COMSOL MODEL REPORT

Contents

1 Global Definitions

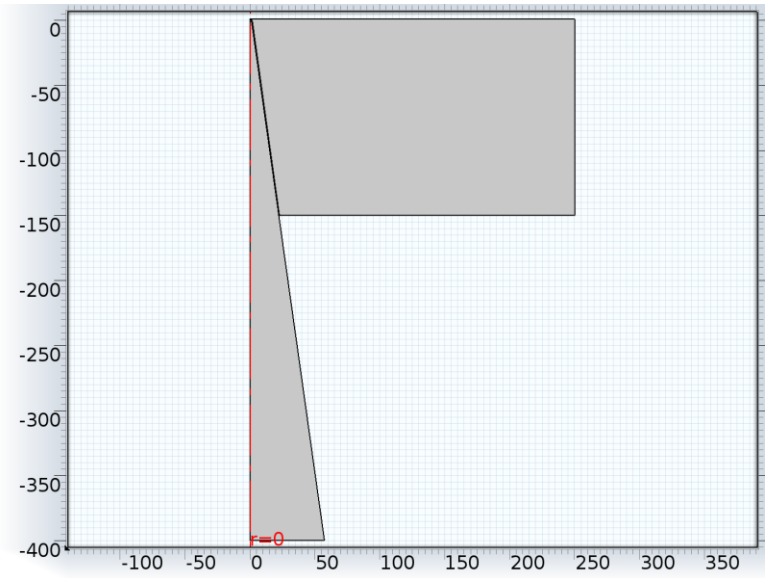
1.1 Parameters 1

Parameters

Name	Expression	Description
RG	1.5	RG of glass
DD	400	limit inside pipette
D	150	limit behind pipette
L	1	distance between pipette and substrate
RS	250	limit of substrate
tan	0.1405	tangent of pipette angle
DR	1	diffusion coefficient of reduced form
DO	1	diffusion coefficient of oxidized form
gamma	1.41	ratio of D in two phases
K	2	partition coefficient
C	1	initial concentration of R
M	10000	stiff-spring velocity
EXPN	10000	steady state

2 Model 1 (mod1)

2.1 Geometry 1



2.1.1 Bézier Polygon 2 (b2)

Polygon segments

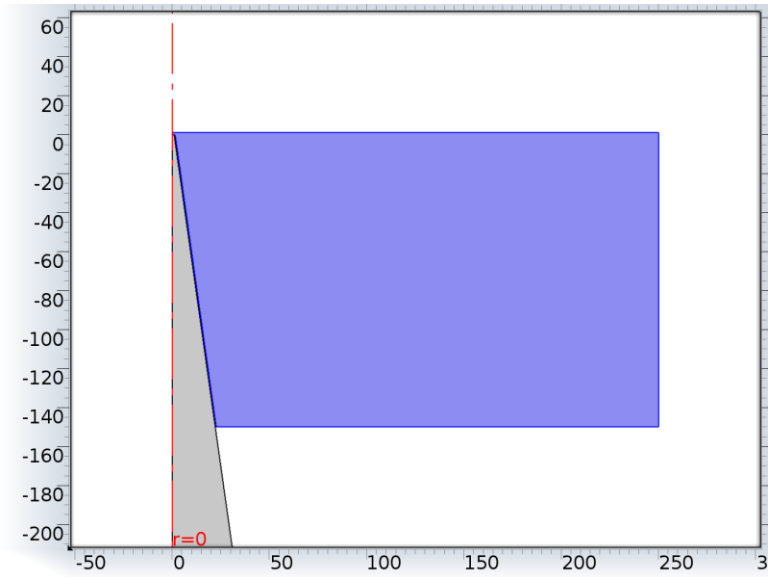
Name	Value
Control points	{{0, 1, 1 + DD*tan, 0, 0}, {0, 0, DD, DD, 0}}
Degree	{1, 1, 1, 1}
Weights	{1, 1, 1, 1, 1, 1, 1, 1}
Valid vertex coordinates	{{0, 0}, {1, 0}, {57.2, 400}, {0, 400}, {0, 0}}

2.1.2 Bézier Polygon 1 (b1)

Polygon segments

Name	Value
Control points	{{0, 1, RG, RG + D*tan, RS, RS, 40, 0, 0}, {0, 0, 0, D, D, L, L, L, 0}}
Degree	{1, 1, 1, 1, 1, 1, 1, 1}
Weights	{1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1}
Valid vertex coordinates	{{0, 0}, {1, 0}, {1.5, 0}, {22.575000000000003, 150}, {250, 150}, {250, 1}, {40, 1}, {0, 1}, {0, 0}}

