBr	mol/m^4	Concentration gradient, r component	Domain 2
chds.gradphi_cTMB	0	mol/m^4	Concentration gradient, phi component	Domain 2
chds.gradz_cTMB	cTMBz	mol/m^4	Concentration gradient, z component	Domain 2

Name	Expression	Unit	Description	Selection
chds.dfluxMag_cTMB	sqrt(chds.dfluxr_cTMB^2+chds.dfluxphi_cTMB^2+chds.dfluxz_cTMB^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds.tfluxMag_cTMB	sqrt(chds.tfluxr_cTMB^2+chds.tfluxphi_cTMB^2+chds.tfluxz_cTMB^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds.Drr_cTMB1	D	m^2/s	Diffusion coefficient, rr component	Domain 2
chds.Dphir_cTMB1	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chds.Dzr_cTMB1	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chds.Drphi_cTMB1	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chds.Dphiphi_cTMB1	D	m^2/s	Diffusion coefficient, phiphi component	Domain 2
chds.Dzphi_cTMB1	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chds.Drz_cTMB1	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chds.Dphiz_cTMB1	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chds.Dzz_cTMB1	D	m^2/s	Diffusion coefficient, zz component	Domain 2
chds.Dav_cTMB1	0.5*(chds.Drr_cTMB1+chds.Dzz_cTMB1)	m^2/s	Average diffusion coefficient	Domain 2
chds.tfluxr_cTMB1	-chds.Drr_cTMB1*cTMB1r-chds.Drz_cTMB1*cTMB1z	mol/(m^2*s)	Total flux, r component	Domain 2
chds.tfluxphi_c	-chds.Dphir_cTMB1*cTMB1r-	mol/(m^2*s)	Total flux, phi	Domain 2

Name	Expression	Unit	Description	Selection
TMB1	chds.Dphiz_cTMB1*cTMB1z		component	
chds.tfluxz_cTMB1	-chds.Dzr_cTMB1*cTMB1r-chds.Dzz_cTMB1*cTMB1z	mol/(m^2*s)	Total flux, z component	Domain 2
chds.dfluxr_cTMB1	-chds.Drr_cTMB1*cTMB1r-chds.Drz_cTMB1*cTMB1z	mol/(m^2*s)	Diffusive flux, r component	Domain 2
chds.dfluxphi_cTMB1	-chds.Dphir_cTMB1*cTMB1r-chds.Dphiz_cTMB1*cTMB1z	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chds.dfluxz_cTMB1	-chds.Dzr_cTMB1*cTMB1r-chds.Dzz_cTMB1*cTMB1z	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds.gradr_cTMB1	cTMB1r	mol/m^4	Concentration gradient, r component	Domain 2
chds.gradphi_cTMB1	0	mol/m^4	Concentration gradient, phi component	Domain 2
chds.gradz_cTMB1	cTMB1z	mol/m^4	Concentration gradient, z component	Domain 2
chds.dfluxMag_cTMB1	sqrt(chds.dfluxr_cTMB1^2+chds.dfluxphi_cTMB1^2+chds.dfluxz_cTMB1^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds.tfluxMag_cTMB1	sqrt(chds.tfluxr_cTMB1^2+chds.tfluxphi_cTMB1^2+chds.tfluxz_cTMB1^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds.Drr_cTMB2	D	m^2/s	Diffusion coefficient, rr component	Domain 2
chds.Dphir_cTMB2	0	m^2/s	Diffusion coefficient, phir component	Domain 2
chds.Dzr_cTMB2	0	m^2/s	Diffusion coefficient, zr component	Domain 2
chds.Drphi_cTMB2	0	m^2/s	Diffusion coefficient, rphi component	Domain 2
chds.Dphiphi_cTMB2	D	m^2/s	Diffusion coefficient, phiphi	Domain 2

Name	Expression	Unit	Description	Selection
			component	
chds.Dzphi_cTMB2	0	m^2/s	Diffusion coefficient, zphi component	Domain 2
chds.Drz_cTMB2	0	m^2/s	Diffusion coefficient, rz component	Domain 2
chds.Dphiz_cTMB2	0	m^2/s	Diffusion coefficient, phiz component	Domain 2
chds.Dzz_cTMB2	D	m^2/s	Diffusion coefficient, zz component	Domain 2
chds.Dav_cTMB2	0.5*(chds.Drr_cTMB2+chds.Dzz_cTMB2)	m^2/s	Average diffusion coefficient	Domain 2
chds.tfluxr_cTMB2	-chds.Drr_cTMB2*cTMB2r-chds.Drz_cTMB2*cTMB2z	mol/(m^2*s)	Total flux, r component	Domain 2
chds.tfluxphi_cTMB2	-chds.Dphir_cTMB2*cTMB2r-chds.Dphiz_cTMB2*cTMB2z	mol/(m^2*s)	Total flux, phi component	Domain 2
chds.tfluxz_cTMB2	-chds.Dzr_cTMB2*cTMB2r-chds.Dzz_cTMB2*cTMB2z	mol/(m^2*s)	Total flux, z component	Domain 2
chds.dfluxr_cTMB2	-chds.Drr_cTMB2*cTMB2r-chds.Drz_cTMB2*cTMB2z	mol/(m^2*s)	Diffusive flux, r component	Domain 2
chds.dfluxphi_cTMB2	-chds.Dphir_cTMB2*cTMB2r-chds.Dphiz_cTMB2*cTMB2z	mol/(m^2*s)	Diffusive flux, phi component	Domain 2
chds.dfluxz_cTMB2	-chds.Dzr_cTMB2*cTMB2r-chds.Dzz_cTMB2*cTMB2z	mol/(m^2*s)	Diffusive flux, z component	Domain 2
chds.gradr_cTMB2	cTMB2r	mol/m^4	Concentration gradient, r component	Domain 2
chds.gradphi_cTMB2	0	mol/m^4	Concentration gradient, phi component	Domain 2
chds.gradz_cTMB2	cTMB2z	mol/m^4	Concentration gradient, z component	Domain 2

Name	Expression	Unit	Description	Selection
chds.dfluxMag_cTMB2	sqrt(chds.dfluxr_cTMB2^2+chds.dfluxphi_cTMB2^2+chds.dfluxz_cTMB2^2)	mol/(m^2*s)	Diffusive flux magnitude	Domain 2
chds.tfluxMag_cTMB2	sqrt(chds.tfluxr_cTMB2^2+chds.tfluxphi_cTMB2^2+chds.tfluxz_cTMB2^2)	mol/(m^2*s)	Total flux magnitude	Domain 2
chds.helem	h	m	Element size	Domain 2
chds.glim_mass	0.1[mol/m^3]/chds.helem	mol/m^4	Lower gradient limit	Domain 2
chds.Ck_mass	0.5	1	Tuning parameter	Domain 2
chds.Res_cDMA	-chds.R_cDMA	mol/(m^3*s)	Equation residual	Domain 2
chds.Res_cDMARadic	-chds.R_cDMARadic	mol/(m^3*s)	Equation residual	Domain 2
chds.Res_cTMB	-chds.R_cTMB	mol/(m^3*s)	Equation residual	Domain 2
chds.Res_cTMB1	-chds.R_cTMB1	mol/(m^3*s)	Equation residual	Domain 2
chds.Res_cTMB2	-chds.R_cTMB2	mol/(m^3*s)	Equation residual	Domain 2

