

Supporting Information

The Observation of Local Redox Events at Individual Au Nanoparticles Using Electrogenerated Chemiluminescence Microscopy

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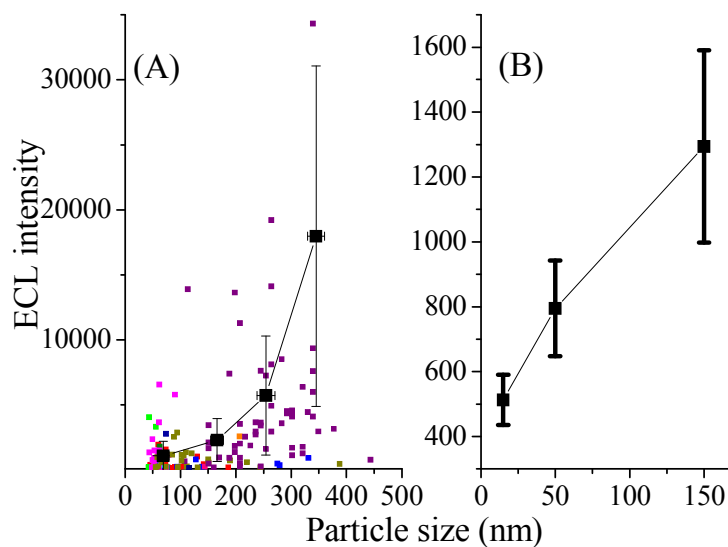


Figure S1. (A) Measured ECL intensity vs. particle diameter of each single electrodeposited Au NPs. ECL intensity data points of various colors of left panel are from Au NPs whose diameter were measured by either dark field scattering or SEM. Different colors represent data collected from different samples. Connected solid squares in black are the average ECL intensity of particles with indicated average Au NP sizes. (B) ECL vs. particle size of the pre-synthesized Au NPs. Average particle size and ECL intensity are summarized in table S1.

Average Electrodeposited polydisperse Au NP size and ECL intensity	
<i>Average particle size/nm</i>	<i>Average ECL intensity</i>
69	1093 (+/-1117)
166	2302 (+/-1648)
254	5727 (+/-4570)
345	17978 (+/-13093)
<i>Note: ECL spots are not correlated to particle sizes of the same Au NPs. Refer table 1 of the main text for correlated particle size and ECL from the same particle.</i>	
Pre-synthesized Au NPs	
<i>Average particle size/nm</i>	<i>Average ECL intensity</i>
15	513 (+/-77)
50	795 (+/-147)
150	1294 (+/-297)

Table S1. Average ECL intensity dependence on particle sizes.

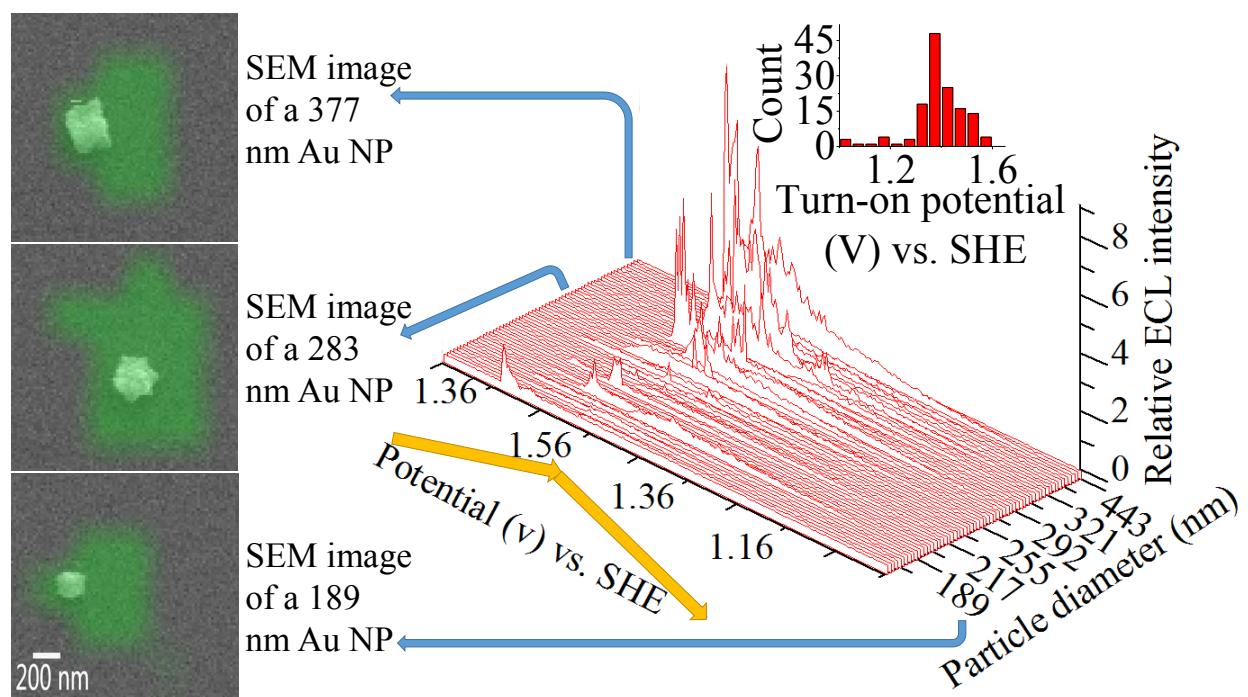


Figure S2. SEM image (B/W) overlaid with ECL image (green) showing that ECL emission from individual Au NPs instead of clusters on ITO.

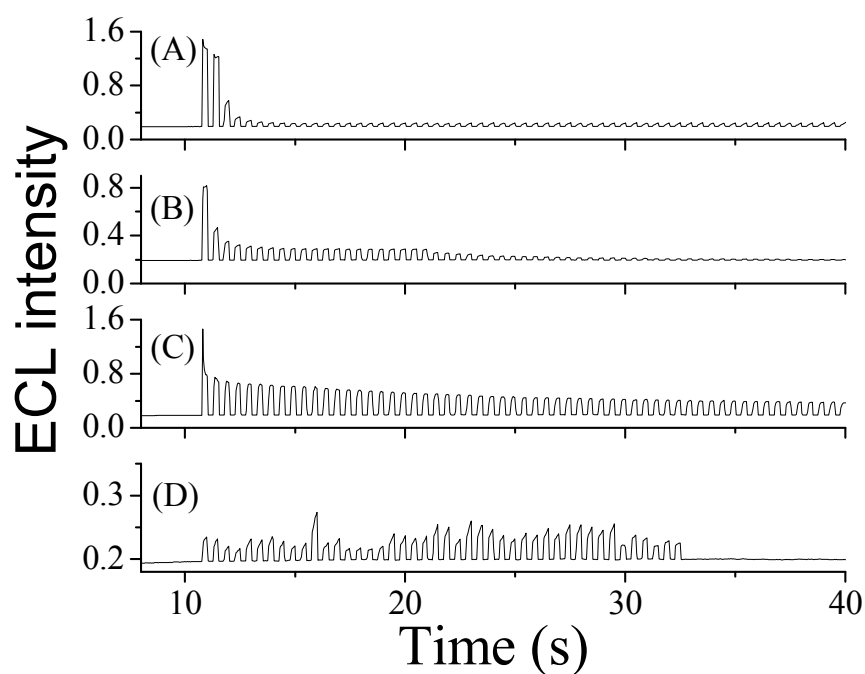


Figure S3. ECL intensity under 1.56 V vs. SHE pulse potential with a pulse width of 0.25 s. (A) ECL generated at Au NP modified ITO substrate from ECL solution containing 0.1 M TrPA, 5 mM Ru(bpy)₃Cl₂ in 0.1 M PBS buffer at a pH of 7.4; (B) ECL generated on Au NPs after adding 10 mM NaCl into ECL solution. (C) ECL generated on Au NPs using ECL solution that has been mixed with 5 mM Ag₂SO₄ followed by removal of AgCl precipitate; (D) ECL generated on bare ITO using original ECL solution under the same condition as panel A.