2.2 Transport of Diluted Species (chds)



Transport of Diluted Species

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

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

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

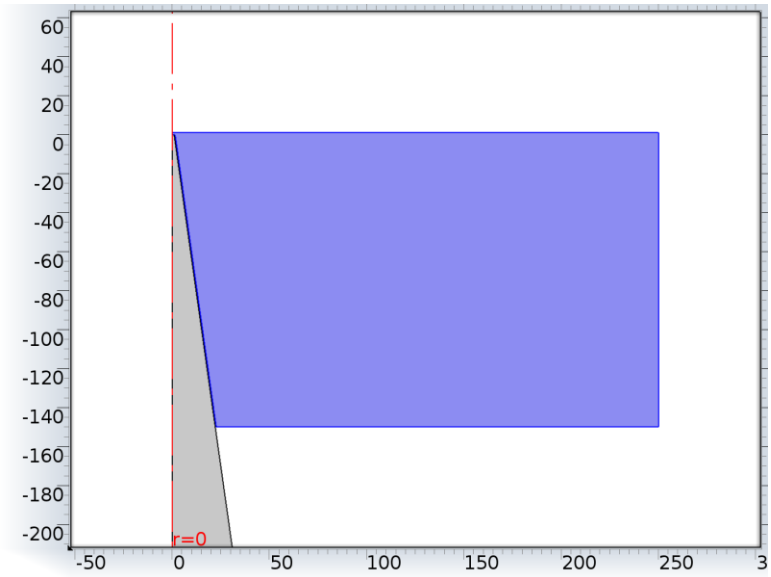
Settings

Description	Value
Convection	0
Show equation assuming	std1/stat

Used products

COMSOL Multiphysics
Chemical Reaction Engineering Module

2.2.1 Diffusion



Diffusion

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

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

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

Settings

Settings

Description	Value
Diffusion coefficient	{{DR, 0, 0}, {0, DR, 0}, {0, 0, DR}}
Diffusion coefficient	{{DO, 0, 0}, {0, DO, 0}, {0, 0, DO}}

Used products

COMSOL Multiphysics

Variables

Shape functions

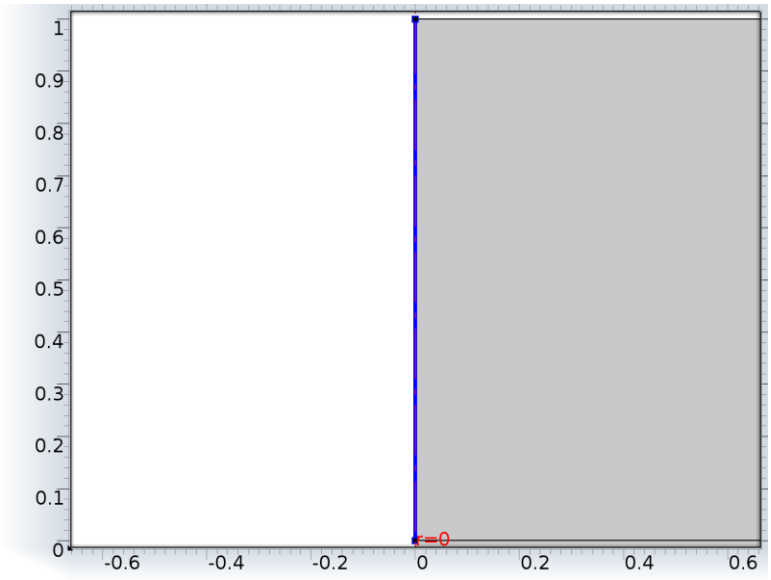
Name	Shape function	Description	Shape frame	Selection
cR1	Lagrange (Linear)	Concentration	Material	Domain 2

Name	Shape function	Description	Shape frame	Selection
cO1	Lagrange (Linear)	Concentration	Material	Domain 2

Weak expressions

Weak expression	Integration frame	Selection
2*(cR1t*test(cR1) - (chds.Drr_cR1*cR1r + chds.Drz_cR1*cR1z)*test(cR1r) - (chds.Dzr_cR1*cR1r + chds.Dzz_cR1*cR1z)*test(cR1z))*pi*r	Material	Domain 2
2*(cO1t*test(cO1) - (chds.Drr_cO1*cO1r + chds.Drz_cO1*cO1z)*test(cO1r) - (chds.Dzr_cO1*cO1r + chds.Dzz_cO1*cO1z)*test(cO1z))*pi*r	Material	Domain 2
2*chds.streamline*pi*r	Material	Domain 2
2*chds.crosswind*pi*r	Material	Domain 2

