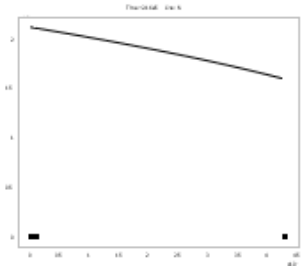
COMSOL Model Report



1. Table of Contents

2. Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Jan 25, 2010 2:40:23 PM
Creation date	Jan 14, 2010 7:30:51 PM
COMSOL version	COMSOL 3.5.0.603

File name: C:\Documents and Settings\s23988\My Documents\Thesis\Kinetics Modelling\Kinetic model formulations\1 D model with delta moving bound jan 25.mph

Application modes and modules used in this model:

- Geom1 (1D)
  - Moving Mesh (ALE)

- PDE, General Form
- PDE, General Form

3. Constants

Name	Expression	Value	Description
R	8.3145[J/(K*mol)]		J/K.mol
K	(100/0.00043)[K/m]		deg/m (T grad)
Qalphastar	3015[K]*R		J/mol (p.27)
Dalpha0	0.5*2.17e-03[cm^2/s]		m^2s^-1
Qalpha	4170[K]*R		J/mol
Nalpha0	8.5e04		ppm
Ddelta0	1.09e-03[cm^2/s]		m^2s^-1 (p.27 in Sawat)
Qdelta	5730[K]*R		J/mol
Qdeltastar	653[K]*R		J/mol
Ndelta	1.6e04		ppm
H	3820[K]*R		J/mol
intN	129.99547		ppm

