Supporting Information

Nanoscale Mechanism of Molecular Transport through the Nuclear Pore Complex as Studied by Scanning Electrochemical Microscopy

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COMSOL Model Report

1. Table of Contents

2. Model Properties

| Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Aug 29, 2012 4:31:42 PM
Creation date	Aug 28, 2012 9:58:45 PM
COMSOL version	COMSOL 3.5.0.603

Application modes and modules used in this model:

- Geom1 (3D)
  - o Diffusion (Chemical Engineering Module)
  - o Diffusion (Chemical Engineering Module)
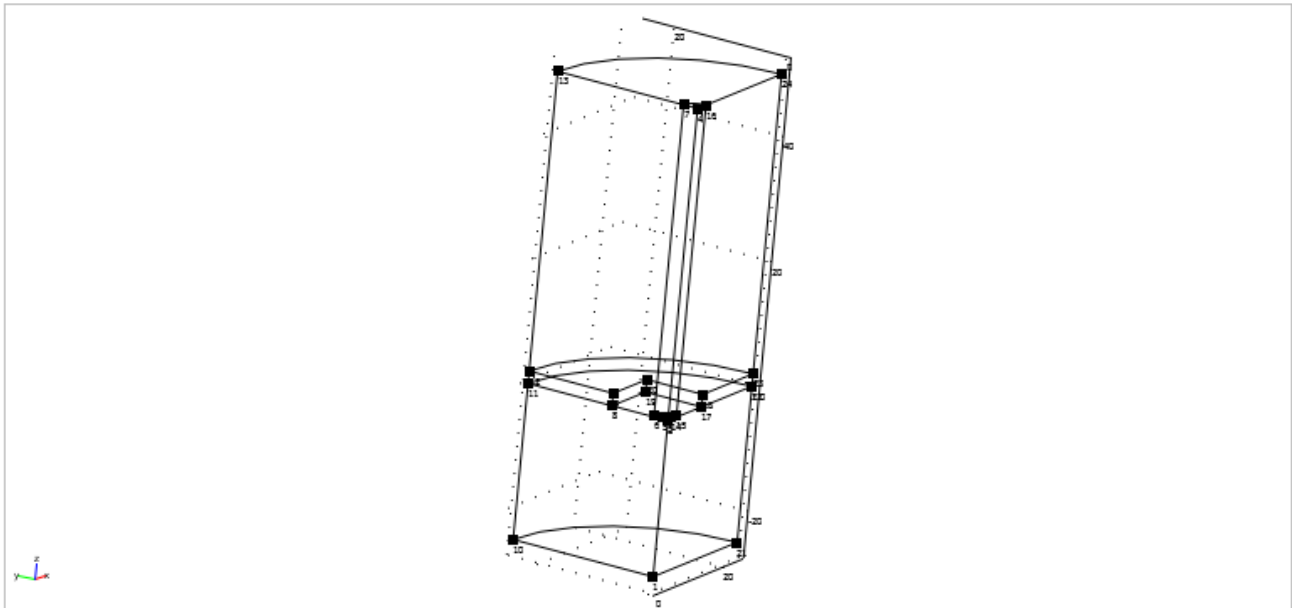- Geom3 (2D)
- Geom2 (2D)
- Geom4 (2D)

