

MOB version 3

Report date	Aug 4, 2015 6:43:53 PM
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1 Global Definitions

Date	Aug 4, 2015 12:25:27 PM
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Global settings

Name	MOB version LM.mph
Path	C:\Users\lmurtoma\AppData\Local\Microsoft\Windows\Temporary Internet Files\Content.IE5\O63EV1ZP\MOB version_LM.mph
COMSOL version	COMSOL 5.1 (Build: 180)
Unit system	SI

Used products

COMSOL Multiphysics
Batteries & Fuel Cells Module

1.1 Parameters 1

Parameters

Name	Expression	Value	Description
L	1.38e-3[m]	0.00138 m	length of the microchamber
d	50e-6[m]	5E-5 m	leagth of the bacteria
Km	9.44e-6[mole/l]	0.00944 mol/m ³	Kmax
Vmax	1.48e-3[mole/l/s]	1.48 mol/(m ³ ·s)	Vmax
Dp	3.98e-6[m ² /s]	3.98E-6 m ² /s	Diffusion coefficient of product
Ds	1.96e-06[m ² /s]	1.96E-6 m ² /s	Diffusion coefficient of substrate
S	10e-3[mole/l]	10 mol/m ³	substrate concentration

1.2 Variables

1.2.1 Variables 1

2 Component 1

Date	Jul 14, 2015 10:09:31 AM
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Component settings

Unit system	SI
Geometry shape order	automatic

2.1 Definitions

2.1.1 Variables

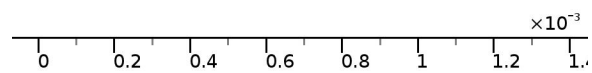
Variables 2

Selection

Geometric entity level	Entire model
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Name	Expression	Unit	Description
Rsp	$V_{max} \cdot c^2 / (K_m + c^2)$	$\text{mol}/(\text{m}^3 \cdot \text{s})$	

2.2 Geometry 1



Geometry 1

Units

Length unit	m
Angular unit	deg

Geometry statistics

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

2.2.1 Interval 1 (I1)

Interval

Description	Value
Number of intervals	One
Left endpoint	0
Right endpoint	L

2.2.2 Point 1 (pt1)

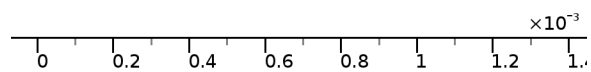
Point

Description	Value
Point coordinate	d

2.3 Transport of Diluted Species

Used products

COMSOL Multiphysics
Batteries & Fuel Cells Module



Transport of Diluted Species

Selection

Geometric entity level	Domain
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Selection	Domains 1-2
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Equations

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

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

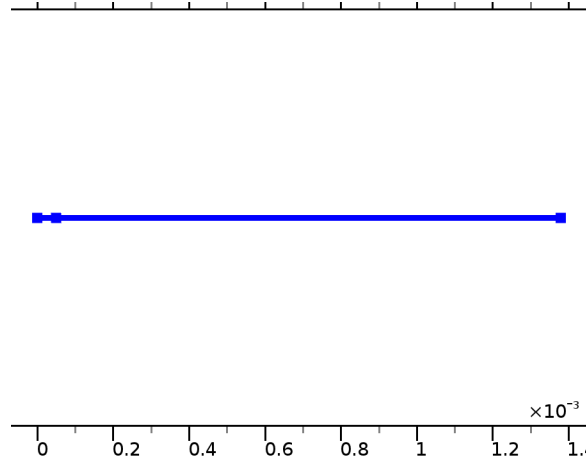
Settings

Description	Value
Concentration	Linear
Compute boundary fluxes	On
Apply smoothing to boundary fluxes	On
Value type when using splitting of complex variables	Real
Streamline diffusion	On
Crosswind diffusion	On
Crosswind diffusion type for free flow	Do Carmo and Galeão
Equation residual	Approximate residual
Convective term	Non - conservative form
Convection	Off
Migration in electric field	Off
Adsorption in porous media	Off
Dispersion in porous media	Off
Volatilization in partially saturated porous media	Off

Variables

Name	Expression	Unit	Description	Selection
domflux.c1x	chds.dflux_c1x	mol/(m ² *s)	Domain flux, x component	Domains 1-2
domflux.c2x	chds.dflux_c2x	mol/(m ² *s)	Domain flux, x component	Domains 1-2
chds.R_c1	0	mol/(m ³ *s)	Total rate expression	Domains 1-2
chds.R_c2	0	mol/(m ³ *s)	Total rate expression	Domains 1-2

2.3.1 Convection and Diffusion 1



Convection and Diffusion 1

Selection

Geometric entity level	Domain
Selection	Domains 1–2

Equations

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

.....