2.2.2 Axial Symmetry 1



Axial Symmetry 1

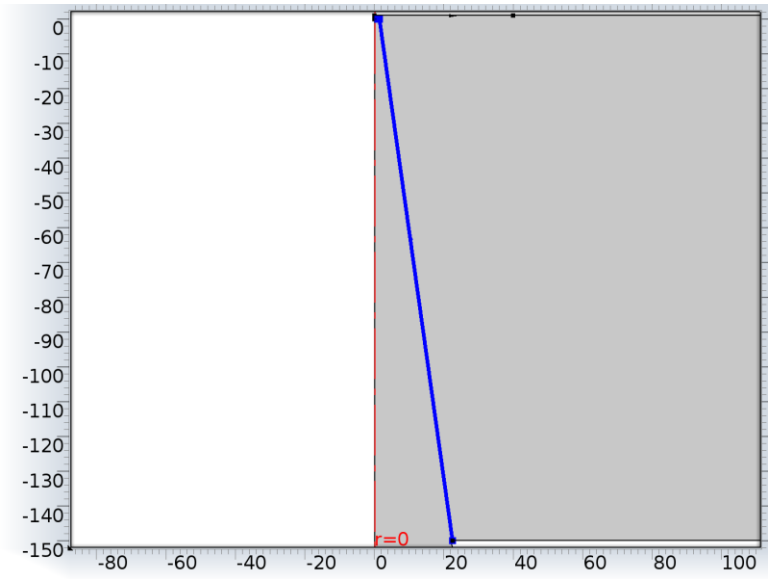
Selection

Geometric entity level	Boundary
Selection	Boundary 3

Used products

COMSOL Multiphysics

2.2.3 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 6, 8

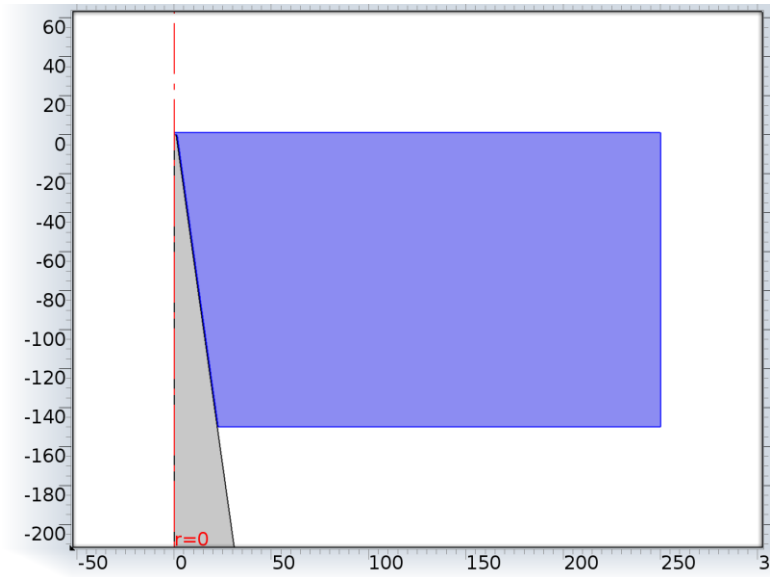
Equations

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

Used products

COMSOL Multiphysics

2.2.4 Initial Values 1



Initial Values 1

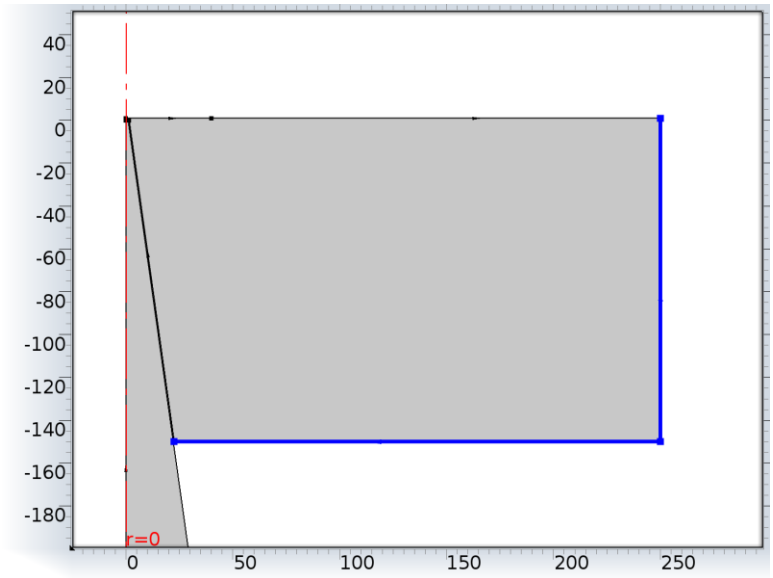
Selection

Geometric entity level	Domain
Selection	Domain 2

Used products

COMSOL Multiphysics

2.2.5 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 9, 11

Equations

$$c_i = c_{0i}$$

Settings

Settings

Description	Value
Species cR1	1
Species cO1	1

Used products

COMSOL Multiphysics

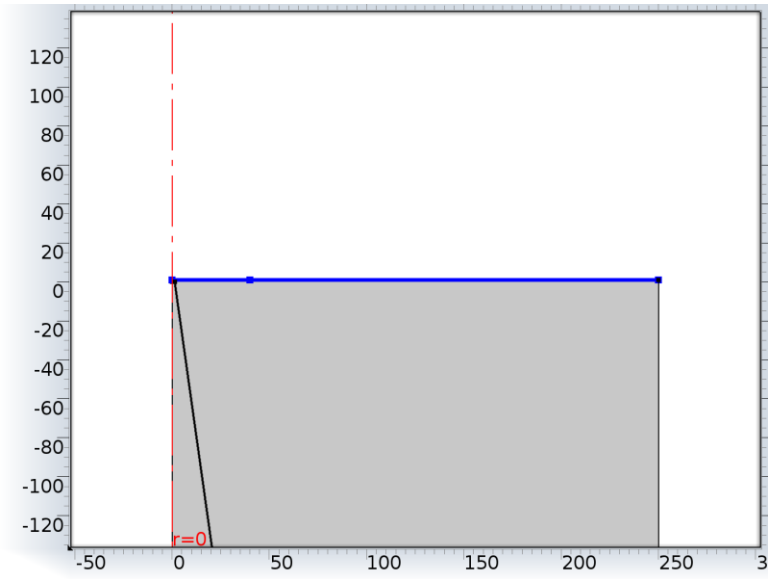
Variables

Name	Expression	Description	Selection
chds.c0_cR1	0	Concentration	Boundaries 9, 11
chds.c0_cO1	0	Concentration	Boundaries 9, 11