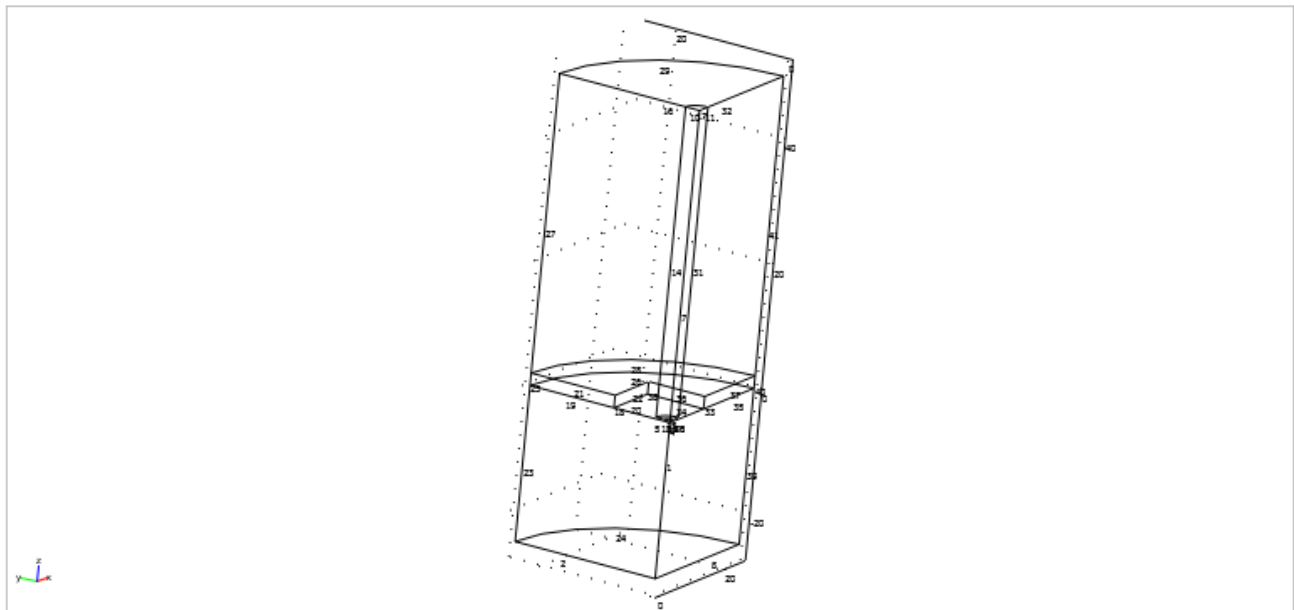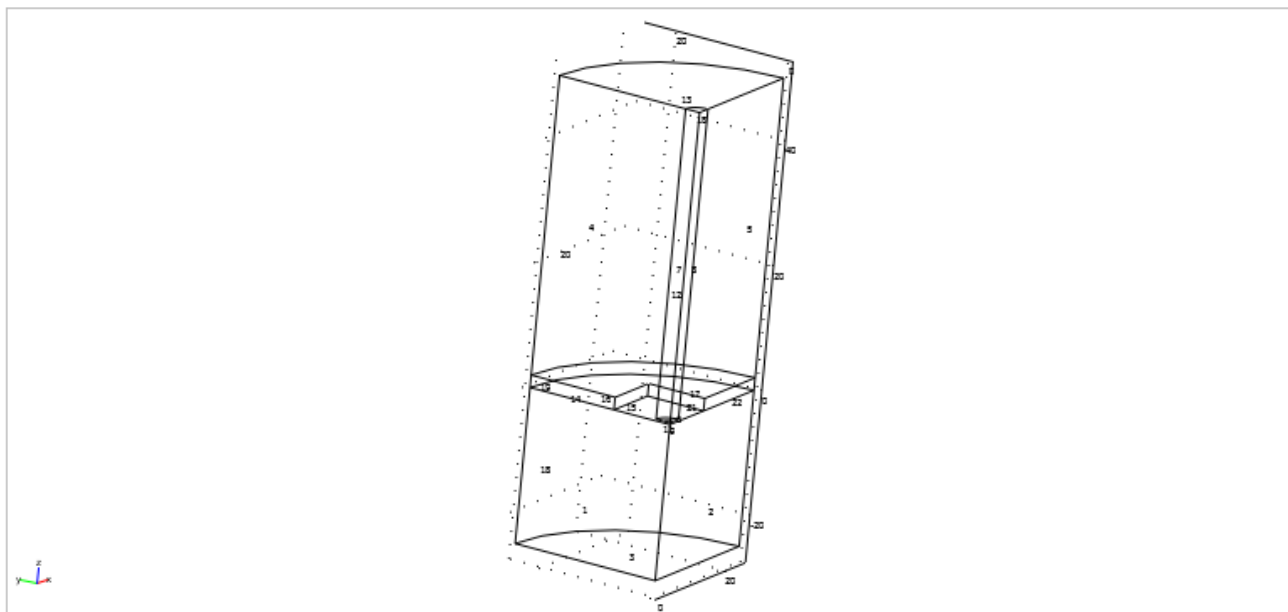# 3. Geometry