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

Settings

Description	Value
Material	None
Diffusion coefficient	{{Dp, 0, 0}, {0, Dp, 0}, {0, 0, Dp}}
Diffusion coefficient	User defined
Diffusion coefficient	User defined
Diffusion coefficient	{{Ds, 0, 0}, {0, Ds, 0}, {0, 0, Ds}}

Used products

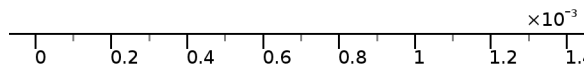
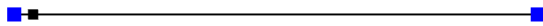
COMSOL Multiphysics

Variables

Name	Expression	Unit	Description	Selection
chds.D_c1xx	Dp	m ² /s	Diffusion coefficient, xx component	Domains 1–2

Name	Expression	Unit	Description	Selection
chds.D_c2yy	Ds	m ² /s	Diffusion coefficient, yy component	Domains 1-2

2.3.2 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 1, 3

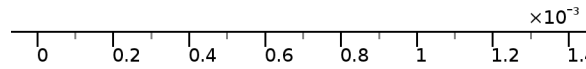
Equations

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

Used products

COMSOL Multiphysics

2.3.3 Initial Values 1



Initial Values 1

Selection

Geometric entity level	Domain
Selection	Domains 1–2

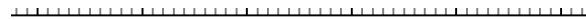
Settings

Description	Value
Concentration	{0, S}

Used products

COMSOL Multiphysics

2.3.4 Reactions 1



Reactions 1

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

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

Settings

Description	Value
Total rate expression	Rsp
Total rate expression	User defined
Reacting volume	Total volume
Total rate expression	User defined
Total rate expression	-Rsp

Used products

COMSOL Multiphysics

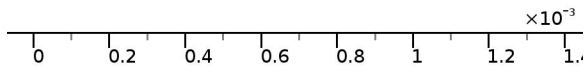
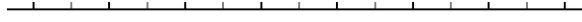
Variables

Name	Expression	Unit	Description	Selection
chds.R_c1	chds.reac1.R_c1	mol/(m ³ *s)	Total rate expression	Domain 1
chds.R_c2	chds.reac1.R_c2	mol/(m ³ *s)	Total rate expression	Domain 1

2.4 Mesh 1

Mesh statistics

Description	Value
Minimum element quality	1.0
Average element quality	1.0
Edge elements	200
Vertex elements	3



Mesh 1

2.4.1 Size (size)

Settings

Description	Value
Maximum element size	2.76E-5
Minimum element size	1.03E-7
Curvature factor	0.25
Maximum element growth rate	1.2
Predefined size	Extra fine

2.4.2 Edge 1 (edg1)

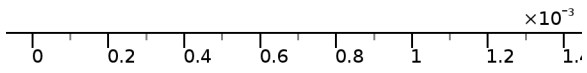
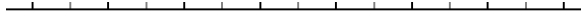
Selection

Geometric entity level	Remaining
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Distribution 1 (dis1)

Selection

Geometric entity level	Domain
Selection	Domains 1-2



Distribution 1

Settings

Description	Value
Distribution properties	Predefined distribution type
Number of elements	100
Element ratio	10

3 Study 1

Computation information

Computation time	2 s
CPU	Intel(R) Core(TM) i5-3437U CPU @ 1.90GHz, 2 cores
Operating system	Windows 7

3.1 Time Dependent

Study settings

Description	Value
Include geometric nonlinearity	Off

Times	Unit
$0,10^{\{\text{range}(-6,0.2,0)\}}$	s

Physics and variables selection

Physics interface	Discretization
Transport of Diluted Species (chds)	physics

Mesh selection

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.2 Solver Configurations

3.2.1 Solver 1

Compile Equations: Time Dependent (st1)

Study and step

Description	Value
Use study	Study 1
Use study step	Time Dependent

Dependent Variables 1 (v1)

General

Description	Value
Defined by study step	Time Dependent

Initial values of variables solved for

Description	Value
Solution	Zero

Values of variables not solved for

Description	Value
Solution	Zero

Concentration (comp1.c1) (comp1_c1)

General

Description	Value
Field components	comp1.c1

Concentration (comp1.c2) (comp1_c2)