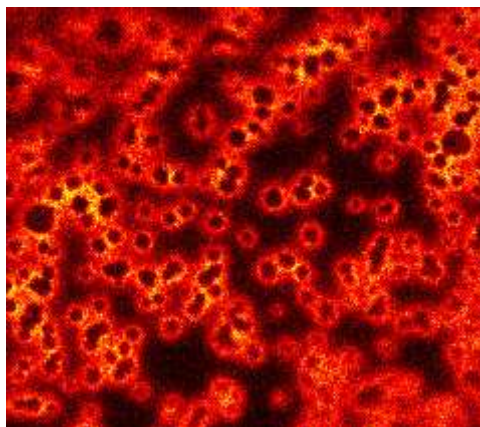


Figure S4. A $20\ \mu\text{m} \times 20\ \mu\text{m}$ ECL image of large gold particles (diameter $> 1\ \mu\text{m}$) electrodeposited onto ITO.

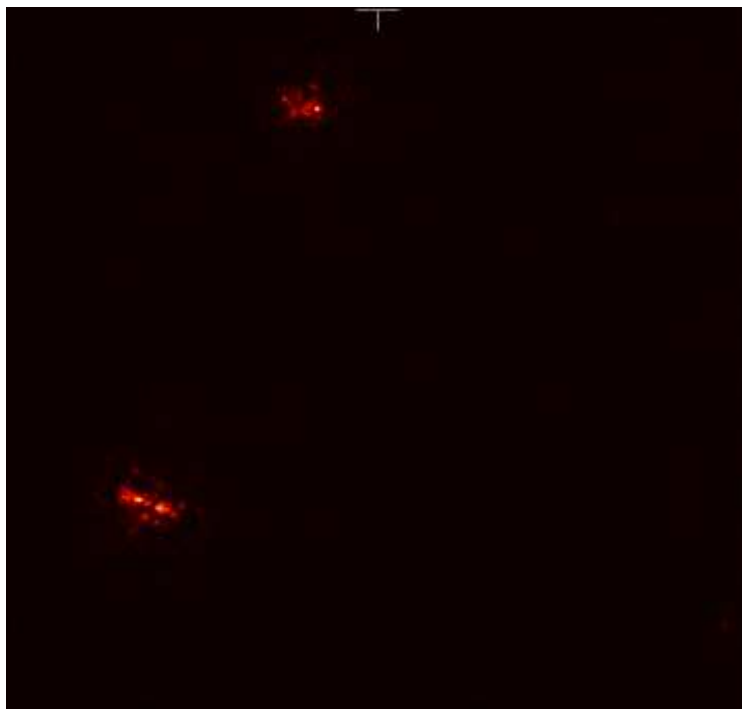
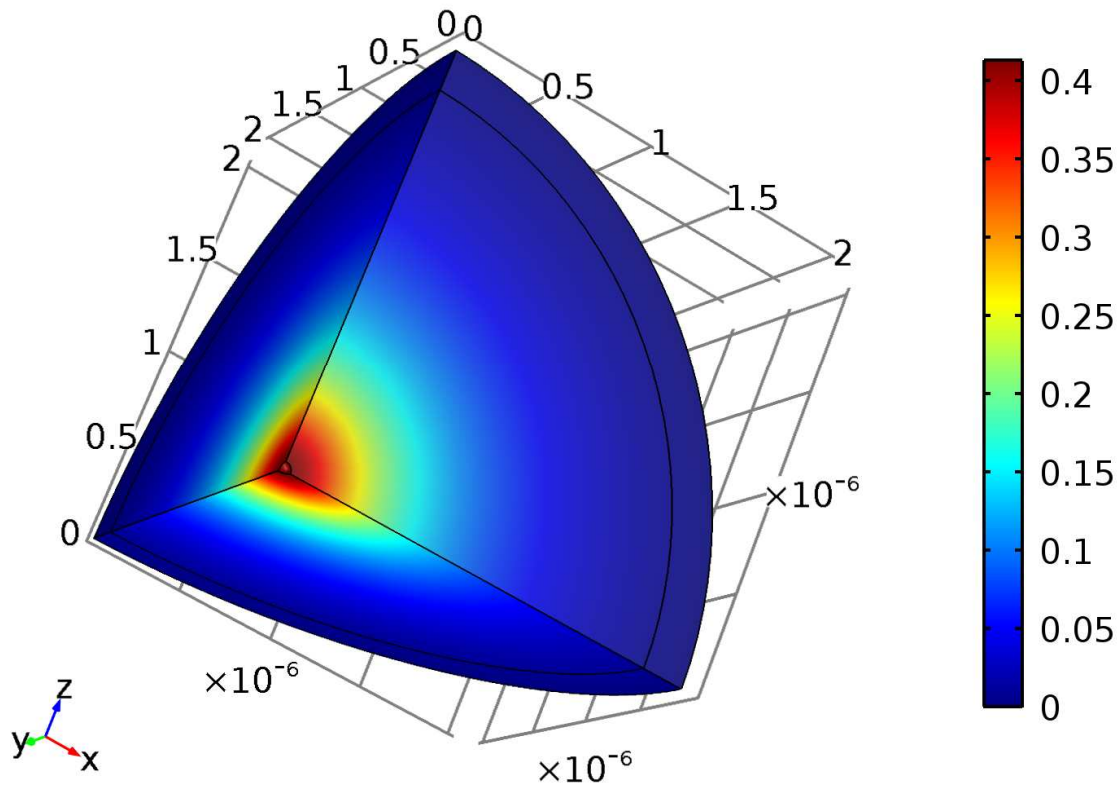


Figure S5. ECL images of pre-synthesized gold nanowires with a diameter of 70 nm and length of 1 μm .

ECL simulation Report

Time=6.841 s Surface: Concentration (mol/m³)



Report date	Jun 28, 2015 10:17:33 PM
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1 Global Definitions

Date	Jun 28, 2015 10:12:44 PM
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Global settings

Name	Final-ECL modified nanosphere electrode 3D.mph
Path	/Applications/COMSOL51/Multiphysics/applications/Electrochemistry_Module/Electroanalysis/final-ECL modified nanosphere electrode 3D.mph
COMSOL version	COMSOL 5.1 (Build: 180)
Unit system	SI

Used products

COMSOL Multiphysics
Electrochemistry Module

1.1 Parameters 1

Parameters

Name	Expression	Value	Description
v	0.1[V/s]	0.1 V/s	Voltammetric scan rate
V_therm	298.15[K]*R_const/F_const	0.025693 V	Thermal volt
cRu_bulk	5[mmol/L]	5 mol/m ³	Reactant concentration
re	40[nm]	4E-8 m	Electrode radius
DA	1e-9[m^2/s]	1E-9 m ² /s	Reactant diffusion coefficient
DB	1e-9[m^2/s]	1E-9 m ² /s	Product diffusion coefficient
k01	0.01[m/s]	0.01 m/s	Reaction rate
E_vertex1	0.8[V]	0.8 V	Start potential
E_vertex2	1.65[V]	1.65 V	Switching potential
L	6*sqrt(DA*2*abs(E_vertex1 - E_vertex2)/v)	7.823E-4 m	Outer bound on diffusion layer
r1	50*re	2E-6 m	
r2	5*re	2E-7 m	
cTrPA_bulk	0.1[mol/L]	100 mol/m ³	

Name	Expression	Value	Description
Ef1	1.26[V]	1.26 V	
Ef2	1.1[V]	1.1 V	
k02	0.006[m/s]	0.006 m/s	

2 Component 1

Date	Jun 26, 2015 10:52:04 PM
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Component settings