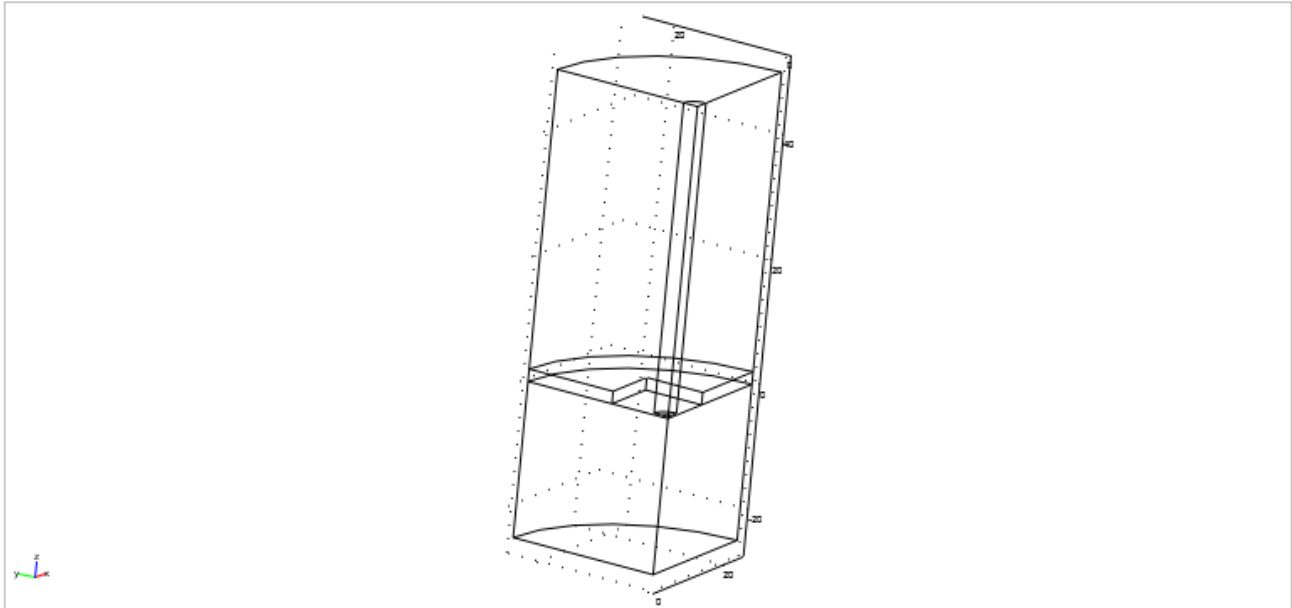Number of geometries: 4

3.1. Geom1
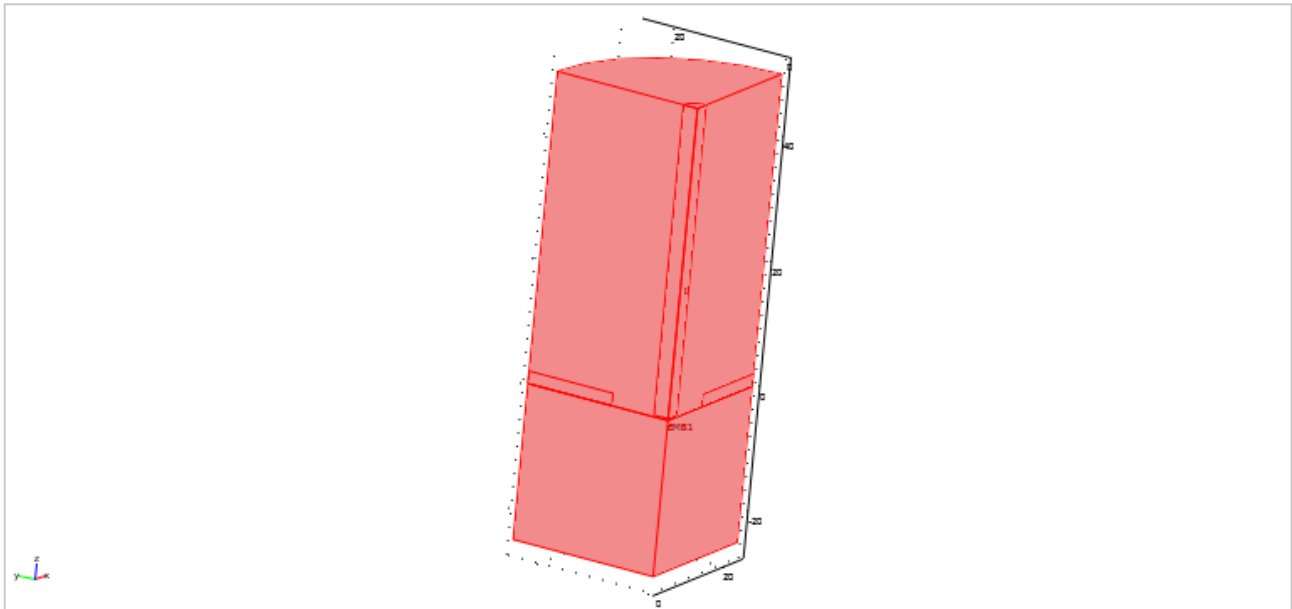
3.1.1. Point mode

3.1.2. Edge mode

3.1.3. Boundary mode

