

SUPPLEMENTARY INFORMATION (2)

COMSOL Report

Antimicrobial effects of silver nanoparticle-microspots on the mechanical properties of single bacteria

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1 Global Definitions

Date	Dec 8, 2023, 10:34:17 PM
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GLOBAL SETTINGS

Version	COMSOL Multiphysics 6.1 (Build: 357)
Unit system	SI

USED PRODUCTS

COMSOL Multiphysics

COMPUTER INFORMATION

CPU	Intel64 Family 6 Model 85 Stepping 4, 2 sockets, 8 cores, 254.65 GB RAM
Operating system	Windows 10

1.1 PARAMETERS

1.1.1 Silver Parameters

SILVERPARAMETERS

Name	Expression	Value	Description
diamdisc	5 [um]	5E-6 m	Diameter of disc
startheightdisc	36.7 [nm]	3.67E-8 m	Height presumed from starting NPs
endheight	31.4 [nm]	3.14E-8 m	Height presumed from end NPs
densityag	10.49[g/cm^3]	10490 kg/m ³	Density of silver
mwag	107.87[g/mol]	0.10787 kg/mol	MW of Silver
time	6[h]	21600 s	Time
startvolume	$((\text{diamdisc}/2)^2 \cdot \pi) \cdot \text{startheightdisc}$	7.206E-19 m ³	
endvolume	$((\text{diamdisc}/2)^2 \cdot \pi) \cdot \text{endheight}$	6.1654E-19 m ³	
changevolume	startvolume-endvolume	1.0407E-19 m ³	
molsilverlost	$(\text{changevolume} \cdot \text{densityag}) / \text{mwag}$	1.012E-14 mol	

Name	Expression	Value	Description
fluxsilver	$\text{molsilverlost}/(\text{time}*((\text{diamdisc}/2)^2*\pi))$	2.3861E-8 mol/(m ² .s)	Flux of silver (linear) for first 6 hours
D _{Ag}	$1.648*10^{-9}[\text{m}^2/\text{s}]$	1.648E-9 m ² /s	

1.1.2 Geometry

GEOMETRY

Name	Expression	Value	Description
boxshape	100000[um]	0.1 m	
middle	boxshape/2	0.05 m	
nopart	4	4	
distapart	100[um]	1E-4 m	
usegeom	50[um]	5E-5 m	

2 Component 1

SETTINGS

Description	Value
Geometry shape function	Automatic

2.1 DEFINITIONS

2.1.1 Probes

Point Probe 1

Probe type	Point probe
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SELECTION

Geometric entity level	Point
Selection	Geometry geom1: Dimension 0: Point 40

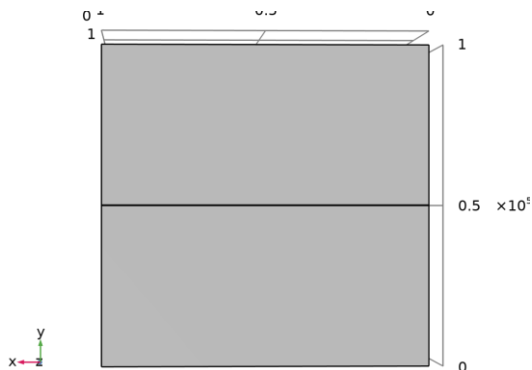
EXPRESSION

Description	Value
Expression	cAg
Table and plot unit	mol/m ³
Description	Concentration

TABLE AND WINDOW SETTINGS

Description	Value
Output table	Probe Table 1
Plot window	Probe Plot 1

2.2 GEOMETRY 1



Geometry 1

UNITS

Length unit	μm
Angular unit	deg

GEOMETRY STATISTICS

Description	Value
Space dimension	3
Number of domains	1
Number of boundaries	33
Number of edges	102
Number of vertices	79