Constraints

Constraint	Constraint force	Shape function	Selection
-cR1 + chds.c0_cR1	test(cR1 + chds.c0_cR1)	Lagrange (Linear)	Boundaries 9, 11
-cO1 + chds.c0_cO1	test(cO1 + chds.c0_cO1)	Lagrange (Linear)	Boundaries 9, 11

2.2.6 Flux 1



Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 5, 10

Equations

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

Settings

Settings

Description	Value
Species cR1	1
Species cO1	1
Inward flux	{M*(cO1 - cR1*EXPN), M*(cR1*EXPN - cO1)}

Used products

COMSOL Multiphysics

Variables

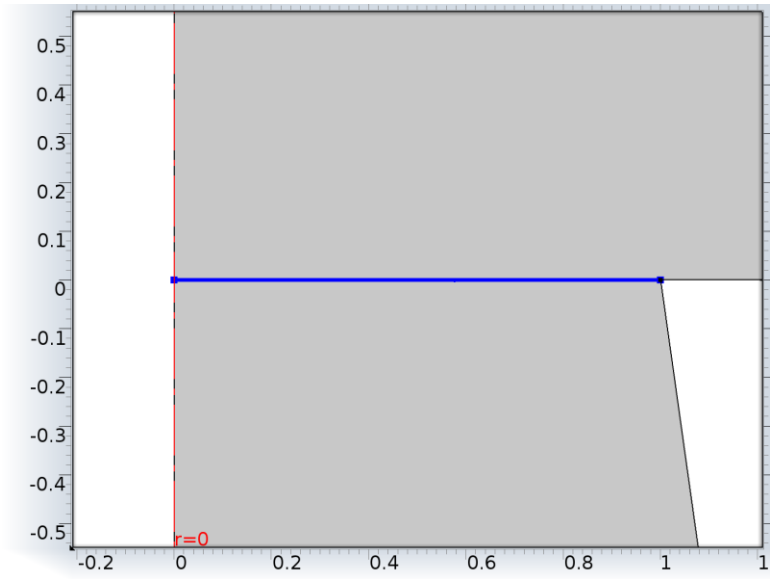
Name	Expression	Description	Selection
chds.cb_cR1	0	Bulk concentration	Boundaries 5, 10
chds.kc_cR1	0	Mass transfer coefficient	Boundaries 5, 10
chds.cb_cO1	0	Bulk concentration	Boundaries 5, 10

Name	Expression	Description	Selection
chds.kc_cO1	0	Mass transfer coefficient	Boundaries 5, 10

Weak expressions

Weak expression	Integration frame	Selection
2*M*(cO1 - cR1*EXPN)*test(cR1)*pi*r	Material	Boundaries 5, 10
2*M*(cR1*EXPN - cO1)*test(cO1)*pi*r	Material	Boundaries 5, 10

2.2.7 Flux 2



Flux 2

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Equations

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

Settings

Settings

Description	Value
Species cR1	1
Species cO1	1
Inward flux	{M*(cR2 - K*cR1), M*(cO2 - cO1*EXPN)}

Used products

COMSOL Multiphysics

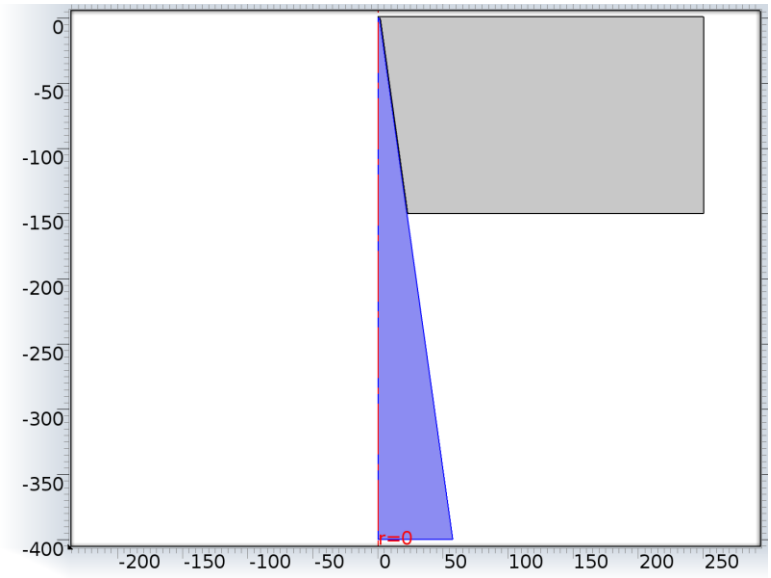
Variables

Name	Expression	Description	Selection
chds.cb_cR1	0	Bulk concentration	Boundary 4
chds.kc_cR1	0	Mass transfer coefficient	Boundary 4
chds.cb_cO1	0	Bulk concentration	Boundary 4
chds.kc_cO1	0	Mass transfer coefficient	Boundary 4