General

Description	Value
Field components	comp1.c2

Time-Dependent Solver 1 (t1)

General

Description	Value
Defined by study step	Time Dependent
Time	{0, 1.0E-6, 1.584893192461114E-6, 2.5118864315095823E-6, 3.981071705534969E-6, 6.30957344480193E-6, 1.0E-5, 1.584893192461114E-5, 2.5118864315095822E-5, 3.9810717055349695E-5, 6.309573444801929E-5, 1.0E-4, 1.5848931924611142E-4, 2.511886431509582E-4, 3.9810717055349735E-4, 6.309573444801936E-4, 0.001, 0.001584893192461114, 0.002511886431509582, 0.003981071705534973, 0.006309573444801936, 0.01, 0.01584893192461114, 0.025118864315095822, 0.039810717055349776, 0.06309573444801943, 0.1, 0.15848931924611143, 0.25118864315095824, 0.39810717055349776, 0.6309573444801942, 1}

Absolute tolerance

Description	Value
Tolerance	0.0010

Time stepping

Description	Value
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Description	Value
Initial step	0.0010
Maximum BDF order	2
Fraction of initial step for Backward Euler	0.0010

Log

Fully Coupled 1 (fc1)

General

Description	Value
Linear solver	Direct 1

Method and termination

Description	Value
Damping factor	0.9
Jacobian update	Once per time step
Maximum number of iterations	8

Direct 1 (d1)

General

Description	Value
Solver	PARDISO

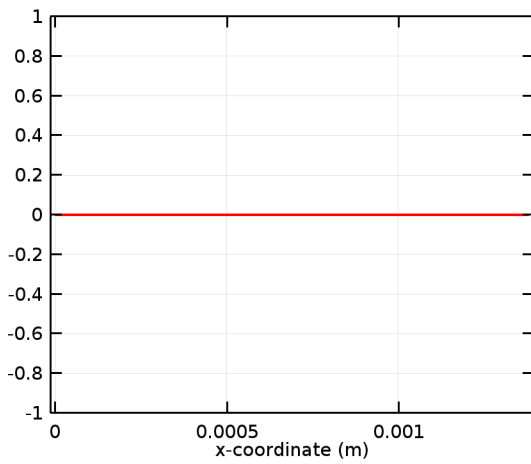
4 Results

4.1 Data Sets

4.1.1 Solution 1

Solution

Description	Value
Solution	Solver 1
Component	Save Point Geometry 1

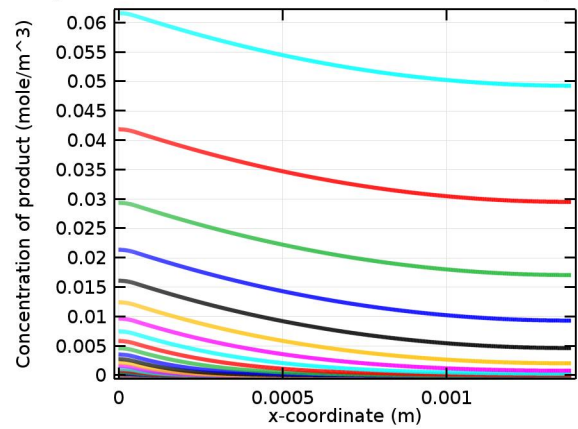


Data set: Solution 1

4.2 Plot Groups

4.2.1 Product

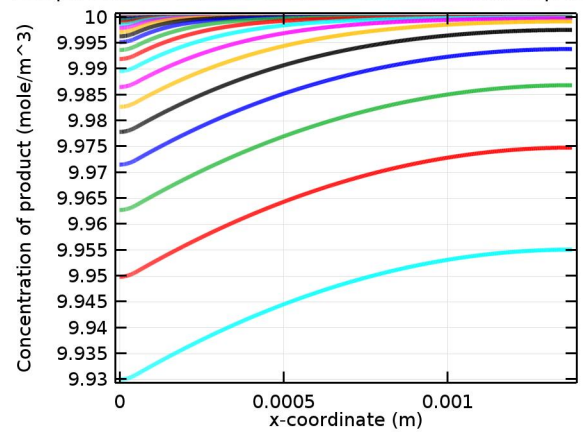
Graph: Distance from the electrode Vs Concentration of prod



Line Graph: Distance from the electrode Vs Concentration of product

4.2.2 Substrate

Graph: Distance from the electrode Vs Concentration of prod



Line Graph: Distance from the electrode Vs Concentration of product