2.3.1.4 Shape functions

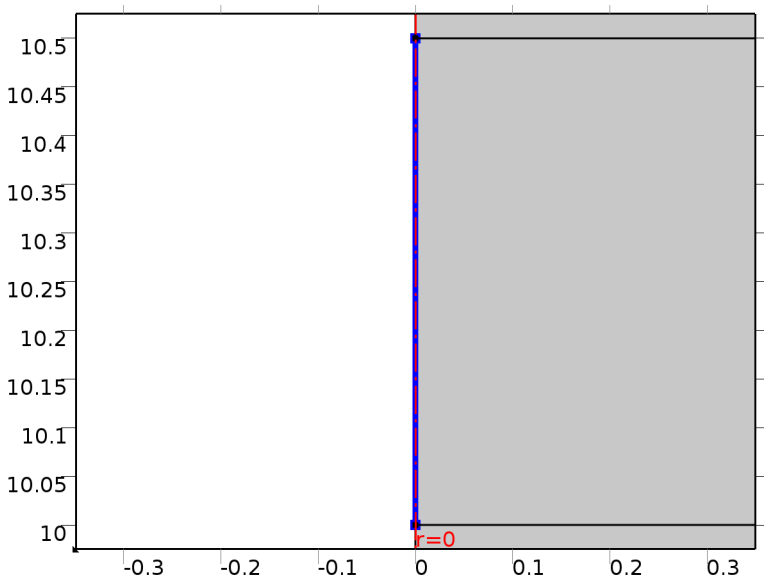
Name	Shape function	Unit	Description	Shape frame	Selection
cDMA	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
cDMARadic	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
cTMB	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
cTMB1	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2
cTMB2	Lagrange (Linear)	mol/m^3	Concentration	Material	Domain 2

2.3.1.5 Weak expressions

Weak expression	Integration frame	Selection
2*(-d(cDMA,t)*test(cDMA)-(chds.Drr_cDMA*cDMAr+chds.Drz_cDMA*cDMAz)*test(cDMAr)-(chds.Dzr_cDMA*cDMAr+chds.Dzz_cDMA*cDMAz)*test(cDMAz))*pi*r	Material	Domain 2

Weak expression	Integration frame	Selection
2*(-d(cDMARadic,t)*test(cDMARadic)-(chds.Drr_cDMARadic*cDMARadicr+chds.Drz_cDMARadic*cDMARadicz)*test(cDMARadicr)-(chds.Dzr_cDMARadic*cDMARadicr+chds.Dzz_cDMARadic*cDMARadicz)*test(cDMARadicz))*pi*r	Material	Domain 2
2*(-d(cTMB,t)*test(cTMB)-(chds.Drr_cTMB*cTMBr+chds.Drz_cTMB*cTMBz)*test(cTMBr)-(chds.Dzr_cTMB*cTMBr+chds.Dzz_cTMB*cTMBz)*test(cTMBz))*pi*r	Material	Domain 2
2*(-d(cTMB1,t)*test(cTMB1)-(chds.Drr_cTMB1*cTMB1r+chds.Drz_cTMB1*cTMB1z)*test(cTMB1r)-(chds.Dzr_cTMB1*cTMB1r+chds.Dzz_cTMB1*cTMB1z)*test(cTMB1z))*pi*r	Material	Domain 2
2*(-d(cTMB2,t)*test(cTMB2)-(chds.Drr_cTMB2*cTMB2r+chds.Drz_cTMB2*cTMB2z)*test(cTMB2r)-(chds.Dzr_cTMB2*cTMB2r+chds.Dzz_cTMB2*cTMB2z)*test(cTMB2z))*pi*r	Material	Domain 2
2*chds.streamline*pi*r	Material	Domain 2
2*chds.crosswind*pi*r	Material	Domain 2