3.1.4. Subdomain mode

3.2. Geom3
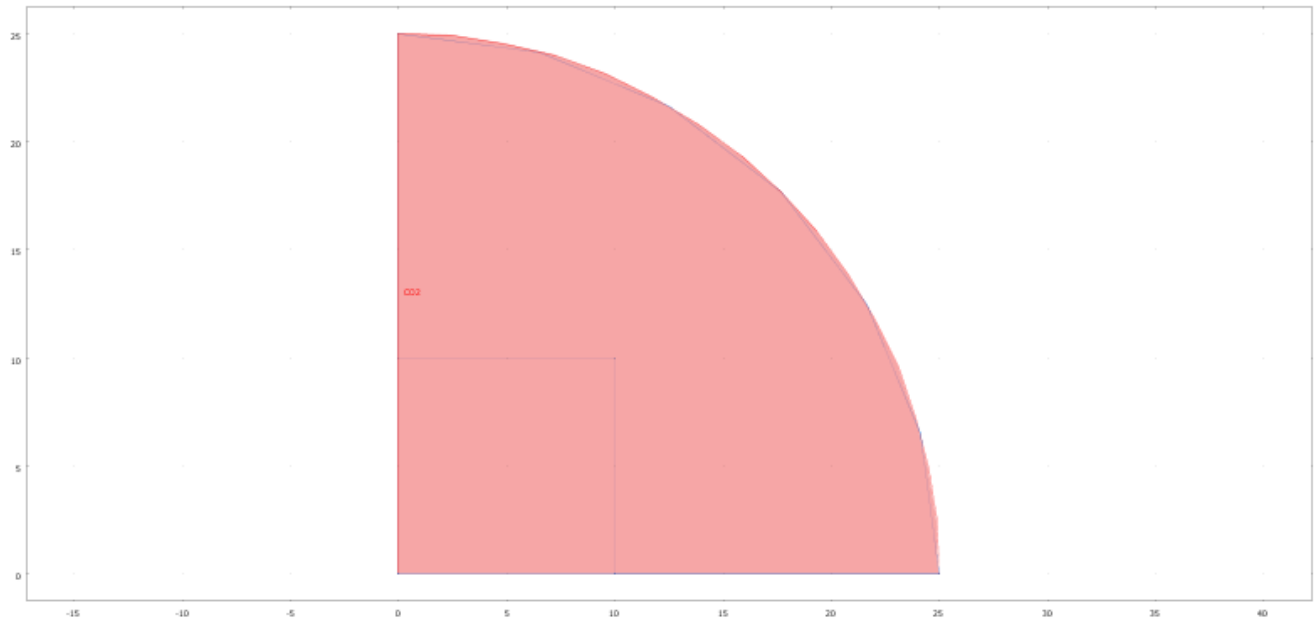
3.3. Geom2
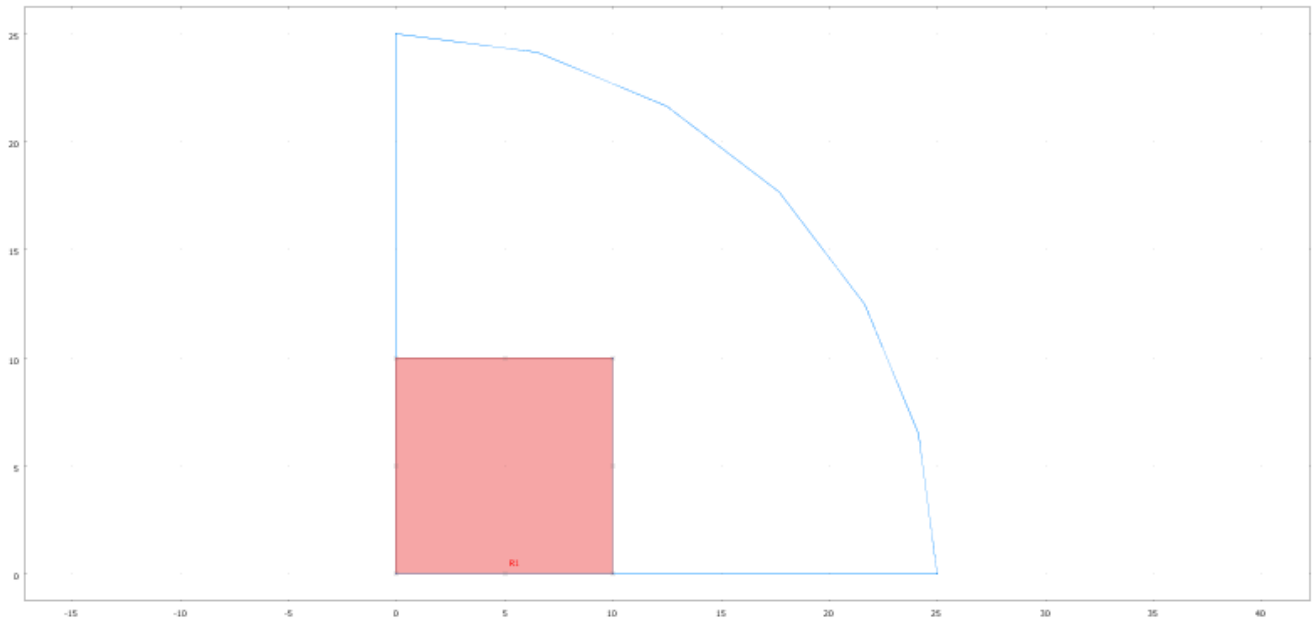
3.4. Geom4
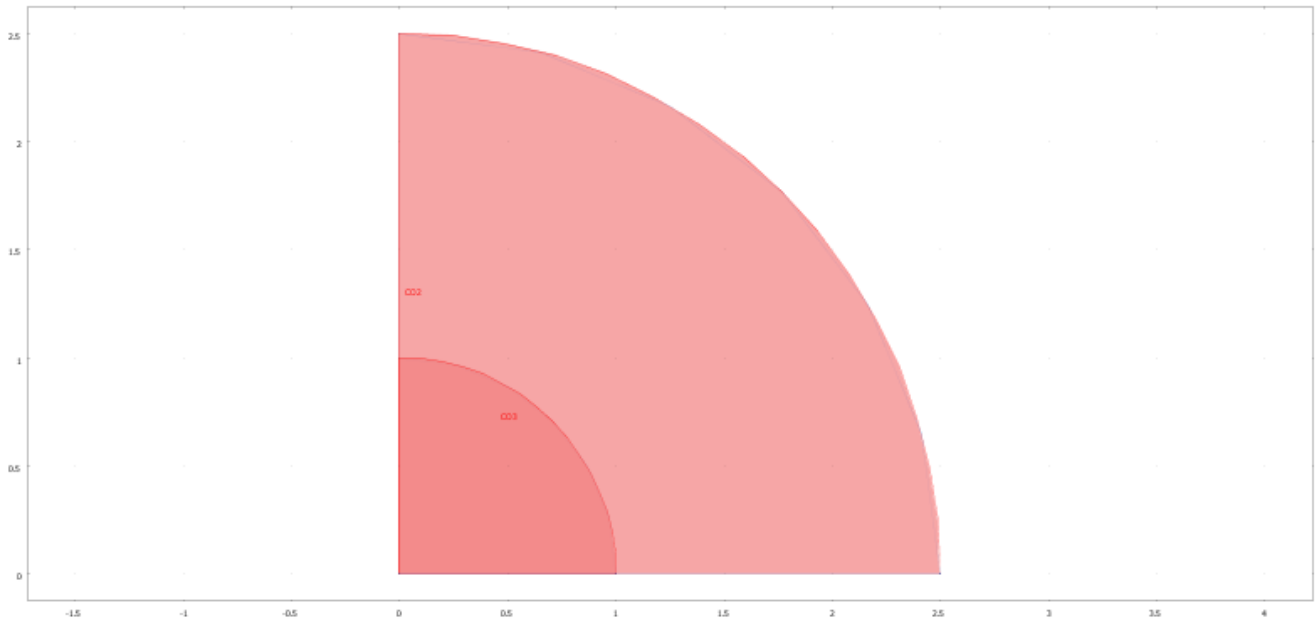
4. Geom1