2.2.1 Block 1 (blk1)

POSITION

Description	Value
Position	{0, 0, 0}

AXIS

Description	Value
Axis type	z - axis

SIZE AND SHAPE

Description	Value
Width	boxshape
Depth	boxshape
Height	boxshape

2.2.2 Work Plane 1 (wp1)

UNITE OBJECTS

Description	Value
Unite objects	On

Plane Geometry (sequence2D)

Circle 1 (c1)

POSITION

Description	Value
Position	{50000 - 3*usegeom, 50000 - 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 2 (c2)

POSITION

Description	Value
Position	{50000 - 3*usegeom, 50000 - 1*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 3 (c3)

POSITION

Description	Value
Position	{50000 - 3*usegeom, 50000 + 1*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 4 (c4)

POSITION

Description	Value
Position	{50000 - 3*usegeom, 50000 + 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 5 (c5)

POSITION

Description	Value
Position	{50000 - usegeom, 50000 - 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 6 (c6)

POSITION

Description	Value
Position	{50000 - usegeom, 50000 - usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 7 (c7)

POSITION

Description	Value
Position	{50000 - usegeom, 50000 + usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 8 (c8)

POSITION

Description	Value
Position	{50000 - usegeom, 50000 + 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 9 (c9)

POSITION

Description	Value
Position	{50000 + usegeom, 50000 - 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 10 (c10)

POSITION

Description	Value
Position	{50000 + usegeom, 50000 - usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 11 (c11)

POSITION

Description	Value
Position	{50000 + usegeom, 50000 + usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 12 (c12)

POSITION

Description	Value
Position	{50000 + usegeom, 50000 + 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 13 (c13)

POSITION

Description	Value
Position	{50000 + 3*usegeom, 50000 - 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 14 (c14)

POSITION

Description	Value
Position	{50000 + 3*usegeom, 50000 - usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 15 (c15)

POSITION

Description	Value
Position	{50000 + 3*usegeom, 50000 + usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Circle 16 (c16)

POSITION

Description	Value
Position	{50000 + 3*usegeom, 50000 + 3*usegeom}

SIZE AND SHAPE

Description	Value
Radius	diamdisc/2

Point 1 (pt1)

POINT

Description	Value
Point coordinate	{50000, 50000}

Line Segment 1 (ls1)

SETTINGS

Description	Value
Specify	Coordinates
Coordinates	{0, 50000}
Specify	Coordinates
Coordinates	{1E5, 50000}

Line Segment 2 (ls2)

SETTINGS

Description	Value
Specify	Coordinates
Coordinates	{0, 50050}
Specify	Coordinates
Coordinates	{1E5, 50050}

Line Segment 3 (ls3)

SETTINGS

Description	Value
Specify	Coordinates
Coordinates	{0, 50150}
Specify	Coordinates
Coordinates	{1E5, 50150}

2.3 TRANSPORT OF DILUTED SPECIES

USED PRODUCTS

COMSOL Multiphysics

EQUATIONS

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i$$

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

2.3.1 Transport Properties 1

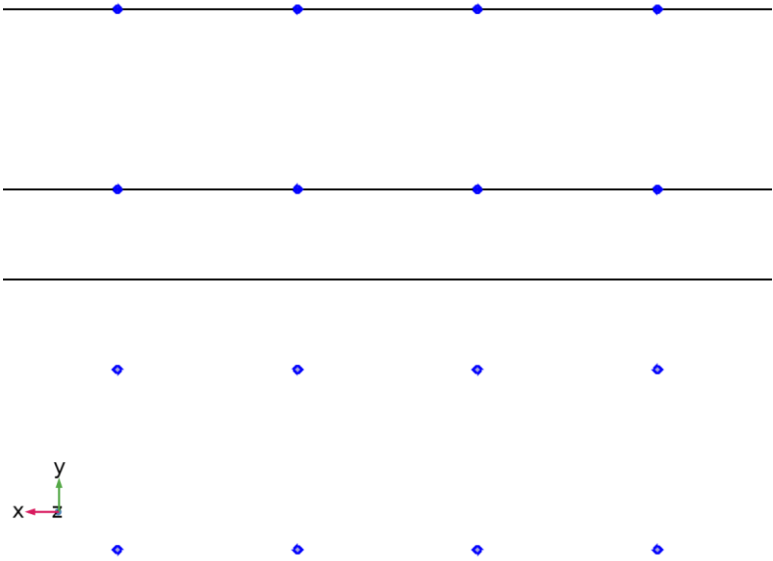
EQUATIONS

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \mathbf{J}_i + \mathbf{u} \cdot \nabla c_i = R_i$$

.....