2.3.2 Axial Symmetry 1



Axial Symmetry 1

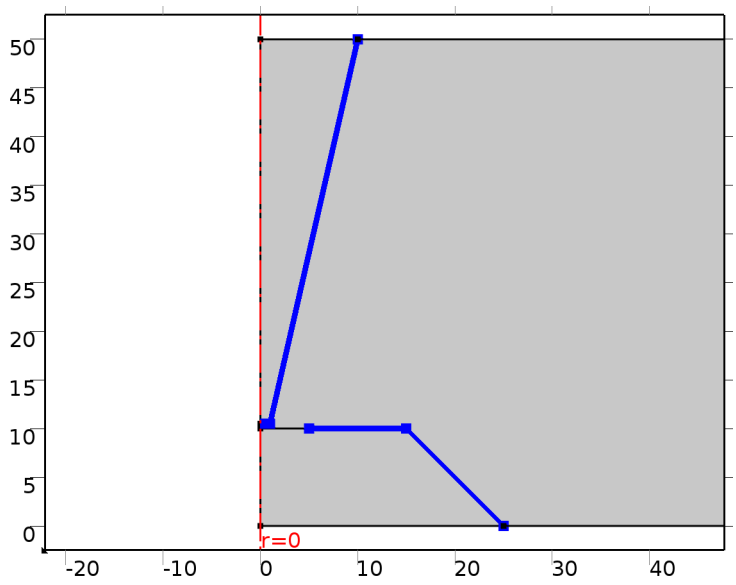
Selection

Geometric entity level	Boundary
Selection	Boundary 3

2.3.2.1 Used products

COMSOL Multiphysics

2.3.3 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 8–10, 12

Equations

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

2.3.3.1 Settings

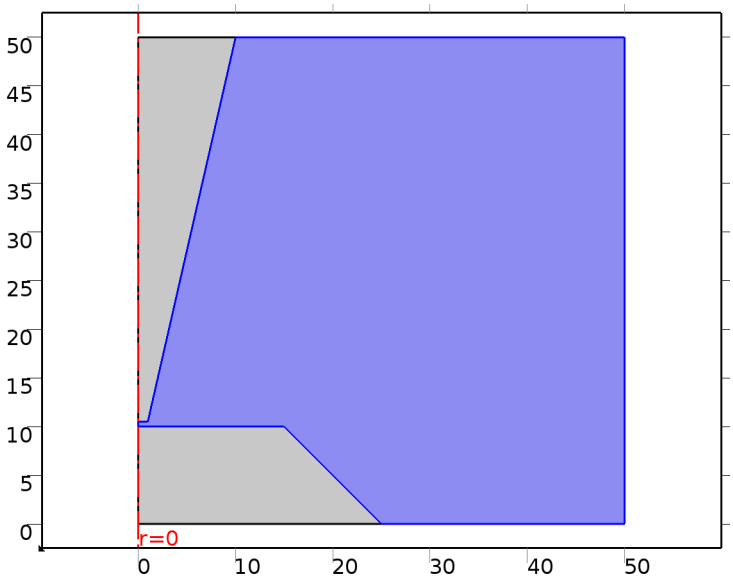
Settings

Description	Value
Apply for all species	Apply for all species

2.3.3.2 Used products

COMSOL Multiphysics

2.3.4 Initial Values 1



Initial Values 1

Selection

Geometric entity level	Domain
Selection	Domain 2

2.3.4.1 Settings

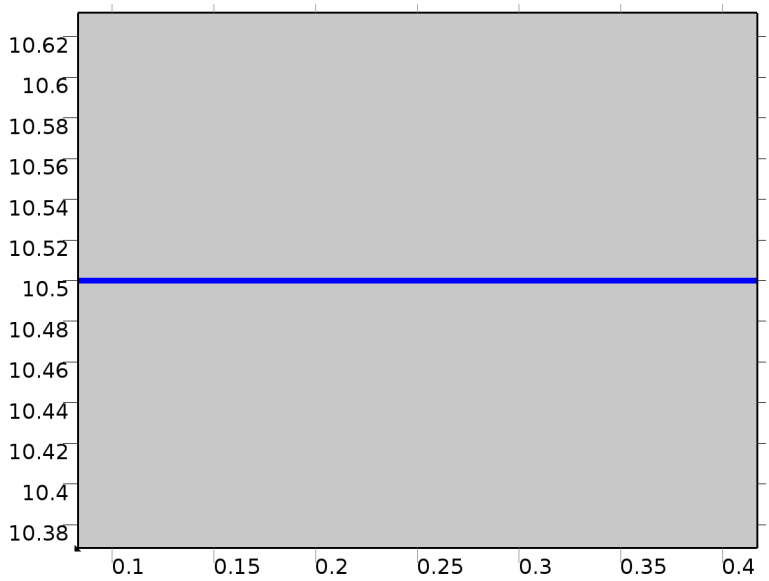
Settings

Description	Value
Concentration	cini
Concentration	0
Concentration	0
Concentration	0
Concentration	0

2.3.4.2 Used products

COMSOL Multiphysics

2.3.5 Flux 1



Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundary 6

Equations

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

2.3.5.1 Settings

Settings

Description	Value
Species cDMA	On
Species cDMARadic	On
Species cTMB	On
Species cTMB1	On
Species cTMB2	On
Inward flux	{-kbt*cDMA + kft*cDMARadic, kbt*cDMA - kft*cDMARadic, -kbtTMB*cTMB + kftTMB*cTMB1, kbtTMB*cTMB - kftTMB*cTMB1 + kftTMB1*cTMB2 - kbtTMB1*cTMB1, -kftTMB1*cTMB2 + kbtTMB1*cTMB1}
Flux type	General inward flux

2.3.5.2 Used products

COMSOL Multiphysics

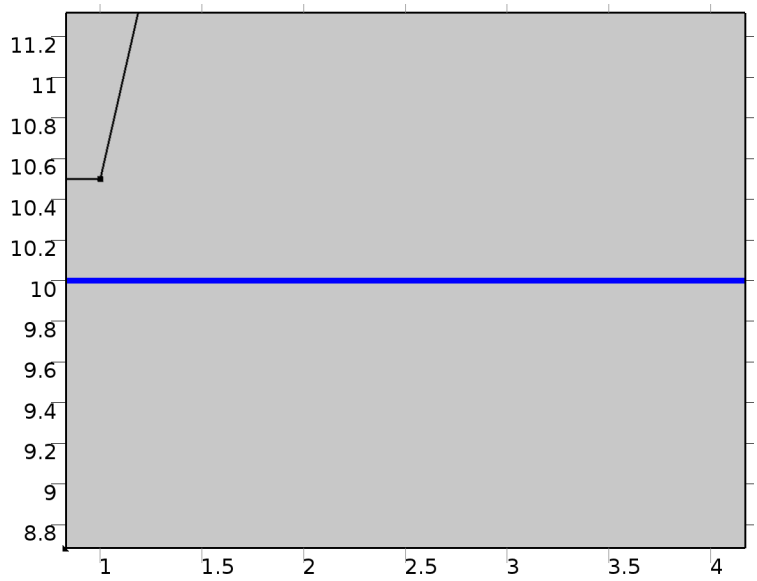
2.3.5.3 Variables

Name	Expression	Unit	Description	Selection
chds.cb_cDMA	0	mol/m^3	Bulk concentration	Boundary 6
chds.kc_cDMA	0	m/s	Mass transfer coefficient	Boundary 6
chds.cb_cDMARadic	0	mol/m^3	Bulk concentration	Boundary 6
chds.kc_cDMARadic	0	m/s	Mass transfer coefficient	Boundary 6
chds.cb_cTMB	0	mol/m^3	Bulk concentration	Boundary 6
chds.kc_cTMB	0	m/s	Mass transfer coefficient	Boundary 6
chds.cb_cTMB1	0	mol/m^3	Bulk concentration	Boundary 6
chds.kc_cTMB1	0	m/s	Mass transfer coefficient	Boundary 6
chds.cb_cTMB2	0	mol/m^3	Bulk concentration	Boundary 6
chds.kc_cTMB2	0	m/s	Mass transfer coefficient	Boundary 6

2.3.5.4 Weak expressions

Weak expression	Integration frame	Selection
2*(-kbt*cDMA+kft*cDMARadic)*test(cDMA)*pi*r	Material	Boundary 6
2*(kbt*cDMA-kft*cDMARadic)*test(cDMARadic)*pi*r	Material	Boundary 6
2*(-kbtTMB*cTMB+kftTMB*cTMB1)*test(cTMB)*pi*r	Material	Boundary 6
2*(kbtTMB*cTMB-kftTMB*cTMB1+kftTMB1*cTMB2-kbtTMB1*cTMB1)*test(cTMB1)*pi*r	Material	Boundary 6
2*(-kftTMB1*cTMB2+kbtTMB1*cTMB1)*test(cTMB2)*pi*r	Material	Boundary 6

2.3.6 Flux 2



Flux 2

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Equations

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

2.3.6.1 Settings

Settings

Description	Value
Species cDMA	On
Species cDMARadic	On
Species cTMB	On
Species cTMB1	On
Species cTMB2	On
Inward flux	{-kbs*cDMA + kfs*cDMARadic, kbs*cDMA - kfs*cDMARadic, -kbsTMB*cTMB + kfsTMB*cTMB1, kbsTMB*cTMB - kfsTMB*cTMB1 + kfsTMB1*cTMB1 - kbsTMB1*cTMB1, -kfsTMB1*cTMB2 + kbsTMB1*cTMB1}
Flux type	General inward flux