Space dimensions: 3D

Independent variables: x, y, z

4.1. Scalar Expressions

Name	Expression	Unit	Description
K	0.5		

4.2. Mesh

4.2.1. Mesh Statistics

Number of degrees of freedom	299204
Number of mesh points	65778
Number of elements	382135
Tetrahedral	382135
Prism	0
Hexahedral	0
Number of boundary elements	38136
Triangular	38136
Quadrilateral	0
Number of edge elements	740
Number of vertex elements	24
Minimum element quality	0.254
Element volume ratio	0
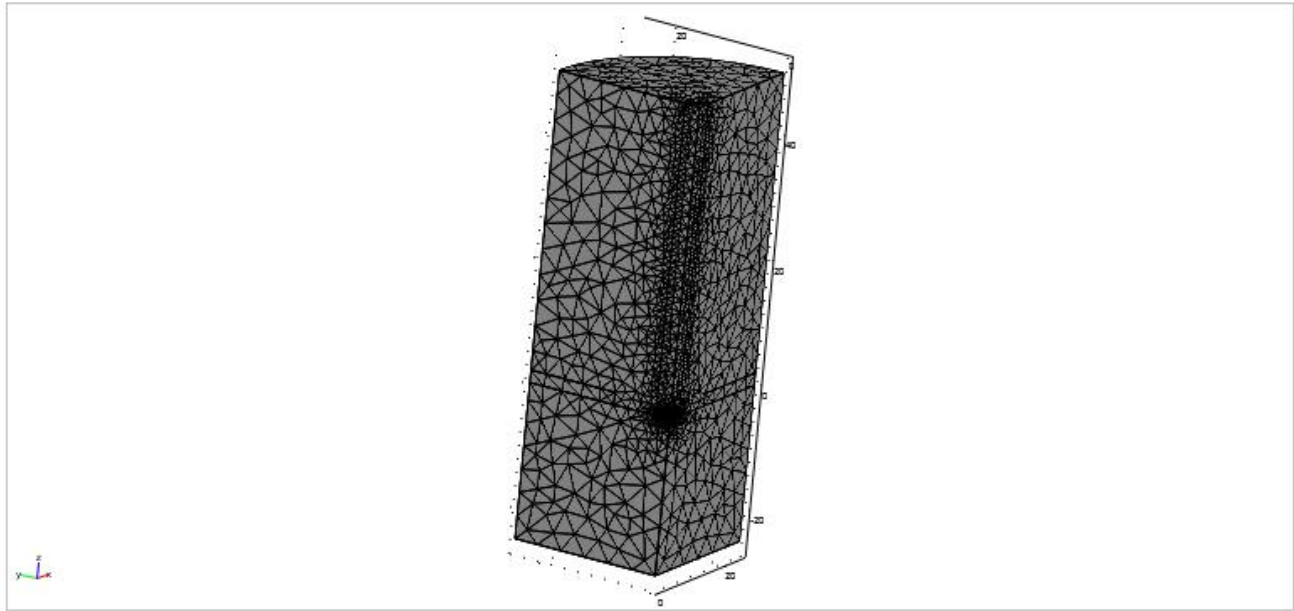
4.3. Application Mode: Diffusion (chdi)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: chdi