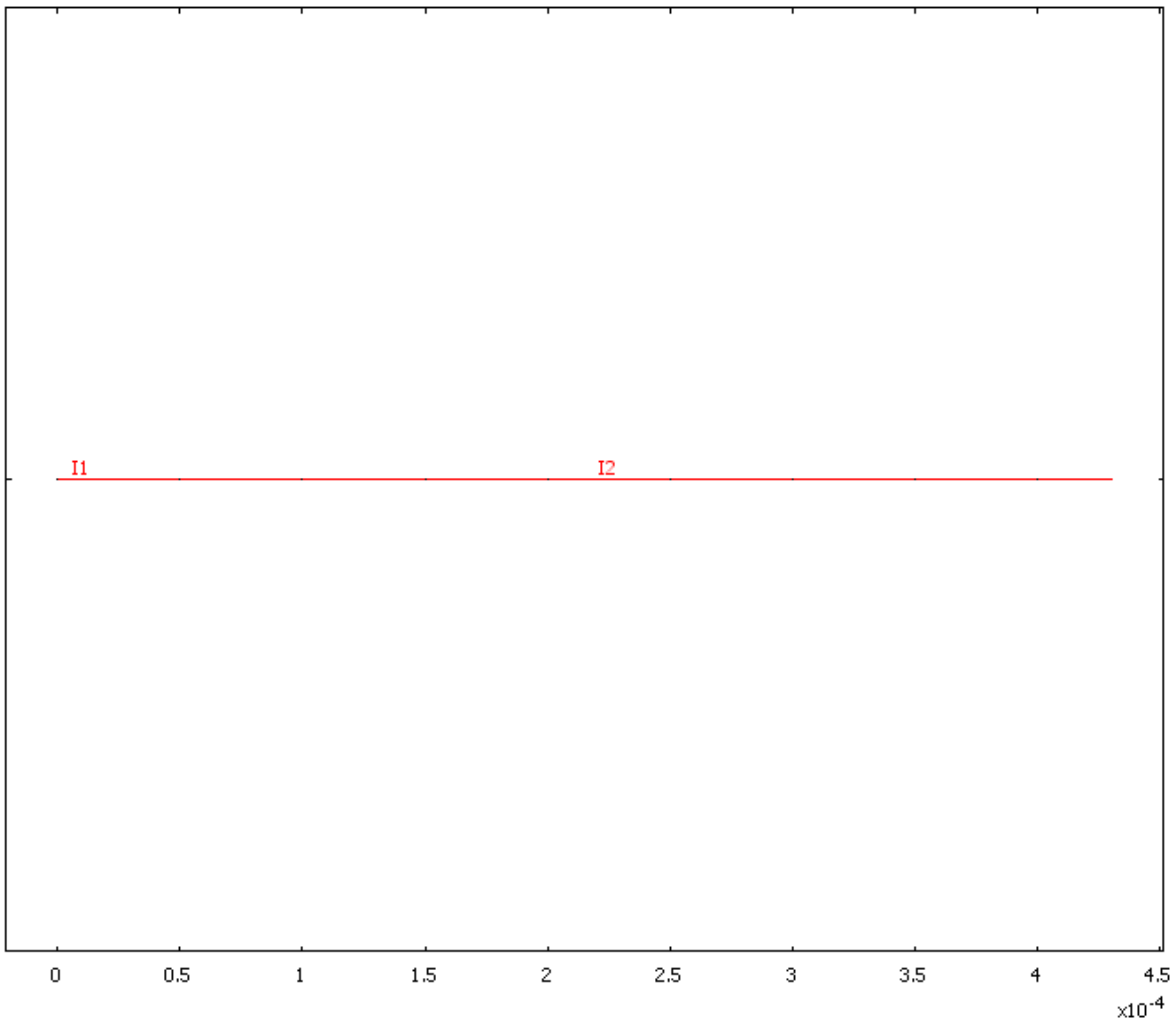
4. Global Expressions

Name	Expression	Unit	Description
T	593-(K*x)	K	600 to 700K across sheath
Dalpha	Dalpha0*exp(-Qalpha/(R*T))	m^2/s	m^2s^-1 Eq. 3 in AECL 1411
Ddelta	Ddelta0*exp(-Qdelta/(R*T))	m^2/s	
Balpha	Qalphastar*K/(R*(T^2))	1/m	
Bdelta	Qdeltastar*K/(R*(T^2))	1/m	
Nalpha	Nalpha0*exp(-H/(R*T))		
flux1	-Dalpha*(N1x+Balpha*N1)		sawat eqn 2
flux2	-Ddelta*(N2x+Bdelta*N2)		
v2	(flux2-flux1)/(N2-N1)		
Bint	18201.6920-4.8398*T	K	concn on interface based on FACT model
Bgas	5638.1761*T^0.2054		