2.3.6.2 Used products

COMSOL Multiphysics

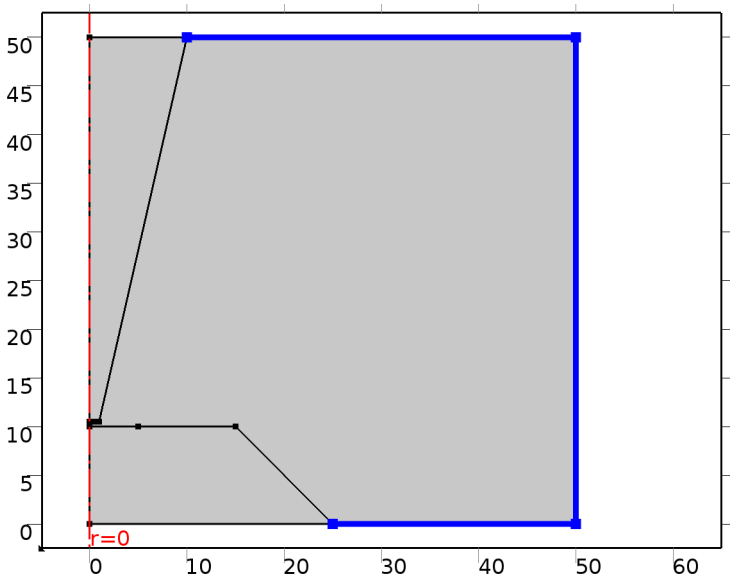
2.3.6.3 Variables

Name	Expression	Unit	Description	Selection
chds.cb_cDMA	0	mol/m^3	Bulk concentration	Boundary 4
chds.kc_cDMA	0	m/s	Mass transfer coefficient	Boundary 4
chds.cb_cDMARadic	0	mol/m^3	Bulk concentration	Boundary 4
chds.kc_cDMARadic	0	m/s	Mass transfer coefficient	Boundary 4
chds.cb_cTMB	0	mol/m^3	Bulk concentration	Boundary 4
chds.kc_cTMB	0	m/s	Mass transfer coefficient	Boundary 4
chds.cb_cTMB1	0	mol/m^3	Bulk concentration	Boundary 4
chds.kc_cTMB1	0	m/s	Mass transfer coefficient	Boundary 4
chds.cb_cTMB2	0	mol/m^3	Bulk concentration	Boundary 4
chds.kc_cTMB2	0	m/s	Mass transfer coefficient	Boundary 4

2.3.6.4 Weak expressions

Weak expression	Integration frame	Selection
2*(-kbs*cDMA+kfs*cDMARadic)*test(cDMA)*pi*r	Material	Boundary 4
2*(kbs*cDMA-kfs*cDMARadic)*test(cDMARadic)*pi*r	Material	Boundary 4
2*(-kbsTMB*cTMB+kfsTMB*cTMB1)*test(cTMB)*pi*r	Material	Boundary 4
2*(kbsTMB*cTMB-kfsTMB*cTMB1+kfsTMB1*cTMB1-kbsTMB1*cTMB1)*test(cTMB1)*pi*r	Material	Boundary 4
2*(-kfsTMB1*cTMB2+kbsTMB1*cTMB1)*test(cTMB2)*pi*r	Material	Boundary 4

2.3.7 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 11, 13–14

Equations

$$c_i = c_{0i}$$

2.3.7.1 Settings

Settings

Description	Value
Concentration	{cini, 0, 0, 0, 0}
Species cDMA	On
Species cDMARadic	On
Species cTMB	On
Species cTMB1	On
Species cTMB2	On
Apply reaction terms on	All physics (symmetric)
Use weak constraints	Off

2.3.7.2 Used products

COMSOL Multiphysics

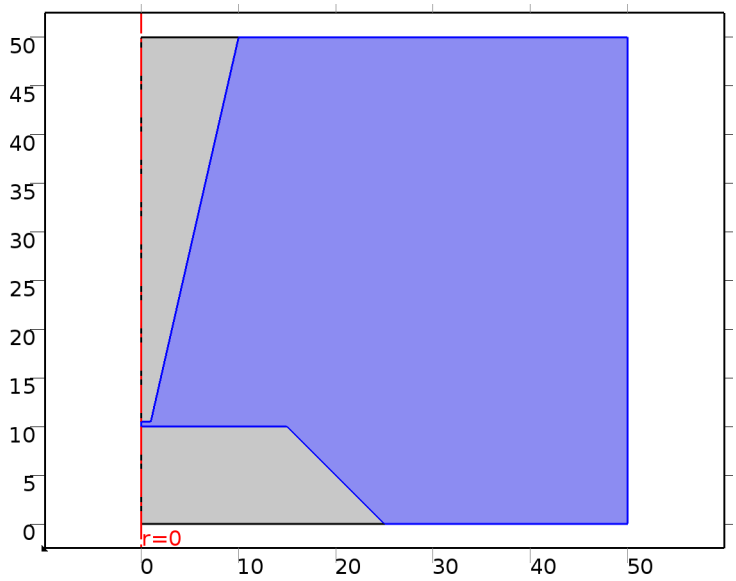
2.3.7.3 Variables

Name	Expression	Unit	Description	Selection
chds.c0_cDMA	cini	mol/m^3	Concentration	Boundaries 11, 13–14
chds.c0_cDMARadic	0	mol/m^3	Concentration	Boundaries 11, 13–14
chds.c0_cTMB	0	mol/m^3	Concentration	Boundaries 11, 13–14
chds.c0_cTMB1	0	mol/m^3	Concentration	Boundaries 11, 13–14
chds.c0_cTMB2	0	mol/m^3	Concentration	Boundaries 11, 13–14

2.3.7.4 Shape functions

Constraint	Constraint force	Shape function	Selection
-cDMA+chds.c0_cDMA	test(-cDMA+chds.c0_cDMA)	Lagrange (Linear)	Boundaries 11, 13–14
-cDMARadic+chds.c0_cDMARadic	test(-cDMARadic+chds.c0_cDMARadic)	Lagrange (Linear)	Boundaries 11, 13–14
-cTMB+chds.c0_cTMB	test(-cTMB+chds.c0_cTMB)	Lagrange (Linear)	Boundaries 11, 13–14
-cTMB1+chds.c0_cTMB1	test(-cTMB1+chds.c0_cTMB1)	Lagrange (Linear)	Boundaries 11, 13–14
-cTMB2+chds.c0_cTMB2	test(-cTMB2+chds.c0_cTMB2)	Lagrange (Linear)	Boundaries 11, 13–14

2.3.8 Reactions 1



Reactions 1

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\nabla \cdot \left(-D_i \nabla c_i\right) = R_i$$

2.3.8.1 Settings

Settings

Description	Value
Total rate expression	{0, -kc*cDMARadic*cDMARadic, kc*cDMARadic*cDMARadic, 0, 0}

2.3.8.2 Used products

COMSOL Multiphysics

2.3.8.3 Variables

Name	Expression	Unit	Description	Selection
chds.R_cDMA	0	mol/(m^3*s)	Total rate expression	Domain 2
chds.R_cDMARadic	-kc*cDMARadic^2	mol/(m^3*s)	Total rate expression	Domain 2
chds.R_cTMB	kc*cDMARadic^2	mol/(m^3*s)	Total rate expression	Domain 2

Name	Expression	Unit	Description	Selection
chds.R_cTMB1	0	mol/(m^3*s)	Total rate expression	Domain 2
chds.R_cTMB2	0	mol/(m^3*s)	Total rate expression	Domain 2