4.3.1. Application Mode Properties

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

4.3.2. Variables

Dependent variables: c

Shape functions: shlag(2,'c')

Interior boundaries not active

4.3.3. Boundary Settings

Boundary		13, 20	4-5, 11-12, 15, 17, 21	9
Type		Concentration	Insulation/Symmetry	Concentration
Mass transfer coefficient (kc)	m/s	0	0	0
Bulk concentration (cb)	mol/m^3	0	0	0
Concentration (c0)	mol/m^3	**1**	0	0

Boundary		6
Type		Flux
Mass transfer coefficient (kc)	m/s	**K**
Bulk concentration (cb)	mol/m^3	**c2**
Concentration (c0)	mol/m^3	0

4.3.4. Subdomain Settings

The subdomain settings only contain default values.

Subdomain initial value		2
Concentration, c (c)	mol/m^3	1

4.4. Application Mode: Diffusion (chdi2)

Application mode type: Diffusion (Chemical Engineering Module)

Application mode name: chdi2

4.4.1. Application Mode Properties

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

4.4.2. Variables

Dependent variables: c2

Shape functions: shlag(2,'c2')

Interior boundaries not active

4.4.3. Boundary Settings

Boundary		1-2, 16	3, 18	6
Type		Insulation/Symmetry	Concentration	Flux
Mass transfer coefficient (kc)	m/s	0	0	**K**
Bulk concentration (cb)	mol/m^3	0	0	**c**
Concentration (c0)	mol/m^3	0	**1**	0

4.4.4. Subdomain Settings

The subdomain settings only contain default values.

Subdomain initial value		1
Concentration, c2 (c2)	mol/m^3	1

5. Geom3

Space dimensions: 2D

Independent variables: x, y, z

6. Geom2

Space dimensions: 2D

Independent variables: x, y, z

7. Geom4

Space dimensions: 2D

Independent variables: x, y, z

8. Solver Settings

Solve using a script: off

Analysis type	Stationary
Auto select solver	On
Solver	Stationary
Solution form	Automatic
Symmetric	auto
Adaptive mesh refinement	Off
Optimization/Sensitivity	Off
Plot while solving	Off

8.1. Conjugate gradients

Solver type: Linear system solver

Parameter	Value
Relative tolerance	1.0E-6
Factor in error estimate	400.0
Maximum number of iterations	10000
Preconditioning	Left

8.1.1. Algebraic multigrid

Solver type: Preconditioner

Parameter	Value
Number of iterations	2
Multigrid cycle	V-cycle
Maximum number of levels	6
Max DOFs at coarsest level	5000
Quality of multigrid hierarchy	3

8.1.1.1. SOR

Solver type: Presmoother

Parameter	Value
Number of iterations	2
Relaxation factor (omega)	1.0
Blocked version	On

8.1.1.2. SORU

Solver type: Postsmoother

Parameter	Value
Number of iterations	2
Relaxation factor (omega)	1.0
Blocked version	On

8.1.1.3. UMFPACK

Solver type: Coarse solver

Parameter	Value
Drop tolerance	0.0
Pivot threshold	0.1
Memory allocation factor	0.7

8.2. Stationary

Parameter	Value
Linearity	Automatic
Relative tolerance	1.0E-6
Maximum number of iterations	25
Manual tuning of damping parameters	Off
Highly nonlinear problem	Off
Initial damping factor	1.0
Minimum damping factor	1.0E-4
Restriction for step size update	10.0