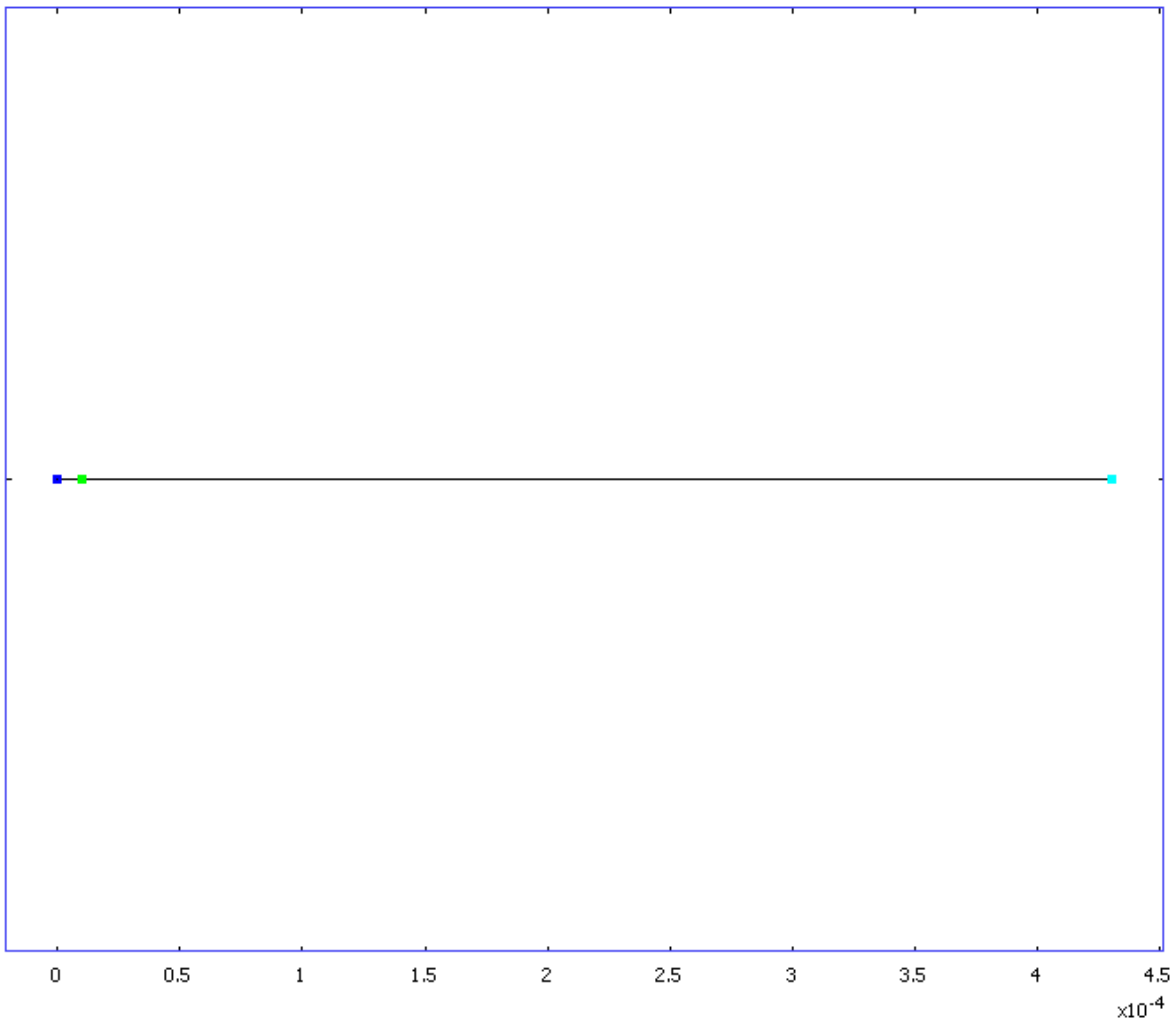
5. Geometry

Number of geometries: 1

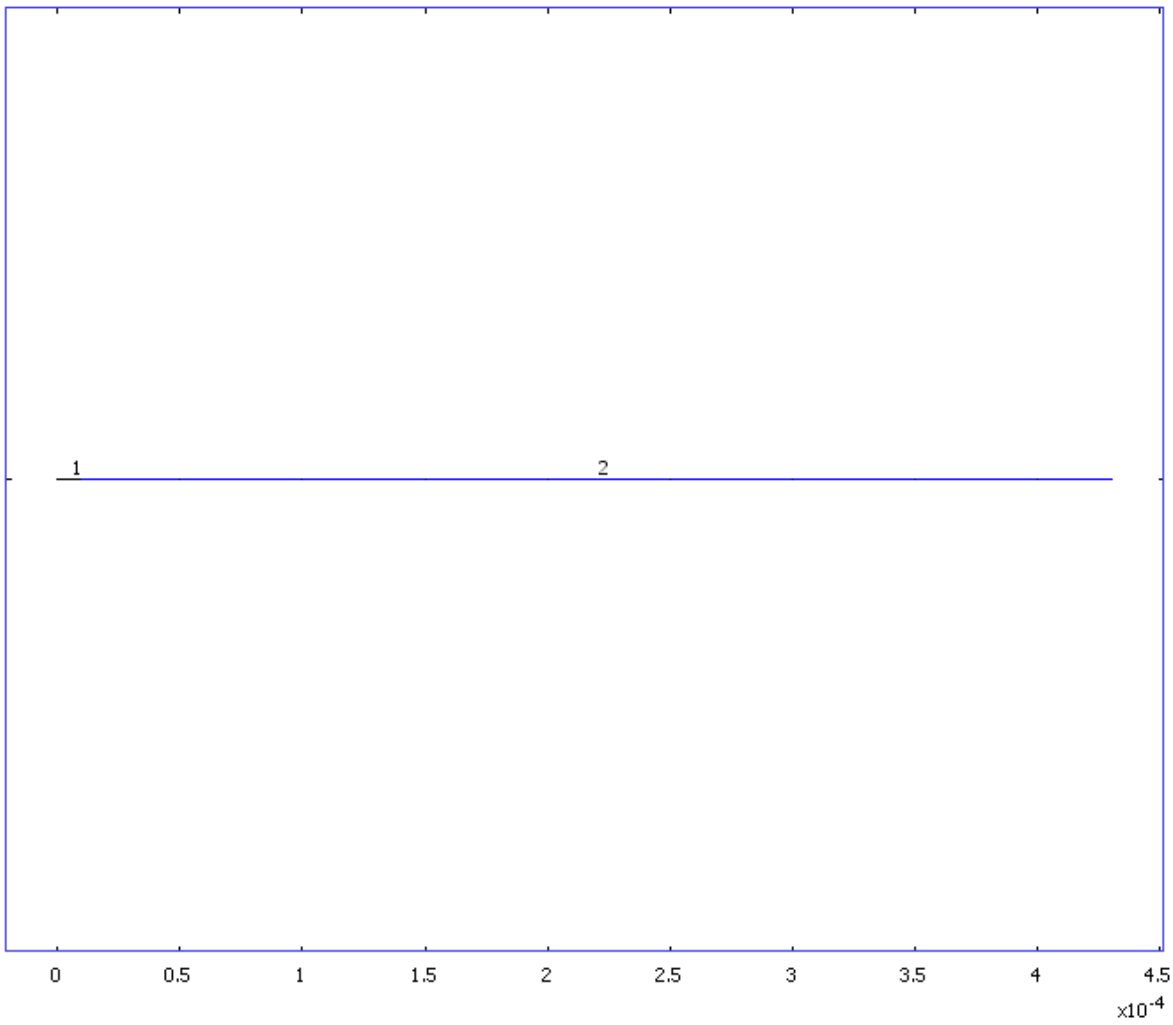
5.1. Geom1



5.1.1. Boundary mode



5.1.2. Subdomain mode



6. Geom1

Space dimensions: 1D

Independent variables: X, Y, Z

6.1. Expressions

6.1.1. Subdomain Expressions

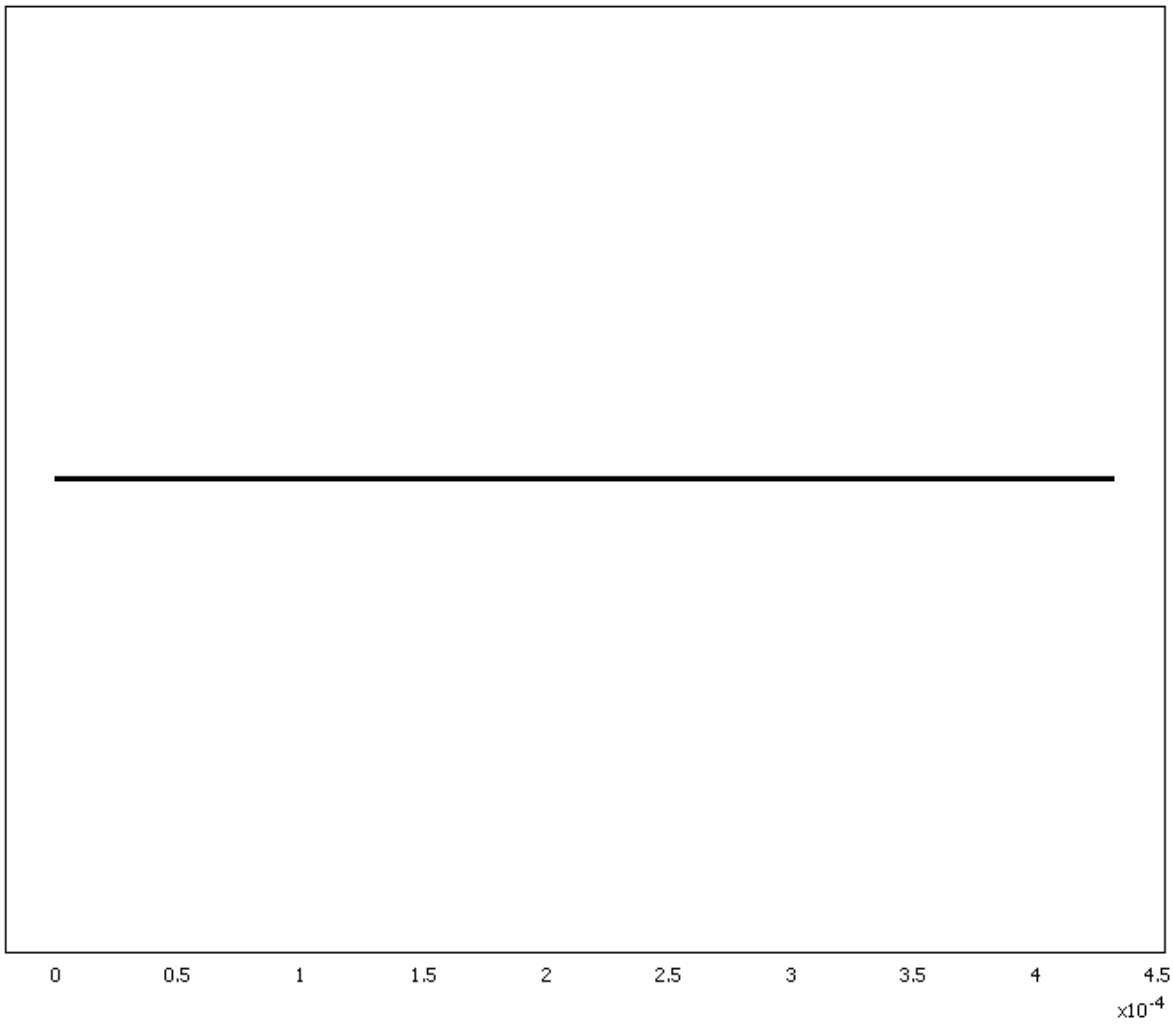
Subdomain		1	2
N		N2	N1

6.2. Mesh

6.2.1. Mesh Statistics

Number of degrees of freedom	1094
Number of mesh points	273
Number of elements	272

Number of boundary elements	3
Element length ratio	0.347



6.3. Application Mode: Moving Mesh (ALE) (ale)

Application mode type: Moving Mesh (ALE)

Application mode name: ale

6.3.1. Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Smoothing method	Laplace
Analysis type	Transient
Allow remeshing	Off
Defines frame	Frame (ale)
Original reference frame	Frame (ale)
Motion relative to	Frame (ref)

Weak constraints	On