Weak expressions

Weak expression	Integration frame	Selection
2*M*(cR2 - K*cR1)*test(cR1)*pi*r	Material	Boundary 4
2*M*(cO2 - cO1*EXPN)*test(cO1)*pi*r	Material	Boundary 4

2.3 Transport of Diluted Species 2 (chds2)



Transport of Diluted Species 2

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

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

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

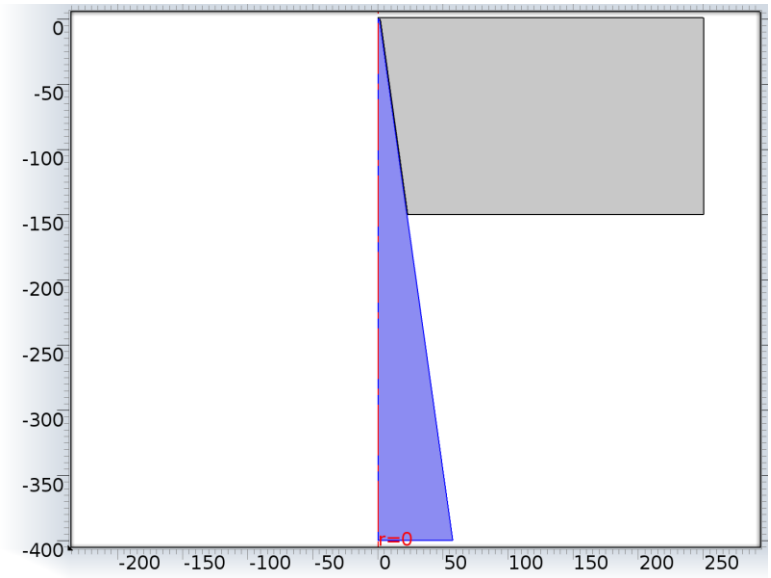
Settings

Description	Value
Convection	0
Show equation assuming	std1/stat

Used products

COMSOL Multiphysics
Chemical Reaction Engineering Module

2.3.1 Diffusion



Diffusion

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

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

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

Settings

Settings

Description	Value
Diffusion coefficient	{{DR*gamma, 0, 0}, {0, DR*gamma, 0}, {0, 0, DR*gamma}}

Description	Value
Diffusion coefficient	{{DO*gamma, 0, 0}, {0, DO*gamma, 0}, {0, 0, DO*gamma}}

Used products

COMSOL Multiphysics

Variables

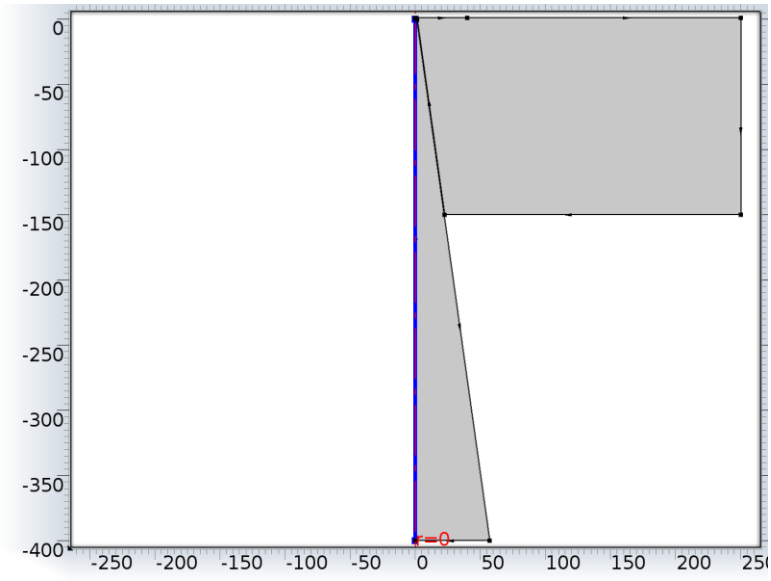
Shape functions

Name	Shape function	Description	Shape frame	Selection
cR2	Lagrange (Linear)	Concentration	Material	Domain 1
cO2	Lagrange (Linear)	Concentration	Material	Domain 1

Weak expressions

Weak expression	Integration frame	Selection
2*(cR2t*test(cR2) - (chds2.Drr_cR2*cR2r + chds2.Drz_cR2*cR2z)*test(cR2r) - (chds2.Dzr_cR2*cR2r + chds2.Dzz_cR2*cR2z)*test(cR2z))*pi*r	Material	Domain 1
2*(cO2t*test(cO2) - (chds2.Drr_cO2*cO2r + chds2.Drz_cO2*cO2z)*test(cO2r) - (chds2.Dzr_cO2*cO2r + chds2.Dzz_cO2*cO2z)*test(cO2z))*pi*r	Material	Domain 1
2*chds2.streamline*pi*r	Material	Domain 1
2*chds2.crosswind*pi*r	Material	Domain 1