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
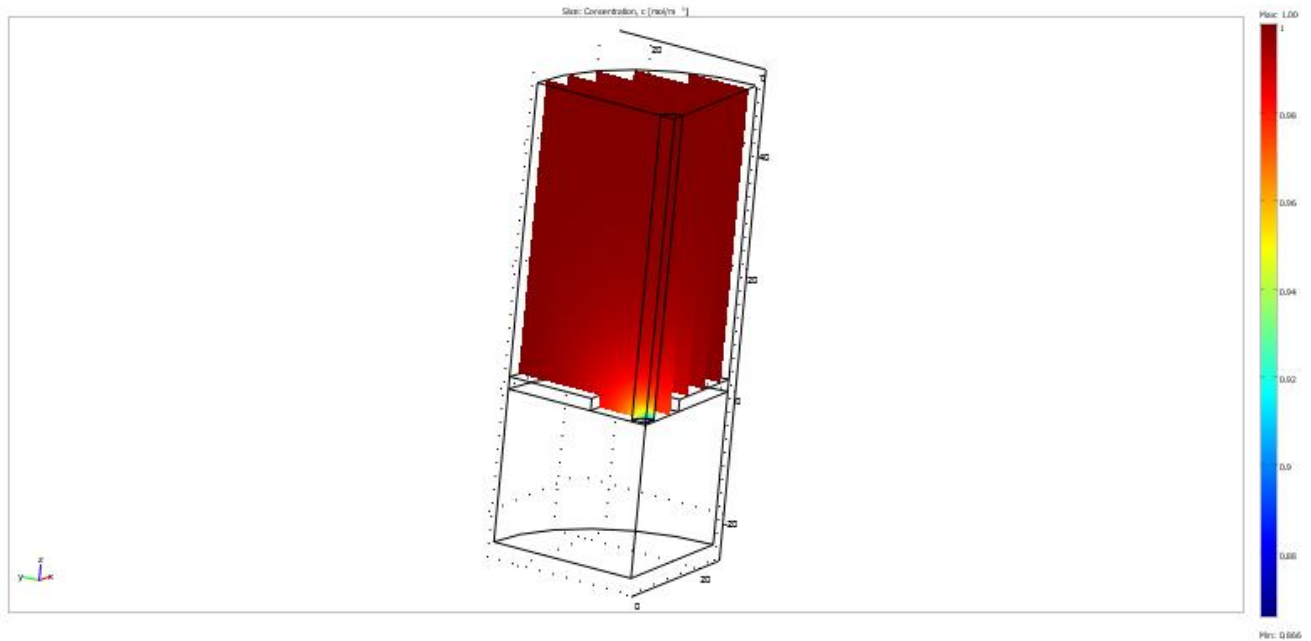
10. Variables

10.1. Boundary

10.1.1. Boundary 1-3, 16, 18

Name	Description	Unit	Expression
ndflux_c_chdi	Normal diffusive flux, c	mol/(m^2*s)	
ndflux_c2_chdi2	Normal diffusive flux, c2	mol/(m^2*s)	nx_chdi2 * dflux_c2_x_chdi2+ny_chdi2 * dflux_c2_y_chdi2+nz_chdi2 * dflux_c2_z_chdi2

10.1.2. Boundary 4-5, 9, 11-13, 15, 17, 20-21

Name	Description	Unit	Expression
ndflux_c_chdi	Normal diffusive flux, c	mol/(m^2*s)	nx_chdi * dflux_c_x_chdi+ny_chdi * dflux_c_y_chdi+nz_chdi * dflux_c_z_chdi
ndflux_c2_chdi2	Normal diffusive flux, c2	mol/(m^2*s)	

10.1.3. Boundary 6

Name	Description	Unit	Expression
ndflux_c_chdi	Normal diffusive flux, c	mol/(m^2*s)	nx_chdi * dflux_c_x_chdi+ny_chdi * dflux_c_y_chdi+nz_chdi * dflux_c_z_chdi
ndflux_c2_chdi2	Normal diffusive flux, c2	mol/(m^2*s)	nx_chdi2 * dflux_c2_x_chdi2+ny_chdi2 * dflux_c2_y_chdi2+nz_chdi2 * dflux_c2_z_chdi2

10.1.4. Boundary 7-8, 10, 14, 19, 22

Name	Description	Unit	Expression
ndflux_c_chdi	Normal diffusive flux, c	mol/(m^2*s)	
ndflux_c2_chdi2	Normal diffusive flux, c2	mol/(m^2*s)	

10.2. Subdomain

10.2.1. Subdomain 1

Name	Description	Unit	Expression
grad_c_x_chdi	Concentration gradient, c, x component	mol/m^4	
dflux_c_x_chdi	Diffusive flux, c, x component	mol/(m^2*s)	
grad_c_y_chdi	Concentration gradient, c, y component	mol/m^4	
dflux_c_y_chdi	Diffusive flux, c, y component	mol/(m^2*s)	
grad_c_z_chdi	Concentration gradient, c, z component	mol/m^4	
dflux_c_z_chdi	Diffusive flux, c, z component	mol/(m^2*s)	
grad_c_chdi	Concentration gradient, c	mol/m^4	
dflux_c_chdi	Diffusive flux, c	mol/(m^2*s)	
grad_c2_x_chdi2	Concentration gradient, c2, x component	mol/m^4	c2x
dflux_c2_x_chdi2	Diffusive flux, c2, x component	mol/(m^2*s)	-Dxx_c2_chdi2 * c2x-Dxy_c2_chdi2 * c2y-Dxz_c2_chdi2 * c2z
grad_c2_y_chdi2	Concentration gradient, c2, y component	mol/m^4	c2y
dflux_c2_y_chdi2	Diffusive flux, c2, y component	mol/(m^2*s)	-Dyx_c2_chdi2 * c2x-Dyy_c2_chdi2 * c2y-Dyz_c2_chdi2 * c2z