Unit system	SI
Geometry shape order	automatic

2.1 Definitions

2.1.1 Coordinate Systems

Boundary System 1

Coordinate system type	Boundary system
Tag	sys1

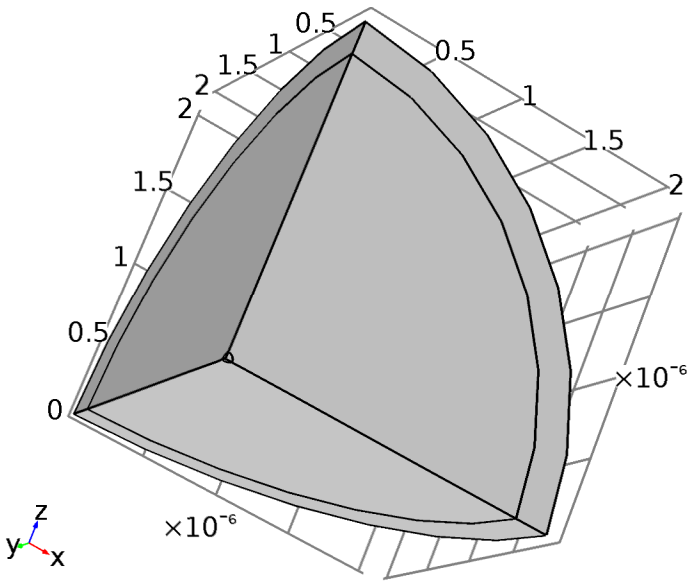
Coordinate names

First (t1)	Second (t2)	Third (n)
t1	t2	n

Settings

Description	Value
Create first tangent direction from	Global Cartesian

2.2 Geometry 1



Geometry 1

Units

Length unit	m
Angular unit	deg

Geometry statistics

Description	Value
Space dimension	3
Number of domains	3
Number of boundaries	12
Number of edges	18
Number of vertices	10

2.2.1 Sphere 1 (sph1)

Position

Description	Value
Position	{0, 0, 0}

Axis

Description	Value
-------------	-------

Description	Value
Axis type	z - axis
Layers	

Size

Description	Value
Radius	re

2.2.2 Block 1 (blk1)

Position

Description	Value
Position	{0, 0, 0}

Axis

Description	Value
Axis type	z - axis

Size and shape

Description	Value
Width	5*re
Depth	5*re
Height	5*re

Layers

Description	Value
Layers	

2.2.3 Sphere 2 (sph2)

Position

Description	Value
Position	{0, 0, 0}

Axis

Description	Value
Axis type	z - axis

Axis

Layer name	Thickness (m)
Layer 1	r2

Size

Description	Value
Radius	re+r1

2.2.4 Block 2 (blk2)

Position

Description	Value
Position	{0, 0, 0}

Axis

Description	Value
Axis type	z - axis

Size and shape

Description	Value
Width	100*re
Depth	100*re
Height	100*re

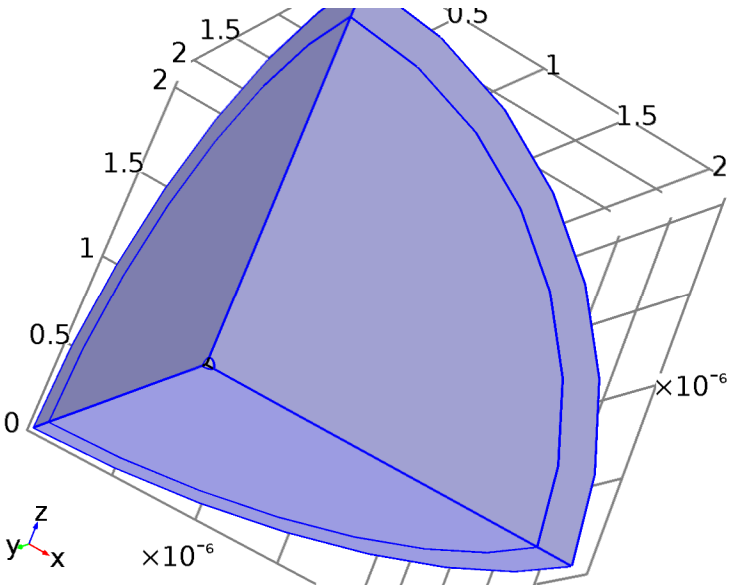
Layers

Description	Value
Layers	

2.3 Electroanalysis

Used products

COMSOL Multiphysics
Electrochemistry Module



Electroanalysis

Selection

Geometric entity level	Domain
Selection	Domains 2-3

Equations

$$\frac{dc_i}{dt} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

$$\phi_1 = 0$$

Settings

Description	Value
Concentration	Linear
Compute boundary fluxes	On
Apply smoothing to boundary fluxes	On
Value type when using splitting of complex variables	Real
Convection	Off
Migration in electric field	Off
Streamline diffusion	On
Crosswind diffusion	On

Description	Value
Equation residual	Approximate residual
Crosswind diffusion type	Do Carmo and Galeão
Convective term	Non - conservative form

Variables

Name	Expression	Unit	Description	Selection
domflux.cRuiix	elan.dflux_cRuiix	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.cRuiiy	elan.dflux_cRuiiy	mol/(m ² *s)	Domain flux, y component	Domains 2–3
domflux.cRuiiz	elan.dflux_cRuiiz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
domflux.cRuix	elan.dflux_cRuix	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.cRuiy	elan.dflux_cRuiy	mol/(m ² *s)	Domain flux, y component	Domains 2–3
domflux.cRuiz	elan.dflux_cRuiz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
domflux.cRuiiix	elan.dflux_cRuiiix	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.cRuiiyy	elan.dflux_cRuiiyy	mol/(m ² *s)	Domain flux, y component	Domains 2–3
domflux.cRuiiiz	elan.dflux_cRuiiiz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
domflux.cRuii_hvx	elan.dflux_cRuii_hvx	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.cRuii_hvy	elan.dflux_cRuii_hvy	mol/(m ² *s)	Domain flux, y component	Domains 2–3
domflux.cRuii_hvz	elan.dflux_cRuii_hvz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
domflux.chvx	elan.dflux_chvx	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.chvy	elan.dflux_chvy	mol/(m ² *s)	Domain flux, y component	Domains 2–3

Name	Expression	Unit	Description	Selection
domflux.chvz	elan.dflux_chvz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
domflux.cTrPAx	elan.dflux_cTrPAx	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.cTrPAy	elan.dflux_cTrPAy	mol/(m ² *s)	Domain flux, y component	Domains 2–3
domflux.cTrPAz	elan.dflux_cTrPAz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
domflux.cTrPAHx	elan.dflux_cTrPAHx	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.cTrPAHy	elan.dflux_cTrPAHy	mol/(m ² *s)	Domain flux, y component	Domains 2–3
domflux.cTrPAHz	elan.dflux_cTrPAHz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
domflux.cTrPA_rx	elan.dflux_cTrPA_rx	mol/(m ² *s)	Domain flux, x component	Domains 2–3
domflux.cTrPA_ry	elan.dflux_cTrPA_ry	mol/(m ² *s)	Domain flux, y component	Domains 2–3
domflux.cTrPA_rz	elan.dflux_cTrPA_rz	mol/(m ² *s)	Domain flux, z component	Domains 2–3
elan.mulstopcond	1	1	Multiplicative stop condition	Global
elan.stopcond	elan.mulstopcond	1	Solver stop condition	Global
elan.nx	nx	1	Normal vector, x component	Boundary 9
elan.ny	ny	1	Normal vector, y component	Boundary 9
elan.nz	nz	1	Normal vector, z component	Boundary 9
elan.nx	unx	1	Normal vector, x component	Boundary 6
elan.ny	uny	1	Normal vector, y component	Boundary 6