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

2.3.2 Flux 1



Flux 1

EQUATIONS

$$-\mathbf{n} \cdot \mathbf{J}_i = j_{0,i}$$

Convection

SETTINGS

Description	Value
Include	Off

Inward Flux

SETTINGS

Description	Value	Unit
Flux type	General inward flux	
Species cAg	On	
	fluxsilver	mol/(m ² ·s)

2.4 MESH 1

2.4.1 Size (size)

SETTINGS

Description	Value
Calibrate for	Fluid dynamics
Maximum element size	3700
Minimum element size	400
Curvature factor	0.4
Resolution of narrow regions	0.9
Predefined size	Finer

2.4.2 Free Tetrahedral 1 (ftet1)

SELECTION

Geometric entity level	Domain
Selection	Remaining

SETTINGS

Description	Value
Avoid inverted curved elements	On
Last build time	80
Built with	COMSOL 6.1.0.357 (win64) 2023 - 12 - 12T10:59:43.785883500

Size 1 (size1)

SELECTION

Geometric entity level	Boundary
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Selection	Geometry geom1: Dimension 2: Boundaries 9–32
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SETTINGS

Description	Value
Minimum element size	20
Minimum element size	Off
Curvature factor	0.2
Curvature factor	Off
Resolution of narrow regions	Off
Maximum element growth rate	1.3
Maximum element growth rate	Off
Predefined size	Extremely fine
Custom element size	Custom

3 Study 2

3.1 TIME DEPENDENT

Times	Unit
range(0,0.1,1), range(1,0.1,2)	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

STUDY SETTINGS

Description	Value
Output times	{0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2}

PHYSICS AND VARIABLES SELECTION

Physics interface	Solve for	Equation form
Transport of Diluted Species (tds)	On	Automatic (Time dependent)

MESH SELECTION

Component	Mesh
Component 1	Mesh 1

3.2 TIME DEPENDENT 2

Times	Unit
$10^{\{\text{range}(\log_{10}(2), 1/5, \log_{10}(100))\}}$	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

STUDY SETTINGS

Description	Value
Output times	{2, 3.1698, 5.0238, 7.9621, 12.619, 20, 31.698, 50.238, 79.621}

PHYSICS AND VARIABLES SELECTION

Physics interface	Solve for	Equation form
Transport of Diluted Species (tds)	On	Automatic (Time dependent)

VALUES OF DEPENDENT VARIABLES

Description	Value
Settings	User controlled
Method	Solution
Study	<u>Study 2</u>

MESH SELECTION

Component	Mesh
Component 1	Mesh 1

3.3 TIME DEPENDENT 3

Times	Unit
$10^{\{\text{range}(\log_{10}(100), 1/5, \log_{10}(21600))\}}$	s

STUDY SETTINGS

Description	Value
Include geometric nonlinearity	Off

STUDY SETTINGS

Description	Value
Output times	{100, 158.49, 251.19, 398.11, 630.96, 1000, 1584.9, 2511.9, 3981.1, 6309.6, 10000, 15849}

PHYSICS AND VARIABLES SELECTION

Physics interface	Solve for	Equation form
Transport of Diluted Species (tds)	On	Automatic (Time dependent)

VALUES OF DEPENDENT VARIABLES

Description	Value
Settings	User controlled
Method	Solution
Study	<u>Study 2</u>

MESH SELECTION

Component	Mesh
Component 1	Mesh 1