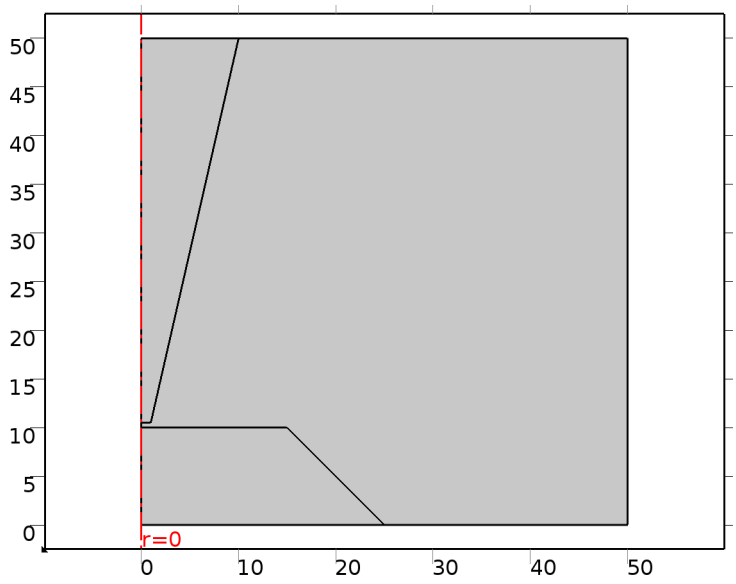
2.3.8.4 Weak expressions

Weak expression	Integration frame	Selection
-2*kc*cDMARadic^2*test(cDMARadic)*pi*r	Material	Domain 2
2*kc*cDMARadic^2*test(cTMB)*pi*r	Material	Domain 2

2.4 Mesh 1

Mesh statistics

Property	Value
Minimum element quality	0.0
Average element quality	0.0



Mesh 1

2.4.1 Size (size)

Settings

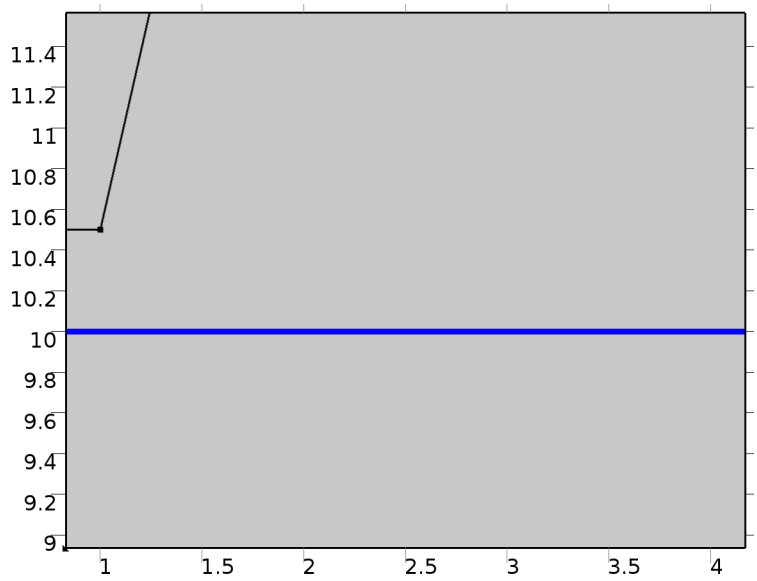
Name	Value
Minimum element size	0.00375
Curvature factor	0.25

Name	Value
Maximum element growth rate	1.2
Predefined size	Extra fine

2.4.2 Edge 1 (edg1)

Selection

Geometric entity level	Boundary
Selection	Boundaries 4, 6

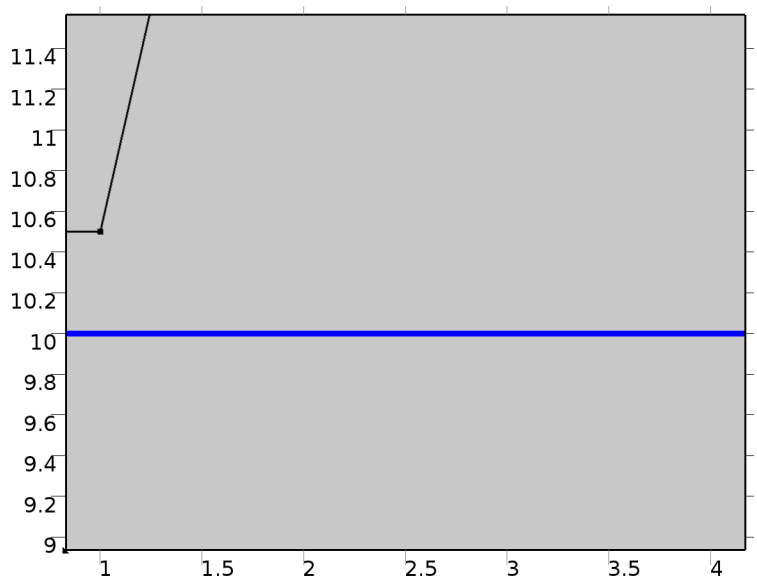


Edge 1

2.4.2.1 Size 1 (size1)

Selection

Geometric entity level	Boundary
Selection	Boundaries 4, 6



Size 1

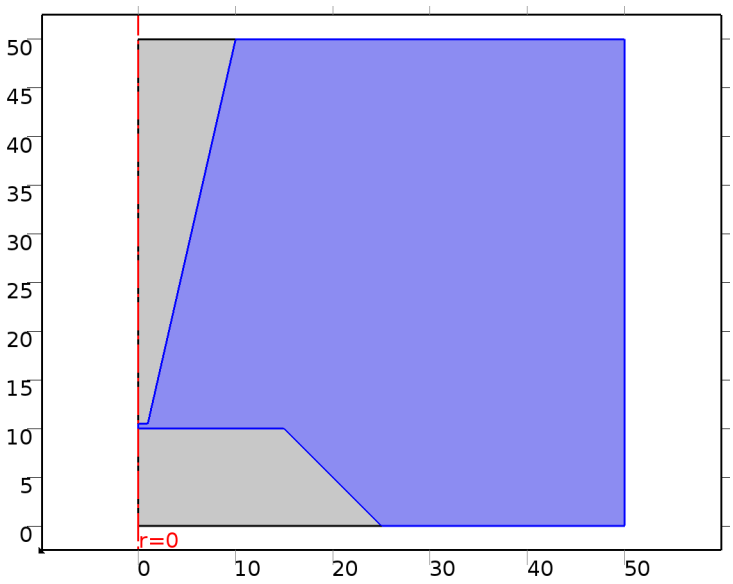
Settings

Name	Value
Maximum element size	0.002
Minimum element size	0.002
Curvature factor	0.3
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Custom element size	Custom

2.4.3 Free Triangular 1 (ftri1)

Selection

Geometric entity level	Domain
Selection	Domain 2



Free Triangular 1

3 Study 1

3.1 Parametric Sweep

Parameter name: tip_h

Parameters:

3.2 Stationary

Study settings

Property	Value
Include geometric nonlinearity	Off

Mesh selection

Geometry	Mesh
Geometry 1 (geom1)	mesh1

Physics selection

Physics	Discretization
Transport of Diluted Species (chds)	physics

3.3 Solver Configurations

3.3.1 Solver 1

3.3.1.1 Compile Equations: Stationary (st1)

Study and step

Name	Value
Use study	Study 1
Use study step	Stationary

3.3.1.2 Dependent Variables 1 (v1)

General

Name	Value
Defined by study step	Stationary

Initial values of variables solved for

Name	Value
Solution	Zero

Values of variables not solved for

Name	Value
Solution	Zero

3.3.1.2.1 Concentration (mod1.cTMB2) (mod1_cTMB2)

General

Name	Value
Field components	mod1.cTMB2

3.3.1.2.2 Concentration (mod1.cDMA) (mod1_cDMA)

General

Name	Value
Field components	mod1.cDMA

3.3.1.2.3 Concentration (mod1.cTMB1) (mod1_cTMB1)

General

Name	Value
Field components	mod1.cTMB1

3.3.1.2.4 Concentration (mod1.cTMB) (mod1_cTMB)

General

Name	Value
Field components	mod1.cTMB

3.3.1.2.5 Concentration (mod1.cDMARadic) (mod1_cDMARadic)

General

Name	Value
Field components	mod1.cDMARadic

3.3.1.3 Stationary Solver 1 (s1)

General

Name	Value
Defined by study step	Stationary

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:48:22.
Nonlinear solver
Number of degrees of freedom solved for: 155915.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1         0.5   0.0100000         0.5    2    1    2 4.4e-011 4.8e-016
   2        0.44   0.1000000         0.5    3    2    4 6.2e-011   5e-016
   3        0.16   0.4418773         0.3    4    3    6 4.6e-011 4.7e-016
   4      0.0056   1.0000000        0.32    5    4    8 1.6e-011 3.8e-013
   5    8.5e-005   1.0000000       0.013    6    5   10 2.2e-011 2.8e-013
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.56 GB
                                 Virtual memory: 1.59 GB
```

3.3.1.3.1 Fully Coupled 1 (fc1)

General

Name	Value
Linear solver	Direct 1

3.3.1.3.2 Direct 1 (d1)

General

Name	Value

Name	Value
Solver	PARDISO

3.3.2 Parametric 2

3.3.2.1 Store Solution 3 (su1)

General

Name	Value
Solution	Store Solution 3

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:45:37.
Nonlinear solver
Number of degrees of freedom solved for: 160250.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.52   0.0100000        0.52    2    1    2 1.3e-011 4.9e-016
   2        0.44   0.1000000         0.5    3    2    4   4e-011 4.9e-016
   3        0.23   0.3204241        0.35    4    3    6 2.1e-011 4.5e-016
   4       0.013   1.0000000        0.36    5    4    8 3.2e-011 8.1e-014
   5     0.00044   1.0000000        0.02    6    5   10 4.5e-011 4.4e-014
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.3 GB
                                 Virtual memory: 1.35 GB
```

3.3.2.2 Store Solution 4 (su2)

General

Name	Value
Solution	Store Solution 4

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:45:50.
Nonlinear solver
Number of degrees of freedom solved for: 160075.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.52   0.0100000        0.52    2    1    2 3.4e-011 5.4e-016
   2        0.44   0.1000000         0.5    3    2    4 3.6e-011   5e-016
   3        0.23   0.3222786        0.35    4    3    6 2.9e-011 4.4e-016
   4       0.013   1.0000000        0.36    5    4    8 2.2e-011 1.1e-013
   5     0.00045   1.0000000       0.019    6    5   10 5.2e-011 4.6e-014
Stationary Solver 1 in Solver 1: Solution time: 13 s
                                 Physical memory: 1.29 GB
                                 Virtual memory: 1.35 GB
```

3.3.2.3 Store Solution 5 (su3)

General

Name	Value
Solution	Store Solution 5

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:46:04.
Nonlinear solver
Number of degrees of freedom solved for: 171715.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.15
Concentration (mod1.cDMA): 0.029
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.029
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.52   0.0100000        0.52    2    1    2 2.4e-012 5.1e-016
   2        0.44   0.1000000         0.5    3    2    4 3.4e-011   5e-016
   3        0.23   0.3230324        0.34    4    3    6 3.9e-011 4.7e-016
   4       0.013   1.0000000        0.36    5    4    8 2.2e-011 1.5e-013
   5     0.00049   1.0000000       0.019    6    5   10 3.7e-011 6.6e-014
Stationary Solver 1 in Solver 1: Solution time: 15 s
                                 Physical memory: 1.42 GB
                                 Virtual memory: 1.48 GB
```

3.3.2.4 Store Solution 6 (su4)

General

Name	Value
Solution	Store Solution 6

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:46:20.
Nonlinear solver
Number of degrees of freedom solved for: 171045.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.15
Concentration (mod1.cDMA): 0.029
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.029
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.51   0.0100000        0.52    2    1    2   1e-011 4.9e-016
   2        0.44   0.1000000         0.5    3    2    4 2.7e-011 5.1e-016
   3        0.23   0.3258443        0.34    4    3    6 3.9e-011 4.8e-016
   4       0.013   1.0000000        0.35    5    4    8   2e-011 1.3e-013
   5      0.0005   1.0000000       0.018    6    5   10 5.5e-011 6.7e-014
Stationary Solver 1 in Solver 1: Solution time: 14 s
                                 Physical memory: 1.44 GB
                                 Virtual memory: 1.5 GB
```

3.3.2.5 Store Solution 7 (su5)

General

Name	Value
Solution	Store Solution 7

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:46:35.
Nonlinear solver
Number of degrees of freedom solved for: 159860.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.52   0.0100000        0.52    2    1    2 1.3e-011 5.3e-016
   2        0.44   0.1000000        0.51    3    2    4 2.2e-011   5e-016
   3        0.23   0.3304127        0.34    4    3    6 2.6e-011 4.3e-016
   4       0.012   1.0000000        0.35    5    4    8 2.6e-011 9.1e-014
   5     0.00048   1.0000000       0.017    6    5   10 4.3e-011 4.8e-014
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.46 GB
                                 Virtual memory: 1.52 GB
```

3.3.2.6 Store Solution 8 (su6)

General

Name	Value

Name	Value
Solution	Store Solution 8

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:46:48.
Nonlinear solver
Number of degrees of freedom solved for: 170495.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.15
Concentration (mod1.cDMA): 0.029
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.029
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.51   0.0100000        0.52    2    1    2   4e-012   5e-016
   2        0.44   0.1000000         0.5    3    2    4 2.2e-011 5.2e-016
   3        0.22   0.3336079        0.34    4    3    6   4e-011 5.1e-016
   4       0.012   1.0000000        0.35    5    4    8 2.4e-011 1.9e-013
   5     0.00049   1.0000000       0.016    6    5   10 4.7e-011 6.8e-014
Stationary Solver 1 in Solver 1: Solution time: 13 s
                                 Physical memory: 1.5 GB
                                 Virtual memory: 1.56 GB
```

3.3.2.7 Store Solution 9 (su7)

General

Name	Value
Solution	Store Solution 9

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:47:02.
Nonlinear solver
Number of degrees of freedom solved for: 159230.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.52   0.0100000        0.52    2    1    2   3e-011 5.4e-016
   2        0.44   0.1000000        0.51    3    2    4 3.8e-011 4.7e-016
   3        0.22   0.3398678        0.34    4    3    6 2.6e-011 4.3e-016
   4       0.012   1.0000000        0.36    5    4    8 3.5e-011   1e-013
   5     0.00047   1.0000000       0.015    6    5   10 4.7e-011 5.9e-014
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.51 GB
                                 Virtual memory: 1.56 GB
```