Name	Expression	Unit	Description	Selection
elan.nz	unz	1	Normal vector, z component	Boundary 6
elan.nx	dnx	1	Normal vector, x component	Boundaries 4-5, 7-8, 10-12
elan.ny	dny	1	Normal vector, y component	Boundaries 4-5, 7-8, 10-12
elan.nz	dnz	1	Normal vector, z component	Boundaries 4-5, 7-8, 10-12
elan.nxmesh	root.nxmesh	1	Normal vector (mesh), x component	Boundary 9
elan.nymesh	root.nymesh	1	Normal vector (mesh), y component	Boundary 9
elan.nzmesh	root.nzmesh	1	Normal vector (mesh), z component	Boundary 9
elan.nxmesh	root.unxmesh	1	Normal vector (mesh), x component	Boundary 6
elan.nymesh	root.unymesh	1	Normal vector (mesh), y component	Boundary 6
elan.nzmesh	root.unzmesh	1	Normal vector (mesh), z component	Boundary 6
elan.nxmesh	root.dnxmesh	1	Normal vector (mesh), x component	Boundaries 4-5, 7-8, 10-12
elan.nymesh	root.dnymesh	1	Normal vector (mesh), y component	Boundaries 4-5, 7-8, 10-12
elan.nzmesh	root.dnzmesh	1	Normal vector (mesh), z	Boundaries 4-5, 7-8, 10-

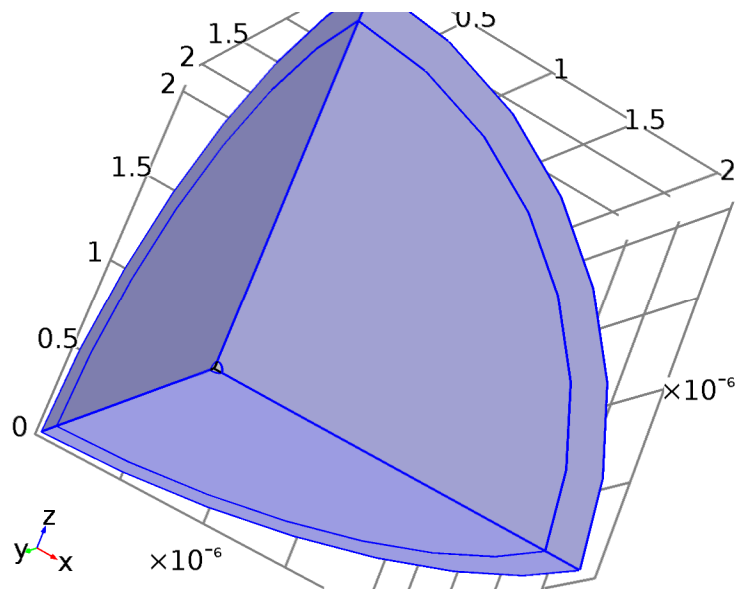
Name	Expression	Unit	Description	Selection
			component	12
elan.nxc	$\text{root.nxc}/\sqrt{\text{root.nxc}^2 + \text{root.nyc}^2 + \text{root.nzc}^2 + \text{eps}}$	1	Normal vector, x component	Boundaries 4–12
elan.nyc	$\text{root.nyc}/\sqrt{\text{root.nxc}^2 + \text{root.nyc}^2 + \text{root.nzc}^2 + \text{eps}}$	1	Normal vector, y component	Boundaries 4–12
elan.nzc	$\text{root.nzc}/\sqrt{\text{root.nxc}^2 + \text{root.nyc}^2 + \text{root.nzc}^2 + \text{eps}}$	1	Normal vector, z component	Boundaries 4–12
elan.ndflux_cRuii	elan.bndFlux_cRuii	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ndflux_cRui	elan.bndFlux_cRui	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ndflux_cRuiii	elan.bndFlux_cRuiii	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ndflux_cRuii_hv	elan.bndFlux_cRuii_hv	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ndflux_chv	elan.bndFlux_chv	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ndflux_cTrPA	elan.bndFlux_cTrPA	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ndflux_cTrPAH	elan.bndFlux_cTrPAH	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ndflux_cTrPA_r	elan.bndFlux_cTrPA_r	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal diffusive flux	Boundaries 4–12
elan.ntflux_cRuii	elan.bndFlux_cRuii	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal total flux	Boundaries 4–12
elan.ntflux_cRui	elan.bndFlux_cRui	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal total flux	Boundaries 4–12
elan.ntflux_cRuiii	elan.bndFlux_cRuiii	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal total flux	Boundaries 4–12
elan.ntflux_cRuii_hv	elan.bndFlux_cRuii_hv	$\text{mol}/(\text{m}^2 \cdot \text{s})$	Normal total flux	Boundaries 4–12

Name	Expression	Unit	Description	Selection
elan.ntflux_chv	elan.bndFlux_chv	mol/(m ² *s)	Normal total flux	Boundaries 4–12
elan.ntflux_cTrPA	elan.bndFlux_cTrPA	mol/(m ² *s)	Normal total flux	Boundaries 4–12
elan.ntflux_cTrPAH	elan.bndFlux_cTrPAH	mol/(m ² *s)	Normal total flux	Boundaries 4–12
elan.ntflux_cTrPA_r	elan.bndFlux_cTrPA_r	mol/(m ² *s)	Normal total flux	Boundaries 4–12
elan.bndFlux_cRuii	-dflux_spatial(cRuii)	mol/(m ² *s)	Boundary flux	Boundaries 4–5, 7–8, 10–12
elan.bndFlux_cRuii	-uflux_spatial(cRuii)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_cRuii	0.5*(uflux_spatial(cRuii)-dflux_spatial(cRuii))	mol/(m ² *s)	Boundary flux	Boundary 9
elan.bndFlux_cRui	-dflux_spatial(cRui)	mol/(m ² *s)	Boundary flux	Boundaries 4–5, 7–8, 10–12
elan.bndFlux_cRui	-uflux_spatial(cRui)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_cRui	0.5*(uflux_spatial(cRui)-dflux_spatial(cRui))	mol/(m ² *s)	Boundary flux	Boundary 9
elan.bndFlux_cRuiii	-dflux_spatial(cRuiii)	mol/(m ² *s)	Boundary flux	Boundaries 4–5, 7–8, 10–12
elan.bndFlux_cRuiii	-uflux_spatial(cRuiii)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_cRuiii	0.5*(uflux_spatial(cRuiii)-dflux_spatial(cRuiii))	mol/(m ² *s)	Boundary flux	Boundary 9
elan.bndFlux_cRuii_hv	-dflux_spatial(cRuii_hv)	mol/(m ² *s)	Boundary flux	Boundaries 4–5, 7–8, 10–12
elan.bndFlux_cRuii_hv	-uflux_spatial(cRuii_hv)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_cRuii_hv	0.5*(uflux_spatial(cRuii_hv)-dflux_spatial(cRuii_hv))	mol/(m ² *s)	Boundary flux	Boundary 9

Name	Expression	Unit	Description	Selection
)			
elan.bndFlux_chv	-dflux_spatial(chv)	mol/(m ² *s)	Boundary flux	Boundaries 4-5, 7-8, 10-12
elan.bndFlux_chv	-uflux_spatial(chv)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_chv	0.5*(uflux_spatial(chv)-dflux_spatial(chv))	mol/(m ² *s)	Boundary flux	Boundary 9
elan.bndFlux_cTrPA	-dflux_spatial(cTrPA)	mol/(m ² *s)	Boundary flux	Boundaries 4-5, 7-8, 10-12
elan.bndFlux_cTrPA	-uflux_spatial(cTrPA)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_cTrPA	0.5*(uflux_spatial(cTrPA)-dflux_spatial(cTrPA))	mol/(m ² *s)	Boundary flux	Boundary 9
elan.bndFlux_cTrPAH	-dflux_spatial(cTrPAH)	mol/(m ² *s)	Boundary flux	Boundaries 4-5, 7-8, 10-12
elan.bndFlux_cTrPAH	-uflux_spatial(cTrPAH)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_cTrPAH	0.5*(uflux_spatial(cTrPAH)-dflux_spatial(cTrPAH))	mol/(m ² *s)	Boundary flux	Boundary 9
elan.bndFlux_cTrPA_r	-dflux_spatial(cTrPA_r)	mol/(m ² *s)	Boundary flux	Boundaries 4-5, 7-8, 10-12
elan.bndFlux_cTrPA_r	-uflux_spatial(cTrPA_r)	mol/(m ² *s)	Boundary flux	Boundary 6
elan.bndFlux_cTrPA_r	0.5*(uflux_spatial(cTrPA_r)-dflux_spatial(cTrPA_r))	mol/(m ² *s)	Boundary flux	Boundary 9
elan.R_cRuii	0	mol/(m ³ *s)	Total rate expression	Domains 2-3
elan.R_cRui	0	mol/(m ³ *s)	Total rate expression	Domains 2-3