grad_c2_z_chdi2	Concentration gradient, c2, z component	mol/m^4	c2z
dflux_c2_z_chdi2	Diffusive flux, c2, z component	mol/(m^2*s)	-Dzx_c2_chdi2 * c2x-Dzy_c2_chdi2 * c2y-Dzz_c2_chdi2 * c2z
grad_c2_chdi2	Concentration gradient, c2	mol/m^4	sqrt(grad_c2_x_chdi2^2+grad_c2_y_chdi2^2+grad_c2_z_chdi2^2)
dflux_c2_chdi2	Diffusive flux, c2	mol/(m^2*s)	sqrt(dflux_c2_x_chdi2^2+dflux_c2_y_chdi2^2+dflux_c2_z_chdi2^2)

10.2.2. Subdomain 2

Name	Description	Unit	Expression
grad_c_x_chdi	Concentration gradient, c, x component	mol/m^4	cx
dflux_c_x_chdi	Diffusive flux, c, x component	mol/(m^2*s)	-Dxx_c_chdi * cx-Dxy_c_chdi * cy-Dxz_c_chdi * cz
grad_c_y_chdi	Concentration gradient, c, y component	mol/m^4	cy
dflux_c_y_chdi	Diffusive flux, c, y component	mol/(m^2*s)	-Dyx_c_chdi * cx-Dyy_c_chdi * cy-Dyz_c_chdi * cz
grad_c_z_chdi	Concentration gradient, c, z component	mol/m^4	cz
dflux_c_z_chdi	Diffusive flux, c, z component	mol/(m^2*s)	-Dzx_c_chdi * cx-Dzy_c_chdi * cy-Dzz_c_chdi * cz
grad_c_chdi	Concentration gradient, c	mol/m^4	sqrt(grad_c_x_chdi^2+grad_c_y_chdi^2+grad_c_z_chdi^2)
dflux_c_chdi	Diffusive flux, c	mol/(m^2*s)	sqrt(dflux_c_x_chdi^2+dflux_c_y_chdi^2+dflux_c_z_chdi^2)
grad_c2_x_chdi2	Concentration gradient, c2, x component	mol/m^4	
dflux_c2_x_chdi2	Diffusive flux, c2, x component	mol/(m^2*s)	
grad_c2_y_chdi2	Concentration gradient, c2, y component	mol/m^4	
dflux_c2_y_chdi2	Diffusive flux, c2, y component	mol/(m^2*s)	
grad_c2_z_chdi2	Concentration gradient, c2, z	mol/m^4	

	component		
dflux_c2_z_chdi2	Diffusive flux, c2, z component	mol/(m^2*s)	
grad_c2_chdi2	Concentration gradient, c2	mol/m^4	
dflux_c2_chdi2	Diffusive flux, c2	mol/(m^2*s)	

10.2.3. Subdomain 3-4

Name	Description	Unit	Expression
grad_c_x_chdi	Concentration gradient, c, x component	mol/m^4	
dflux_c_x_chdi	Diffusive flux, c, x component	mol/(m^2*s)	
grad_c_y_chdi	Concentration gradient, c, y component	mol/m^4	
dflux_c_y_chdi	Diffusive flux, c, y component	mol/(m^2*s)	
grad_c_z_chdi	Concentration gradient, c, z component	mol/m^4	
dflux_c_z_chdi	Diffusive flux, c, z component	mol/(m^2*s)	
grad_c_chdi	Concentration gradient, c	mol/m^4	
dflux_c_chdi	Diffusive flux, c	mol/(m^2*s)	
grad_c2_x_chdi2	Concentration gradient, c2, x component	mol/m^4	
dflux_c2_x_chdi2	Diffusive flux, c2, x component	mol/(m^2*s)	
grad_c2_y_chdi2	Concentration gradient, c2, y component	mol/m^4	
dflux_c2_y_chdi2	Diffusive flux, c2, y component	mol/(m^2*s)	
grad_c2_z_chdi2	Concentration gradient, c2, z component	mol/m^4	
dflux_c2_z_chdi2	Diffusive flux, c2, z component	mol/(m^2*s)	
grad_c2_chdi2	Concentration gradient, c2	mol/m^4	
dflux_c2_chdi2	Diffusive flux, c2	mol/(m^2*s)	