2.3.2 Axial Symmetry 1



Axial Symmetry 1

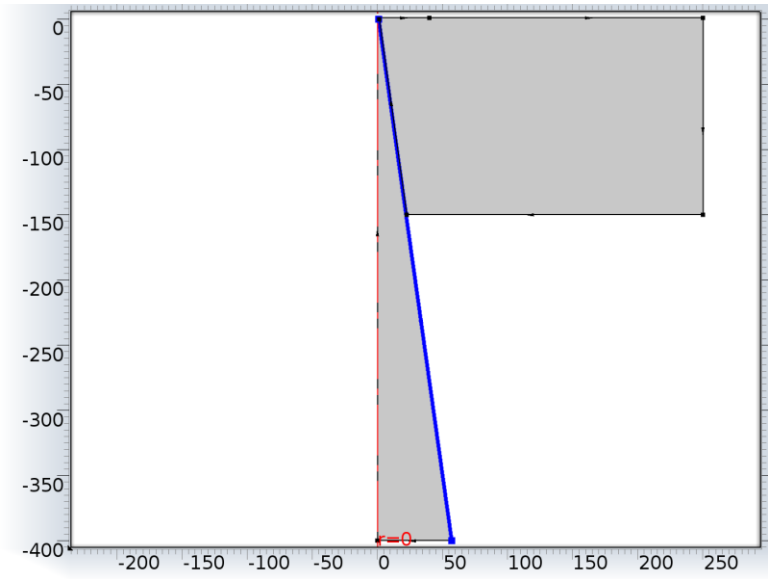
Selection

Geometric entity level	Boundary
Selection	Boundary 1

Used products

COMSOL Multiphysics

2.3.3 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundary 7

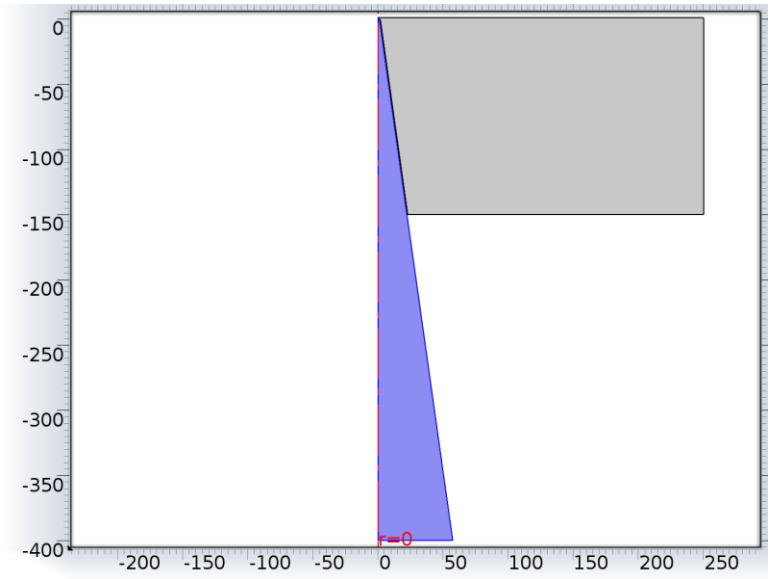
Equations

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

Used products

COMSOL Multiphysics

2.3.4 Initial Values 1



Initial Values 1

Selection

Geometric entity level	Domain
Selection	Domain 1

Settings

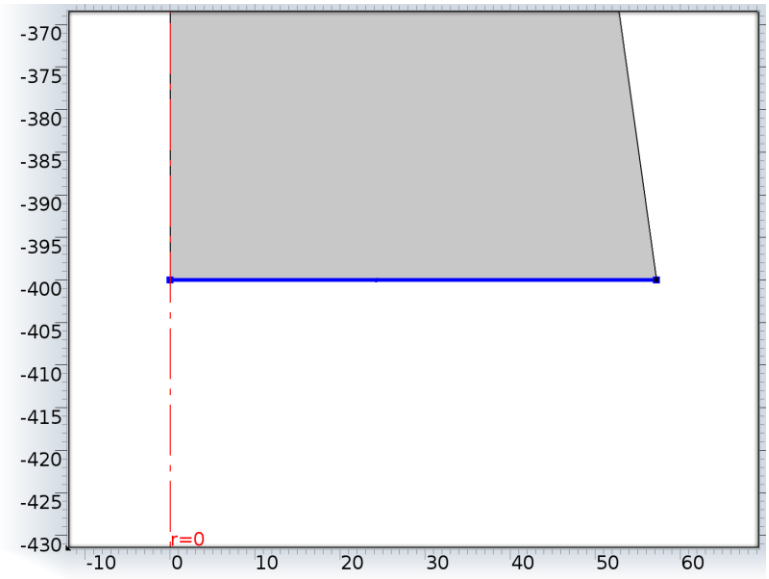
Settings

Description	Value
Concentration	C

Used products

COMSOL Multiphysics

2.3.5 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 2

Equations

$$c_i = c_{0i}$$

Settings

Settings

Description	Value
Concentration	{c, 0}
Species cR2	1
Species cO2	1

Used products

COMSOL Multiphysics

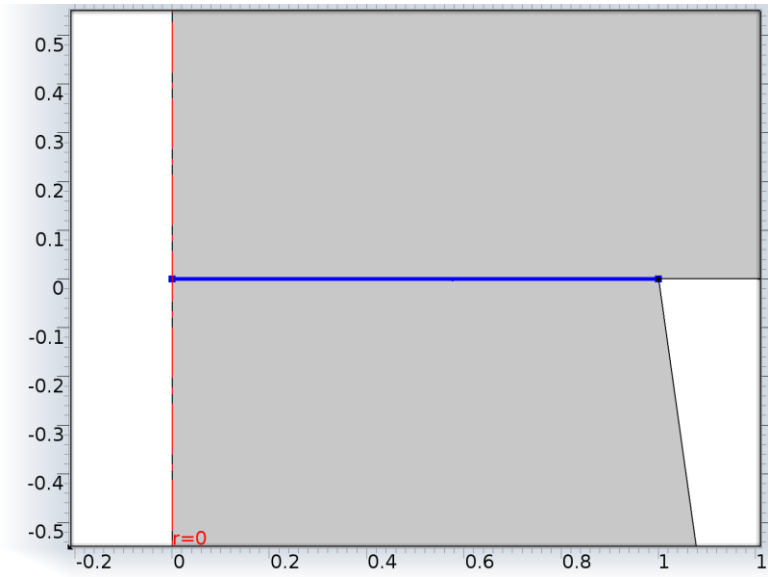
Variables

Name	Expression	Description	Selection
chds2.c0_cR2	C	Concentration	Boundary 2
chds2.c0_cO2	0	Concentration	Boundary 2

Constraints

Constraint	Constraint force	Shape function	Selection
-cR2 + chds2.c0_cR2	test(cR2 + chds2.c0_cR2)	Lagrange (Linear)	Boundary 2
-cO2 + chds2.c0_cO2	test(cO2 + chds2.c0_cO2)	Lagrange (Linear)	Boundary 2

2.3.6 Flux 1



Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Equations

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

Settings

Settings

Description	Value
Species cR2	1
Species cO2	1
Inward flux	{M*(K*cR1 - cR2), M*(cO1*EXPN - cO2)}

Used products

COMSOL Multiphysics

Variables