Name	Expression	Unit	Description	Selection
elan.R_cRuuii	0	mol/(m ³ *s)	Total rate expression	Domains 2-3
elan.R_cRuui_hv	0	mol/(m ³ *s)	Total rate expression	Domains 2-3
elan.R_chv	0	mol/(m ³ *s)	Total rate expression	Domains 2-3
elan.R_cTrPA	0	mol/(m ³ *s)	Total rate expression	Domains 2-3
elan.R_cTrPAH	0	mol/(m ³ *s)	Total rate expression	Domains 2-3
elan.R_cTrPA_r	0	mol/(m ³ *s)	Total rate expression	Domains 2-3
elan.nil	0	A/m ²	Inward electrolyte current density	Domains 2-3

2.3.1 Transport Properties 1



Transport Properties 1

Selection

Geometric entity level	Domain
Selection	Domains 2-3

Equations

$$\frac{dc_i}{dt} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

Settings

Description	Value
Material	None
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}
Diffusion coefficient	User defined
Diffusion coefficient	{{1e-9[m^2/s], 0, 0}, {0, 1e-9[m^2/s], 0}, {0, 0, 1e-9[m^2/s]}}

Variables

Name	Expression	Unit	Description	Selection
elan.D_cRuiixx	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, xx component	Domains 2–3
elan.D_cRuiyx	0	m^2/s	Diffusion coefficient, yx component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.D_cRuiizx	0	m ² /s	Diffusion coefficient, zx component	Domains 2–3
elan.D_cRuiixy	0	m ² /s	Diffusion coefficient, xy component	Domains 2–3
elan.D_cRuiiyy	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, yy component	Domains 2–3
elan.D_cRuiizy	0	m ² /s	Diffusion coefficient, zy component	Domains 2–3
elan.D_cRuiixz	0	m ² /s	Diffusion coefficient, xz component	Domains 2–3
elan.D_cRuiiyz	0	m ² /s	Diffusion coefficient, yz component	Domains 2–3
elan.D_cRuiizz	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, zz component	Domains 2–3
elan.D_cRuixx	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, xx component	Domains 2–3
elan.D_cRuiyx	0	m ² /s	Diffusion coefficient, yx component	Domains 2–3
elan.D_cRuizx	0	m ² /s	Diffusion coefficient, zx component	Domains 2–3
elan.D_cRuixy	0	m ² /s	Diffusion coefficient, xy component	Domains 2–3
elan.D_cRuiyy	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, yy component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.D_cRuizy	0	m ² /s	Diffusion coefficient, zy component	Domains 2–3
elan.D_cRuixz	0	m ² /s	Diffusion coefficient, xz component	Domains 2–3
elan.D_cRuiyz	0	m ² /s	Diffusion coefficient, yz component	Domains 2–3
elan.D_cRuizz	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, zz component	Domains 2–3
elan.D_cRuiiix	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, xx component	Domains 2–3
elan.D_cRuiiixy	0	m ² /s	Diffusion coefficient, yx component	Domains 2–3
elan.D_cRuiiizx	0	m ² /s	Diffusion coefficient, zx component	Domains 2–3
elan.D_cRuiiixy	0	m ² /s	Diffusion coefficient, xy component	Domains 2–3
elan.D_cRuiiiyy	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, yy component	Domains 2–3
elan.D_cRuiiizy	0	m ² /s	Diffusion coefficient, zy component	Domains 2–3
elan.D_cRuiiixz	0	m ² /s	Diffusion coefficient, xz component	Domains 2–3
elan.D_cRuiiiyz	0	m ² /s	Diffusion coefficient, yz component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.D_cRuiizz	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, zz component	Domains 2–3
elan.D_cRui_hvxx	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, xx component	Domains 2–3
elan.D_cRui_hv yx	0	m ² /s	Diffusion coefficient, yx component	Domains 2–3
elan.D_cRui_hvz x	0	m ² /s	Diffusion coefficient, zx component	Domains 2–3
elan.D_cRui_hv xy	0	m ² /s	Diffusion coefficient, xy component	Domains 2–3
elan.D_cRui_hv yy	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, yy component	Domains 2–3
elan.D_cRui_hvz y	0	m ² /s	Diffusion coefficient, zy component	Domains 2–3
elan.D_cRui_hv xz	0	m ² /s	Diffusion coefficient, xz component	Domains 2–3
elan.D_cRui_hv yz	0	m ² /s	Diffusion coefficient, yz component	Domains 2–3
elan.D_cRui_hvz z	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, zz component	Domains 2–3
elan.D_chvxx	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, xx component	Domains 2–3
elan.D_chvyx	0	m ² /s	Diffusion coefficient, yx component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.D_chvzx	0	m ² /s	Diffusion coefficient, zx component	Domains 2–3
elan.D_chvxy	0	m ² /s	Diffusion coefficient, xy component	Domains 2–3
elan.D_chvyy	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, yy component	Domains 2–3
elan.D_chvzy	0	m ² /s	Diffusion coefficient, zy component	Domains 2–3
elan.D_chvxz	0	m ² /s	Diffusion coefficient, xz component	Domains 2–3
elan.D_chvyz	0	m ² /s	Diffusion coefficient, yz component	Domains 2–3
elan.D_chvzz	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, zz component	Domains 2–3
elan.D_cTrPAxx	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, xx component	Domains 2–3
elan.D_cTrPAyx	0	m ² /s	Diffusion coefficient, yx component	Domains 2–3
elan.D_cTrPAzx	0	m ² /s	Diffusion coefficient, zx component	Domains 2–3
elan.D_cTrPAxy	0	m ² /s	Diffusion coefficient, xy component	Domains 2–3
elan.D_cTrPAyy	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, yy component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.D_cTrPAzy	0	m ² /s	Diffusion coefficient, zy component	Domains 2–3
elan.D_cTrPAxz	0	m ² /s	Diffusion coefficient, xz component	Domains 2–3
elan.D_cTrPAyz	0	m ² /s	Diffusion coefficient, yz component	Domains 2–3
elan.D_cTrPAzz	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, zz component	Domains 2–3
elan.D_cTrPAHx x	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, xx component	Domains 2–3
elan.D_cTrPAHy x	0	m ² /s	Diffusion coefficient, yx component	Domains 2–3
elan.D_cTrPAHz x	0	m ² /s	Diffusion coefficient, zx component	Domains 2–3
elan.D_cTrPAHx y	0	m ² /s	Diffusion coefficient, xy component	Domains 2–3
elan.D_cTrPAHy y	1.0E-9[m ² /s]	m ² /s	Diffusion coefficient, yy component	Domains 2–3
elan.D_cTrPAHz y	0	m ² /s	Diffusion coefficient, zy component	Domains 2–3
elan.D_cTrPAHx z	0	m ² /s	Diffusion coefficient, xz component	Domains 2–3
elan.D_cTrPAHy z	0	m ² /s	Diffusion coefficient, yz component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.D_cTrPAHz z	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, zz component	Domains 2-3
elan.D_cTrPA_rx x	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, xx component	Domains 2-3
elan.D_cTrPA_ry x	0	m^2/s	Diffusion coefficient, yx component	Domains 2-3
elan.D_cTrPA_rz x	0	m^2/s	Diffusion coefficient, zx component	Domains 2-3
elan.D_cTrPA_rx y	0	m^2/s	Diffusion coefficient, xy component	Domains 2-3
elan.D_cTrPA_ry y	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, yy component	Domains 2-3
elan.D_cTrPA_rz y	0	m^2/s	Diffusion coefficient, zy component	Domains 2-3
elan.D_cTrPA_rx z	0	m^2/s	Diffusion coefficient, xz component	Domains 2-3
elan.D_cTrPA_ry z	0	m^2/s	Diffusion coefficient, yz component	Domains 2-3
elan.D_cTrPA_rz z	1.0E-9[m^2/s]	m^2/s	Diffusion coefficient, zz component	Domains 2-3
elan.Dav_cRuii	(elan.D_cRuiixx+elan.D_cRuiiyy+elan.D_cRuiizz)/3	m^2/s	Average diffusion coefficient	Domains 2-3
elan.Dav_cRui	(elan.D_cRuiixx+elan.D_cRuiiyy+elan.D_cRuiizz)/3	m^2/s	Average diffusion coefficient	Domains 2-3