3.3.2.8 Store Solution 10 (su8)

General

Name	Value
Solution	Store Solution 10

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:47:15.
Nonlinear solver
Number of degrees of freedom solved for: 158840.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.52   0.0100000        0.52    2    1    2 1.6e-011   5e-016
   2        0.44   0.1000000        0.51    3    2    4 2.1e-011 4.9e-016
   3        0.21   0.3468319        0.33    4    3    6 3.1e-011 4.6e-016
   4       0.011   1.0000000        0.35    5    4    8 1.5e-011 1.2e-013
   5     0.00045   1.0000000       0.015    6    5   10 4.5e-011 6.7e-014
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.52 GB
                                 Virtual memory: 1.57 GB
```

3.3.2.9 Store Solution 11 (su9)

General

Name	Value
Solution	Store Solution 11

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:47:28.
Nonlinear solver
Number of degrees of freedom solved for: 170390.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.15
Concentration (mod1.cDMA): 0.029
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.029
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1         0.5   0.0100000        0.51    2    1    2   4e-012   5e-016
   2        0.44   0.1000000         0.5    3    2    4 5.2e-012   5e-016
   3        0.21   0.3542024        0.32    4    3    6 2.4e-011 4.9e-016
   4       0.011   1.0000000        0.35    5    4    8 2.4e-011 1.7e-013
   5     0.00041   1.0000000       0.015    6    5   10 1.7e-011 9.1e-014
Stationary Solver 1 in Solver 1: Solution time: 13 s
                                 Physical memory: 1.55 GB
                                 Virtual memory: 1.6 GB
```

3.3.2.10 Store Solution 12 (su10)

General

Name	Value
Solution	Store Solution 12

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:47:42.
Nonlinear solver
Number of degrees of freedom solved for: 158725.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.51   0.0100000        0.52    2    1    2 3.3e-011 5.1e-016
   2        0.44   0.1000000        0.51    3    2    4 5.1e-011 4.9e-016
   3         0.2   0.3673017        0.32    4    3    6 3.2e-011 4.4e-016
   4        0.01   1.0000000        0.35    5    4    8 2.2e-011 1.5e-013
   5     0.00034   1.0000000       0.015    6    5   10 2.2e-011 8.5e-014
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.54 GB
                                 Virtual memory: 1.59 GB
```

3.3.2.11 Store Solution 13 (su11)

General

Name	Value

Name	Value
Solution	Store Solution 13

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:47:56.
Nonlinear solver
Number of degrees of freedom solved for: 157990.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.51   0.0100000        0.52    2    1    2 5.9e-011 4.8e-016
   2        0.45   0.1000000        0.51    3    2    4 8.4e-011 5.2e-016
   3        0.19   0.3845094        0.32    4    3    6 2.2e-011 4.7e-016
   4      0.0092   1.0000000        0.34    5    4    8 2.4e-011 1.8e-013
   5     0.00026   1.0000000       0.015    6    5   10 3.1e-011 1.2e-013
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.55 GB
                                 Virtual memory: 1.58 GB
```

3.3.2.12 Store Solution 14 (su12)

General

Name	Value
Solution	Store Solution 14

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:48:09.
Nonlinear solver
Number of degrees of freedom solved for: 157495.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1        0.51   0.0100000        0.51    2    1    2 1.1e-011 5.5e-016
   2        0.44   0.1000000        0.51    3    2    4 4.6e-011 5.1e-016
   3        0.18   0.4075402        0.31    4    3    6 4.7e-011 4.8e-016
   4      0.0078   1.0000000        0.33    5    4    8 2.5e-011 2.4e-013
   5     0.00017   1.0000000       0.014    6    5   10 2.2e-011 1.6e-013
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.56 GB
                                 Virtual memory: 1.59 GB
```

3.3.2.13 Store Solution 15 (su13)

General

Name	Value
Solution	Store Solution 15

Log