Name	Expression	Description	Selection
chds2.cb_cR2	0	Bulk concentration	Boundary 4
chds2.kc_cR2	0	Mass transfer coefficient	Boundary 4
chds2.cb_cO2	0	Bulk concentration	Boundary 4
chds2.kc_cO2	0	Mass transfer coefficient	Boundary 4

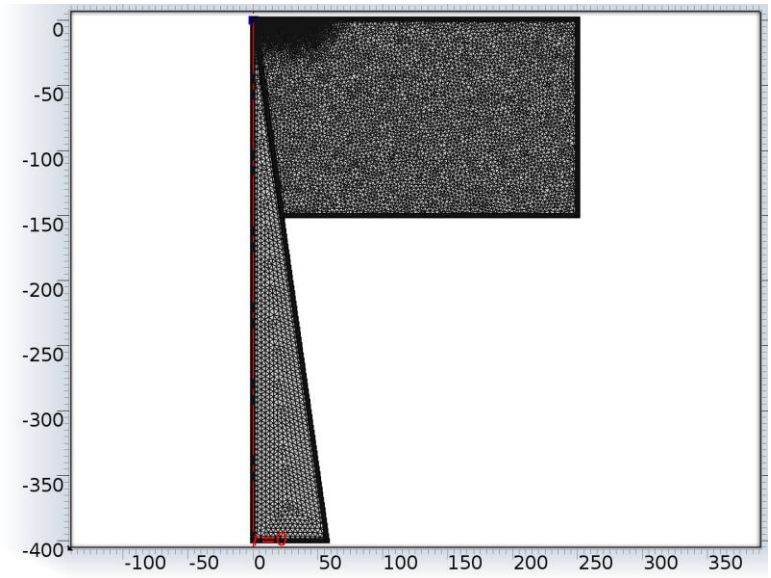
Weak expressions

Weak expression	Integration frame	Selection
2*M*(K*cR1 - cR2)*test(cR2)*pi*r	Material	Boundary 4
2*M*(cO1*EXPN - cO2)*test(cO2)*pi*r	Material	Boundary 4

2.4 Mesh 1

Mesh statistics

Property	Value
Minimum element quality	0.4558
Average element quality	0.9298
Triangular elements	886352
Edge elements	21555
Vertex elements	10



Mesh 1

2.4.1 Size (size)

Settings

Name	Value
Maximum element size	4.01
Minimum element size	0.00802
Resolution of curvature	0.2
Predefined size	Extremely fine

3 Study 1

3.1 Parametric Sweep

Parameter name: L range(1,1,10)

3.2 Solver Configurations

3.2.1 Solver 1

Compile Equations: Stationary (st1)

Study and step

Name	Value
Use study	Study 1
Use study step	Stationary

Stationary Solver 1 (s1)

General

Name	Value
Defined by study step	Stationary

Fully Coupled 1 (fc1)

General

Name	Value
Linear solver	Direct 1

Direct 1 (d1)

General

Name	Value
Solver	PARDISO

3.2.2 Parametric 2

Store Solution 3 (su1)

General

Name	Value
Solution	Store Solution 3

Store Solution 4 (su2)

General

Name	Value
Solution	Store Solution 4

Store Solution 5 (su3)

General

Name	Value
Solution	Store Solution 5

Store Solution 6 (su4)

General

Name	Value
Solution	Store Solution 6

Store Solution 7 (su5)