Name	Expression	Unit	Description	Selection
elan.Dav_cRuii	$(\text{elan.D_cRuiiix} + \text{elan.D_cRuiiyy} + \text{elan.D_cRuiizz})/3$	m^2/s	Average diffusion coefficient	Domains 2–3
elan.Dav_cRuii_hv	$(\text{elan.D_cRuii_hvxx} + \text{elan.D_cRuii_hvyy} + \text{elan.D_cRuii_hvzz})/3$	m^2/s	Average diffusion coefficient	Domains 2–3
elan.Dav_chv	$(\text{elan.D_chvxx} + \text{elan.D_chvy} + \text{elan.D_chvzz})/3$	m^2/s	Average diffusion coefficient	Domains 2–3
elan.Dav_cTrPA	$(\text{elan.D_cTrPAxx} + \text{elan.D_cTrPAyy} + \text{elan.D_cTrPAzz})/3$	m^2/s	Average diffusion coefficient	Domains 2–3
elan.Dav_cTrPA_H	$(\text{elan.D_cTrPAHxx} + \text{elan.D_cTrPAHyy} + \text{elan.D_cTrPAHzz})/3$	m^2/s	Average diffusion coefficient	Domains 2–3
elan.Dav_cTrPA_r	$(\text{elan.D_cTrPA_rxx} + \text{elan.D_cTrPA_ryy} + \text{elan.D_cTrPA_rzz})/3$	m^2/s	Average diffusion coefficient	Domains 2–3
elan.tflux_cRuiix	elan.dflux_cRuiix	$\text{mol}/(\text{m}^2\text{s})$	Total flux, x component	Domains 2–3
elan.tflux_cRuiiy	elan.dflux_cRuiiy	$\text{mol}/(\text{m}^2\text{s})$	Total flux, y component	Domains 2–3
elan.tflux_cRuiiz	elan.dflux_cRuiiz	$\text{mol}/(\text{m}^2\text{s})$	Total flux, z component	Domains 2–3
elan.tflux_cRuix	elan.dflux_cRuix	$\text{mol}/(\text{m}^2\text{s})$	Total flux, x component	Domains 2–3
elan.tflux_cRuiy	elan.dflux_cRuiy	$\text{mol}/(\text{m}^2\text{s})$	Total flux, y component	Domains 2–3
elan.tflux_cRuiz	elan.dflux_cRuiz	$\text{mol}/(\text{m}^2\text{s})$	Total flux, z component	Domains 2–3
elan.tflux_cRuiix x	elan.dflux_cRuiiix	$\text{mol}/(\text{m}^2\text{s})$	Total flux, x component	Domains 2–3
elan.tflux_cRuiiy y	elan.dflux_cRuiiyy	$\text{mol}/(\text{m}^2\text{s})$	Total flux, y component	Domains 2–3
elan.tflux_cRuiiz z	elan.dflux_cRuiiiz	$\text{mol}/(\text{m}^2\text{s})$	Total flux, z	Domains 2–3

Name	Expression	Unit	Description	Selection
z			component	
elan.tflux_cRuii_hvx	elan.dflux_cRuii_hvx	mol/(m ² *s)	Total flux, x component	Domains 2-3
elan.tflux_cRuii_hvy	elan.dflux_cRuii_hvy	mol/(m ² *s)	Total flux, y component	Domains 2-3
elan.tflux_cRuii_hvz	elan.dflux_cRuii_hvz	mol/(m ² *s)	Total flux, z component	Domains 2-3
elan.tflux_chvx	elan.dflux_chvx	mol/(m ² *s)	Total flux, x component	Domains 2-3
elan.tflux_chvy	elan.dflux_chvy	mol/(m ² *s)	Total flux, y component	Domains 2-3
elan.tflux_chvz	elan.dflux_chvz	mol/(m ² *s)	Total flux, z component	Domains 2-3
elan.tflux_cTrPA_x	elan.dflux_cTrPAx	mol/(m ² *s)	Total flux, x component	Domains 2-3
elan.tflux_cTrPA_y	elan.dflux_cTrPAy	mol/(m ² *s)	Total flux, y component	Domains 2-3
elan.tflux_cTrPA_z	elan.dflux_cTrPAz	mol/(m ² *s)	Total flux, z component	Domains 2-3
elan.tflux_cTrPA_Hx	elan.dflux_cTrPAHx	mol/(m ² *s)	Total flux, x component	Domains 2-3
elan.tflux_cTrPA_Hy	elan.dflux_cTrPAHy	mol/(m ² *s)	Total flux, y component	Domains 2-3
elan.tflux_cTrPA_Hz	elan.dflux_cTrPAHz	mol/(m ² *s)	Total flux, z component	Domains 2-3
elan.tflux_cTrPA_rx	elan.dflux_cTrPA_rx	mol/(m ² *s)	Total flux, x component	Domains 2-3
elan.tflux_cTrPA_ry	elan.dflux_cTrPA_ry	mol/(m ² *s)	Total flux, y component	Domains 2-3
elan.tflux_cTrPA_rz	elan.dflux_cTrPA_rz	mol/(m ² *s)	Total flux, z component	Domains 2-3
elan.dfluxMag_cRuii	$\sqrt{\text{elan.dflux_cRuiix}^2 + \text{elan.dflux_cRuiiy}^2 + \text{elan.dflux_cRuiiz}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2-3