```
Stationary Solver 1 in Solver 1 started at 14-十月-2014 23:48:22.
Nonlinear solver
Number of degrees of freedom solved for: 155915.
Nonsymmetric matrix found.
Scales for dependent variables:
Concentration (mod1.cTMB2): 0.16
Concentration (mod1.cDMA): 0.03
Concentration (mod1.cTMB1): 0.4
Concentration (mod1.cTMB): 0.011
Concentration (mod1.cDMARadic): 0.03
Iter      ErrEst     Damping    Stepsize #Res #Jac #Sol   LinErr   LinRes
   1         0.5   0.0100000         0.5    2    1    2 4.4e-011 4.8e-016
   2        0.44   0.1000000         0.5    3    2    4 6.2e-011   5e-016
   3        0.16   0.4418773         0.3    4    3    6 4.6e-011 4.7e-016
   4      0.0056   1.0000000        0.32    5    4    8 1.6e-011 3.8e-013
   5    8.5e-005   1.0000000       0.013    6    5   10 2.2e-011 2.8e-013
Stationary Solver 1 in Solver 1: Solution time: 12 s
                                 Physical memory: 1.56 GB
                                 Virtual memory: 1.59 GB
```

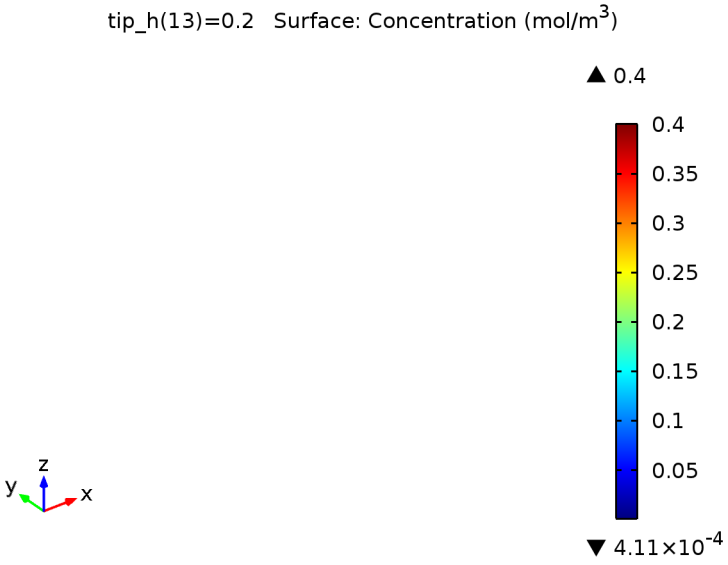
4 Results

4.1 Data Sets

4.1.1 Solution 1

Solution

Name	Value
Solution	Solver 1
Component	Save Point Geometry 1

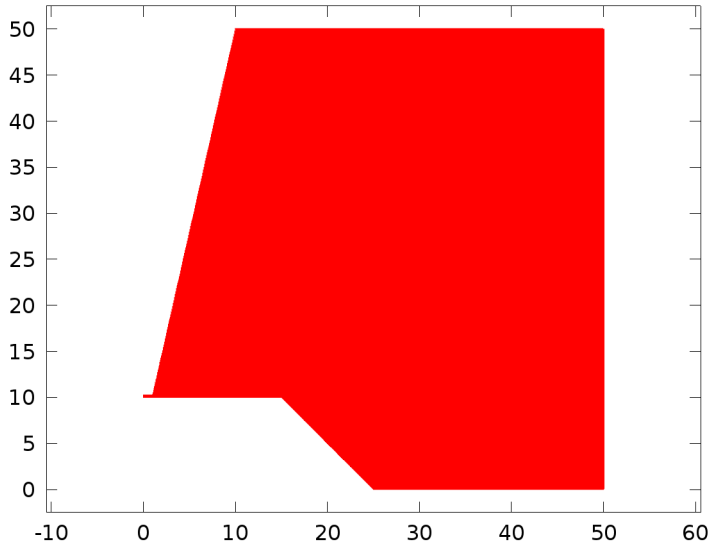


Data set: Solution 1

4.1.2 Solution 2

Solution

Name	Value
Solution	Parametric 2
Component	Save Point Geometry 1



Data set: Solution 2

4.1.3 Revolution 2D 1

Data

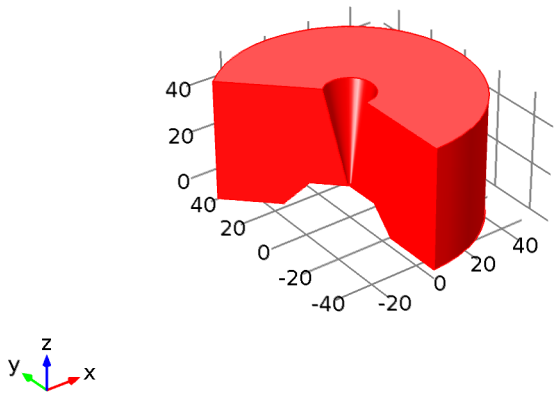
Name	Value
Data set	Solution 2

Axis data

Name	Value
Axis entry method	Two points
Points	{{0, 0}, {0, 1}}

Revolution layers

Name	Value
Start angle	-90
Revolution angle	225



Data set: Revolution 2D 1

4.2 Derived Values

4.2.1 Line Integration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Data

Name	Value
Data set	Solution 2

Expression

Name	Value
Expression	chds.tfluxMag_cTMB2*F
Unit	A
Description	isub TMB2

Integration settings

Name	Value
Integration order	On

4.3 Tables

4.3.1 Table 1

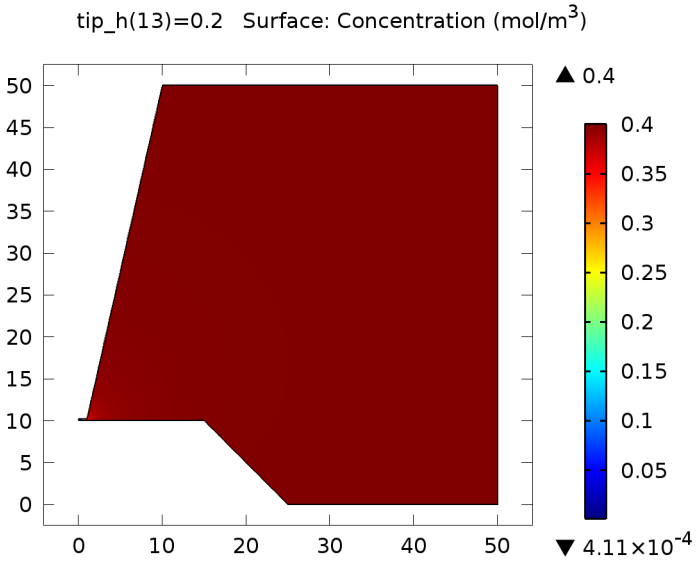
Line Integration 1 (chds.tfluxMag_cDMA*F)

Table 1

tip_h	itip DMA (A)	itip TMB (A)	itip TMB1 (A)	isub DMA Radical (A)	isub TMB (A)	isub TMB1 (A)	isub TMB2 (A)
1.4	1.87968e-10	8.08093e-11	1.35882e-12	3.991e-11	6.00756e-11	1.75749e-11	8.00358e-11
1.3	1.87552e-10	7.96011e-11	1.53012e-12	4.3179e-11	5.89938e-11	1.83541e-11	8.19267e-11
1.2	1.87003e-10	7.81097e-11	1.73146e-12	4.68325e-11	5.75416e-11	1.91269e-11	8.37864e-11
1.1	1.86468e-10	7.63888e-11	1.97502e-12	5.11797e-11	5.58466e-11	1.99112e-11	8.56246e-11
1	1.8633e-10	7.44052e-11	2.27226e-12	5.63089e-11	5.37855e-11	2.06703e-11	8.73929e-11
0.9	1.87191e-10	7.20312e-11	2.63146e-12	6.2272e-11	5.11587e-11	2.13199e-11	8.89136e-11
0.8	1.86184e-10	6.91688e-11	3.05768e-12	6.9682e-11	4.81069e-11	2.18401e-11	9.0139e-11
0.7	1.86927e-10	6.57802e-11	3.57304e-12	7.87725e-11	4.43869e-11	2.20815e-11	9.07692e-11
0.6	1.89063e-10	6.18087e-11	4.18658e-12	9.02909e-11	3.99408e-11	2.19e-11	9.04451e-11
0.5	1.92563e-10	5.62744e-11	4.83367e-12	1.05919e-10	3.48342e-11	2.11217e-11	8.87341e-11
0.4	2.00768e-10	4.96144e-11	5.47873e-12	1.27957e-10	2.89094e-11	1.94368e-11	8.46493e-11
0.3	2.19267e-10	4.13778e-11	5.94824e-12	1.62799e-10	2.22551e-11	1.6584e-11	7.69035e-11
0.2	2.65164e-10	3.09473e-11	5.8238e-12	2.28538e-10	1.49647e-11	1.2373e-11	6.34201e-11

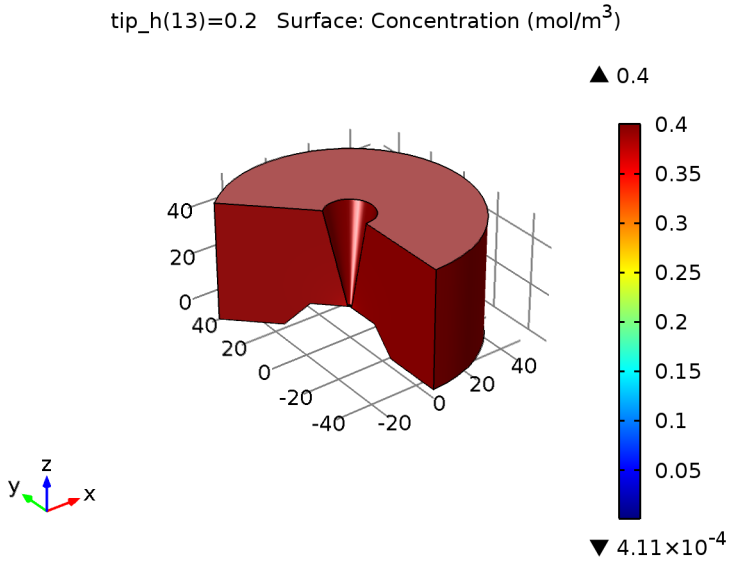
4.4 Plot Groups

4.4.1 Concentration (chds)



tip_h(13)=0.2 Surface: Concentration (mol/m^3)

4.4.2 Concentration, 3D (chds)



tip_h(13)=0.2 Surface: Concentration (mol/m^3)