General

Name	Value
Solution	Store Solution 7

Store Solution 8 (su6)

General

Name	Value
Solution	Store Solution 8

Store Solution 9 (su7)

General

Name	Value
Solution	Store Solution 9

Store Solution 10 (su8)

General

Name	Value
Solution	Store Solution 10

Store Solution 11 (su9)

General

Name	Value
Solution	Store Solution 11

Store Solution 12 (su10)

General

Name	Value
Solution	Store Solution 12

4 Results

4.1 Data Sets

4.1.1 Solution 1

Selection

Geometric entity level	Domain
Selection	Geometry geom1

Solution

Name	Value
Solution	Solver 1
Model	Save Point Geometry 1

4.1.2 Solution 2

Selection

Geometric entity level	Domain
Selection	Geometry geom1

Solution

Name	Value
Solution	Parametric 2
Model	Save Point Geometry 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

Name	Value
Expression	chds2.ndflux_cR2
Description	Normal diffusive flux

Integration settings

Name	Value
Integration order	On

4.2.2 Line Integration 2

Selection

Geometric entity level	Boundary
Selection	Boundary 5

Data

Name	Value
Data set	Solution 2

Expression

Name	Value
Expression	chds.ndflux_cR1
Description	Normal diffusive flux

Integration settings

Name	Value
Integration order	On

4.2.3 Line Integration 3

Selection

Geometric entity level	Boundary
Selection	Boundary 4

Data

Name	Value
Data set	Solution 2

Expression

Name	Value
Expression	chds.ndflux_cO1

Name	Value
Description	Normal diffusive flux

Integration settings

Name	Value
Integration order	On

4.3 Tables

4.3.1 Table 1

Line Integration 1 (chds.ndflux_cR1)

Table 1

L	Normal diffusive flux
1	0.52717
2	0.50913
3	0.50084
4	0.50086
5	0.49609
6	0.49607
7	0.49792
8	0.49475
9	0.49716
10	0.49431

4.3.2 Table 2

Line Integration 2 (chds.ndflux_cO1)

Table 2

L	Normal diffusive flux
1	0.52098
2	0.49365
3	0.47686
4	0.46273
5	0.44947
6	0.43669
7	0.42427

L	Normal diffusive flux
8	0.41197
9	0.40002
10	0.38817

4.3.3 Table 3

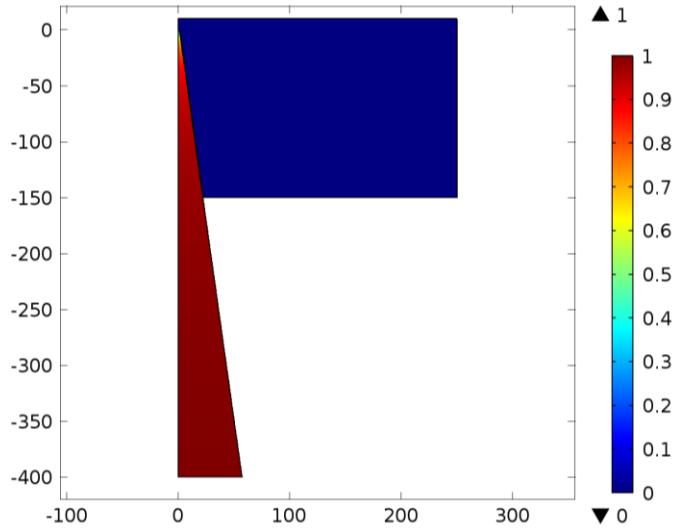
Line Integration 3 (chds2.ndflux_cO2)

Table 3

L	Normal diffusive flux
1	0.24203
2	0.1184
3	0.07408
4	0.05284
5	0.04073
6	0.03293
7	0.02754
8	0.02353
9	0.02051
10	0.01811

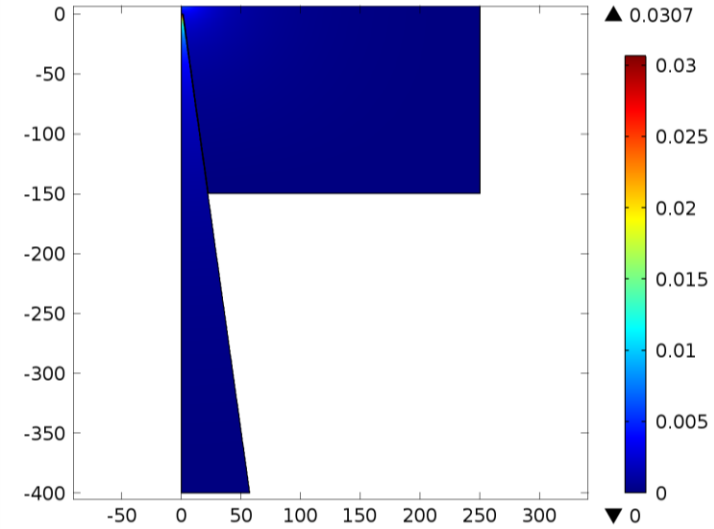
4.4 Plot Groups

4.4.1 Concentration (chds)



d(10)=10 Surface

4.4.2 Concentration (chds2)



d(10)=10 Surface