Name	Expression	Unit	Description	Selection
elan.dfluxMag_cRui	$\sqrt{\text{elan.dflux_cRuix}^2 + \text{elan.dflux_cRuiy}^2 + \text{elan.dflux_cRuiz}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2–3
elan.dfluxMag_cRuiii	$\sqrt{\text{elan.dflux_cRuiiix}^2 + \text{elan.dflux_cRuiiiy}^2 + \text{elan.dflux_cRuiiiz}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2–3
elan.dfluxMag_cRuii_hv	$\sqrt{\text{elan.dflux_cRuii_hvx}^2 + \text{elan.dflux_cRuii_hvy}^2 + \text{elan.dflux_cRuii_hvez}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2–3
elan.dfluxMag_c hv	$\sqrt{\text{elan.dflux_chvx}^2 + \text{elan.dflux_chvy}^2 + \text{elan.dflux_chvz}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2–3
elan.dfluxMag_cTrPA	$\sqrt{\text{elan.dflux_cTrPAx}^2 + \text{elan.dflux_cTrPAy}^2 + \text{elan.dflux_cTrPAz}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2–3
elan.dfluxMag_cTrPAH	$\sqrt{\text{elan.dflux_cTrPAHx}^2 + \text{elan.dflux_cTrPAHy}^2 + \text{elan.dflux_cTrPAHz}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2–3
elan.dfluxMag_cTrPA_r	$\sqrt{\text{elan.dflux_cTrPA_rx}^2 + \text{elan.dflux_cTrPA_ry}^2 + \text{elan.dflux_cTrPA_rz}^2}$	mol/(m ² *s)	Diffusive flux magnitude	Domains 2–3
elan.tfluxMag_cRuii	$\sqrt{\text{elan.tflux_cRuiix}^2 + \text{elan.tflux_cRuiiy}^2 + \text{elan.tflux_cRuiiz}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3
elan.tfluxMag_cRui	$\sqrt{\text{elan.tflux_cRuix}^2 + \text{elan.tflux_cRuiy}^2 + \text{elan.tflux_cRuiz}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3
elan.tfluxMag_cRuiii	$\sqrt{\text{elan.tflux_cRuiiix}^2 + \text{elan.tflux_cRuiiiy}^2 + \text{elan.tflux_cRuiiiz}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3
elan.tfluxMag_cRuii_hv	$\sqrt{\text{elan.tflux_cRuii_hvx}^2 + \text{elan.tflux_cRuii_hvy}^2 + \text{elan.tflux_cRuii_hvez}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3
elan.tfluxMag_c hv	$\sqrt{\text{elan.tflux_chvx}^2 + \text{elan.tflux_chvy}^2 + \text{elan.tflux_chvz}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.tfluxMag_cTrPA	$\sqrt{\text{elan.tflux_cTrPAx}^2 + \text{elan.tflux_cTrPAy}^2 + \text{elan.tflux_cTrPAz}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3
elan.tfluxMag_cTrPAH	$\sqrt{\text{elan.tflux_cTrPAHx}^2 + \text{elan.tflux_cTrPAHy}^2 + \text{elan.tflux_cTrPAHz}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3
elan.tfluxMag_cTrPA_r	$\sqrt{\text{elan.tflux_cTrPA_rx}^2 + \text{elan.tflux_cTrPA_ry}^2 + \text{elan.tflux_cTrPA_rz}^2}$	mol/(m ² *s)	Total flux magnitude	Domains 2–3
elan.dflux_cRuix	$-\text{elan.D_cRuixx} * \text{cRuix} - \text{elan.D_cRuixy} * \text{cRuiiy} - \text{elan.D_cRuixz} * \text{cRuiiz}$	mol/(m ² *s)	Diffusive flux, x component	Domains 2–3
elan.dflux_cRuiy	$-\text{elan.D_cRuiyx} * \text{cRuix} - \text{elan.D_cRuiyy} * \text{cRuiiy} - \text{elan.D_cRuiyz} * \text{cRuiiz}$	mol/(m ² *s)	Diffusive flux, y component	Domains 2–3
elan.dflux_cRuiiz	$-\text{elan.D_cRuiizx} * \text{cRuix} - \text{elan.D_cRuiizy} * \text{cRuiiy} - \text{elan.D_cRuiizz} * \text{cRuiiz}$	mol/(m ² *s)	Diffusive flux, z component	Domains 2–3
elan.dflux_cRuix	$-\text{elan.D_cRuixx} * \text{cRuix} - \text{elan.D_cRuixy} * \text{cRuiy} - \text{elan.D_cRuixz} * \text{cRuiz}$	mol/(m ² *s)	Diffusive flux, x component	Domains 2–3
elan.dflux_cRuiy	$-\text{elan.D_cRuiyx} * \text{cRuix} - \text{elan.D_cRuiyy} * \text{cRuiy} - \text{elan.D_cRuiyz} * \text{cRuiz}$	mol/(m ² *s)	Diffusive flux, y component	Domains 2–3
elan.dflux_cRuiz	$-\text{elan.D_cRuizx} * \text{cRuix} - \text{elan.D_cRuizy} * \text{cRuiy} - \text{elan.D_cRuizz} * \text{cRuiz}$	mol/(m ² *s)	Diffusive flux, z component	Domains 2–3
elan.dflux_cRuiix	$-\text{elan.D_cRuiixx} * \text{cRuiix} - \text{elan.D_cRuiixy} * \text{cRuiiy} - \text{elan.D_cRuiixz} * \text{cRuiiz}$	mol/(m ² *s)	Diffusive flux, x component	Domains 2–3
elan.dflux_cRuiiy	$-\text{elan.D_cRuiiyy} * \text{cRuiiy} - \text{elan.D_cRuiiyy} * \text{cRuiiy} - \text{elan.D_cRuiiyz} * \text{cRuiiz}$	mol/(m ² *s)	Diffusive flux, y component	Domains 2–3
elan.dflux_cRuiiz	$-\text{elan.D_cRuiiizx} * \text{cRuiix} - \text{elan.D_cRuiiizy} * \text{cRuiiy} - \text{elan.D_cRuiiizz} * \text{cRuiiz}$	mol/(m ² *s)	Diffusive flux, z component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.dflux_cRuii_hvx	- elan.D_cRuii_hvxx*cRuii_hv x- elan.D_cRuii_hvxy*cRuii_hv y- elan.D_cRuii_hvzx*cRuii_hv z	mol/(m ² *s)	Diffusive flux, x component	Domains 2-3
elan.dflux_cRuii_hvy	- elan.D_cRuii_hvyx*cRuii_hv x- elan.D_cRuii_hvyy*cRuii_hv y- elan.D_cRuii_hvyz*cRuii_hv z	mol/(m ² *s)	Diffusive flux, y component	Domains 2-3
elan.dflux_cRuii_hvz	- elan.D_cRuii_hvzx*cRuii_hv x- elan.D_cRuii_hvzy*cRuii_hv y- elan.D_cRuii_hvzz*cRuii_hv z	mol/(m ² *s)	Diffusive flux, z component	Domains 2-3
elan.dflux_chvx	-elan.D_chvxx*chvx- elan.D_chvxy*chvy- elan.D_chvxz*chvz	mol/(m ² *s)	Diffusive flux, x component	Domains 2-3
elan.dflux_chvy	-elan.D_chvyx*chvx- elan.D_chvyy*chvy- elan.D_chvyz*chvz	mol/(m ² *s)	Diffusive flux, y component	Domains 2-3
elan.dflux_chvz	-elan.D_chvzx*chvx- elan.D_chvzy*chvy- elan.D_chvzz*chvz	mol/(m ² *s)	Diffusive flux, z component	Domains 2-3
elan.dflux_cTrPAx	-elan.D_cTrPAxx*cTrPAx- elan.D_cTrPAxy*cTrPAy- elan.D_cTrPAxz*cTrPAz	mol/(m ² *s)	Diffusive flux, x component	Domains 2-3
elan.dflux_cTrPAy	-elan.D_cTrPAyx*cTrPAx- elan.D_cTrPAyy*cTrPAy- elan.D_cTrPAyz*cTrPAz	mol/(m ² *s)	Diffusive flux, y component	Domains 2-3
elan.dflux_cTrPAz	-elan.D_cTrPAzx*cTrPAx- elan.D_cTrPAzy*cTrPAy- elan.D_cTrPAzz*cTrPAz	mol/(m ² *s)	Diffusive flux, z component	Domains 2-3

Name	Expression	Unit	Description	Selection
elan.dflux_cTrPAHx	- elan.D_cTrPAHxx*cTrPAHx - elan.D_cTrPAHxy*cTrPAHy - elan.D_cTrPAHxz*cTrPAHz	mol/(m ² *s)	Diffusive flux, x component	Domains 2-3
elan.dflux_cTrPAHy	- elan.D_cTrPAHyx*cTrPAHx - elan.D_cTrPAHyy*cTrPAHy - elan.D_cTrPAHyz*cTrPAHz	mol/(m ² *s)	Diffusive flux, y component	Domains 2-3
elan.dflux_cTrPAHz	- elan.D_cTrPAHzx*cTrPAHx - elan.D_cTrPAHzy*cTrPAHy - elan.D_cTrPAHzz*cTrPAHz	mol/(m ² *s)	Diffusive flux, z component	Domains 2-3
elan.dflux_cTrPA_rx	- elan.D_cTrPA_rxx*cTrPA_rx - elan.D_cTrPA_rxy*cTrPA_ry - elan.D_cTrPA_rxz*cTrPA_rz	mol/(m ² *s)	Diffusive flux, x component	Domains 2-3
elan.dflux_cTrPA_ry	- elan.D_cTrPA_ryx*cTrPA_rx - elan.D_cTrPA_ryy*cTrPA_ry - elan.D_cTrPA_ryz*cTrPA_rz	mol/(m ² *s)	Diffusive flux, y component	Domains 2-3
elan.dflux_cTrPA_rz	- elan.D_cTrPA_rzx*cTrPA_rx - elan.D_cTrPA_rzy*cTrPA_ry - elan.D_cTrPA_rzz*cTrPA_rz	mol/(m ² *s)	Diffusive flux, z component	Domains 2-3
elan.grad_cRuiix	cRuiix	mol/m ⁴	Concentration gradient, x component	Domains 2-3
elan.grad_cRuiiy	cRuiiy	mol/m ⁴	Concentration gradient, y component	Domains 2-3