Constraint type	Non-ideal

6.3.2. Variables

Dependent variables:

Shape functions: shlag(2,'lm5'), shlag(2,'x')

Interior boundaries active

6.3.3. Boundary Settings

Point		1, 3	2
type		Mesh displacement	**Mesh velocity**
Mesh velocity (veldeform)	m/s	0	**v2**
defflag		**1**	0
veldefflag		0	**1**
Shape functions (wcshape)		**shlag(2,'lm5') shlag(2,'x')**	**shlag(2,'lm5') shlag(2,'x')**

6.3.4. Subdomain Settings

Subdomain		1-2
Shape functions (shape)		**shlag(2,'lm5') shlag(2,'x')**

Subdomain initial value		1-2
Spatial coordinate (x)	m	xinit_ale

6.4. Application Mode: PDE, General Form (hydride)

Application mode type: PDE, General Form

Application mode name: hydride

6.4.1. Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Wave extension	Off
Frame	Frame (ale)
Weak constraints	Off

6.4.2. Variables

Dependent variables: N2, N2_t

Shape functions: shlag(2,'N2')

Interior boundaries not active

6.4.3. Boundary Settings

Point		3	1	2
(r)		-N2	**Bgas-N2**	**Bint-N2**

6.4.4. Subdomain Settings

Subdomain		1
Source term (f)		**0**
Conservative flux source term (ga)		**flux2**

Subdomain initial value		1
N2		Ndelta

6.5. Application Mode: PDE, General Form (alphamatrix)

Application mode type: PDE, General Form

Application mode name: alphamatrix

6.5.1. Application Mode Properties

Property	**Value**
Default element type	Lagrange - Quadratic
Wave extension	Off
Frame	Frame (ale)
Weak constraints	Off

6.5.2. Variables

Dependent variables: N1, N1_t

Shape functions: shlag(2,'N1')

Interior boundaries not active

6.5.3. Boundary Settings

Point		1	3	2
(g)		0	0	**(N2-N1)*v2-flux2**
type		Dirichlet boundary condition	**Neumann boundary condition**	**Neumann boundary condition**

6.5.4. Subdomain Settings

Subdomain		2
Source term (f)		**0**
Conservative flux source term (ga)		**flux1**

7. Solver Settings

Solve using a script: off

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

7.1. Direct (SPOOLES)

Solver type: Linear system solver

Parameter	**Value**
Pivot threshold	0.1
Preordering algorithm	Nested dissection

7.2. Time Stepping

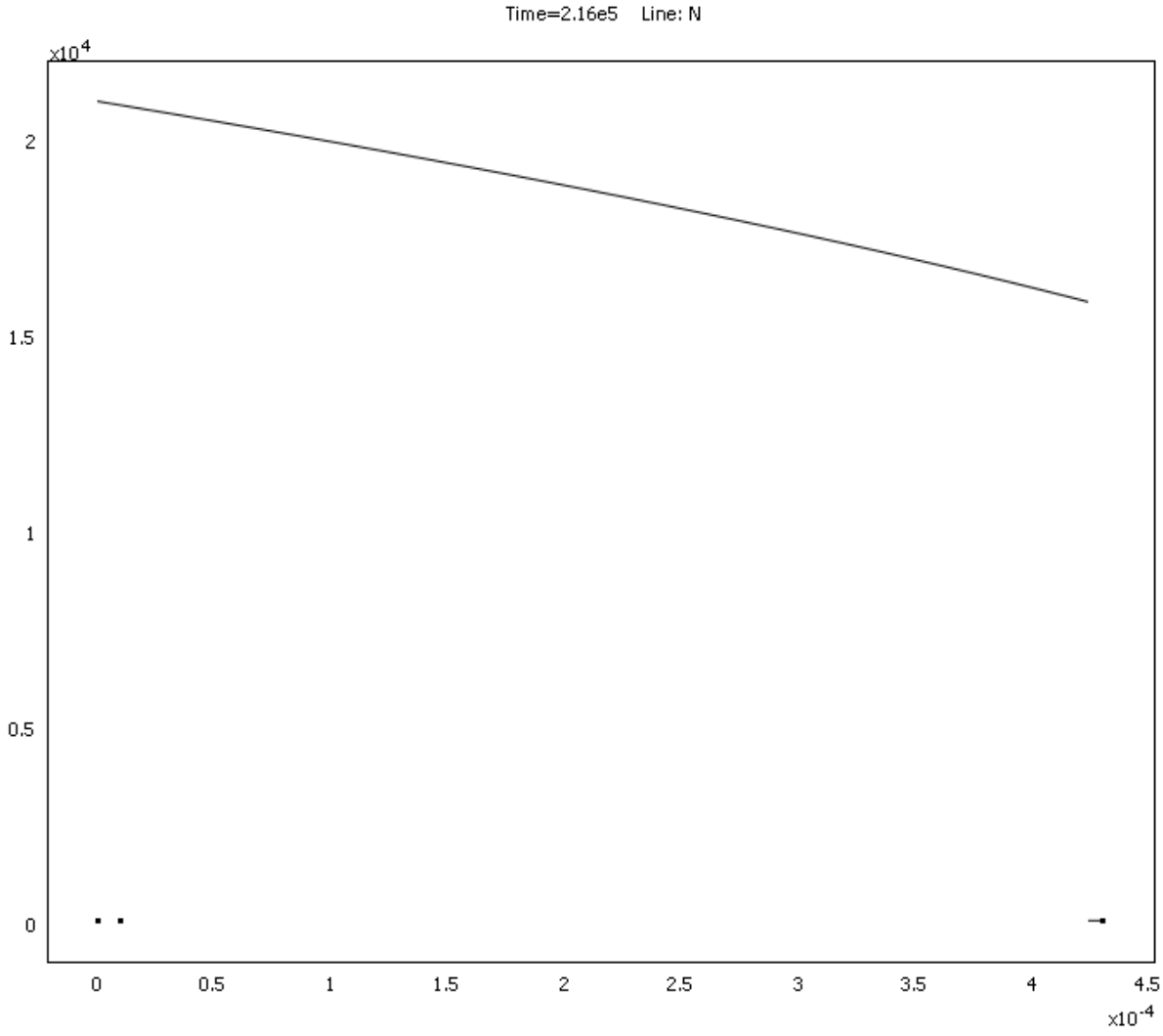
Parameter	**Value**
Times	range(0,360,3600*60)
Relative tolerance	1e-4
Absolute tolerance	1e-5
Times to store in output	Specified times
Time steps taken by solver	Free
Maximum BDF order	5
Singular mass matrix	Maybe
Consistent initialization of DAE systems	Backward Euler
Error estimation strategy	Include algebraic
Allow complex numbers	Off

7.3. 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

8. Postprocessing



9. Variables

9.1. Boundary

Name	Description	Unit	Expression
xinit_ale	x coordinate initial value	m	X

9.2. Subdomain

Name	Description	Unit	Expression
xinit_ale	x coordinate initial value	m	X
dx_ale	x-displacement	m	x-X