Name	Expression	Unit	Description	Selection
elan.grad_cRuiiz	cRuiiz	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.grad_cRuix	cRuix	mol/m ⁴	Concentration gradient, x component	Domains 2–3
elan.grad_cRuiy	cRuiy	mol/m ⁴	Concentration gradient, y component	Domains 2–3
elan.grad_cRuiz	cRuiz	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.grad_cRuiix x	cRuiix	mol/m ⁴	Concentration gradient, x component	Domains 2–3
elan.grad_cRuiiy y	cRuiiy	mol/m ⁴	Concentration gradient, y component	Domains 2–3
elan.grad_cRuiiz z	cRuiiz	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.grad_cRuii_hvx	cRuii_hvx	mol/m ⁴	Concentration gradient, x component	Domains 2–3
elan.grad_cRuii_hvy	cRuii_hvy	mol/m ⁴	Concentration gradient, y component	Domains 2–3
elan.grad_cRuii_hvz	cRuii_hvz	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.grad_chvx	chvx	mol/m ⁴	Concentration gradient, x component	Domains 2–3
elan.grad_chvy	chvy	mol/m ⁴	Concentration gradient, y component	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.grad_chvz	chvz	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.grad_cTrPA _x	cTrPA _x	mol/m ⁴	Concentration gradient, x component	Domains 2–3
elan.grad_cTrPA _y	cTrPA _y	mol/m ⁴	Concentration gradient, y component	Domains 2–3
elan.grad_cTrPA _z	cTrPA _z	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.grad_cTrPA _{Hx}	cTrPA _{Hx}	mol/m ⁴	Concentration gradient, x component	Domains 2–3
elan.grad_cTrPA _{Hy}	cTrPA _{Hy}	mol/m ⁴	Concentration gradient, y component	Domains 2–3
elan.grad_cTrPA _{Hz}	cTrPA _{Hz}	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.grad_cTrPA _{_rx}	cTrPA _{rx}	mol/m ⁴	Concentration gradient, x component	Domains 2–3
elan.grad_cTrPA _{_ry}	cTrPA _{ry}	mol/m ⁴	Concentration gradient, y component	Domains 2–3
elan.grad_cTrPA _{_rz}	cTrPA <sub_rz< sub=""></sub_rz<>	mol/m ⁴	Concentration gradient, z component	Domains 2–3
elan.phil	0	V	Electrolyte potential	Domains 2–3
elan.Res_cRuii	-elan.R_cRuii	mol/(m ³ *s)	Equation residual	Domains 2–3
elan.Res_cRui	-elan.R_cRui	mol/(m ³ *s)	Equation residual	Domains 2–3

Name	Expression	Unit	Description	Selection
elan.Res_cRuiii	-elan.R_cRuiii	mol/(m ³ *s)	Equation residual	Domains 2-3
elan.Res_cRuii_hv	-elan.R_cRuii_hv	mol/(m ³ *s)	Equation residual	Domains 2-3
elan.Res_chv	-elan.R_chv	mol/(m ³ *s)	Equation residual	Domains 2-3
elan.Res_cTrPA	-elan.R_cTrPA	mol/(m ³ *s)	Equation residual	Domains 2-3
elan.Res_cTrPAH	-elan.R_cTrPAH	mol/(m ³ *s)	Equation residual	Domains 2-3
elan.Res_cTrPA_r	-elan.R_cTrPA_r	mol/(m ³ *s)	Equation residual	Domains 2-3

Shape functions

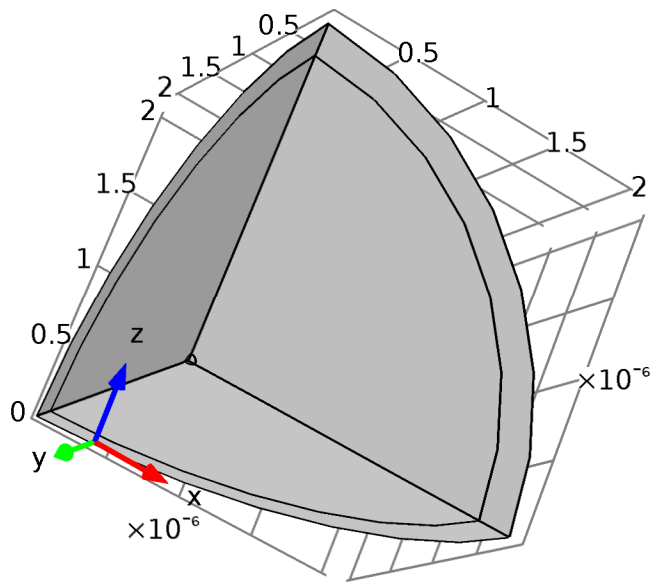
Name	Shape function	Unit	Description	Shape frame	Selection
cRuii	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3
cRui	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3
cRuiii	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3
cRuii_hv	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3
chv	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3
cTrPA	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3
cTrPAH	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3
cTrPA_r	Lagrange (Linear)	mol/m ³	Concentration	Material	Domains 2-3

Weak expressions

Weak expression	Integration frame	Selection
- cRuii*test(cRuii)+elan.dflux_cRuiix*test(cRuiix)+elan.dflux_cRuiiy*test(cRuiiy)+elan.dflux_cRuiiz*test(cRuiiz)	Material	Domains 2-3
- cRui*test(cRui)+elan.dflux_cRuix*test(cRuix)+elan.dflux_cRuiy*test(cRuiy)+elan.dflux_cRuiz*test(cRuiz)	Material	Domains 2-3
-	Material	Domains 2-3

Weak expression	Integration frame	Selection
cRuiiit*test(cRuiii)+elan.dflux_cRuiiix*test(cRuiiix)+elan.dflux_cRuiiiy*test(cRuiiiy)+elan.dflux_cRuiiiz*test(cRuiiiz)		
- cRuii_hvt*test(cRuii_hv)+elan.dflux_cRuii_hvx*test(cRuii_hvx)+elan.dflux_cRuii_hvy*test(cRuii_hvy)+elan.dflux_cRuii_hvz*test(cRuii_hvz)	Material	Domains 2-3
- chvt*test(chv)+elan.dflux_chvx*test(chvx)+elan.dflux_chvy*test(chvy)+elan.dflux_chvz*test(chvz)	Material	Domains 2-3
- cTrPA_t*test(cTrPA)+elan.dflux_cTrPAx*test(cTrPAx)+elan.dflux_cTrPAy*test(cTrPAy)+elan.dflux_cTrPAz*test(cTrPAz)	Material	Domains 2-3
- cTrPAH_t*test(cTrPAH)+elan.dflux_cTrPAHx*test(cTrPAHx)+elan.dflux_cTrPAHy*test(cTrPAHy)+elan.dflux_cTrPAHz*test(cTrPAHz)	Material	Domains 2-3
- cTrPA_rt*test(cTrPA_r)+elan.dflux_cTrPA_rx*test(cTrPA_rx)+elan.dflux_cTrPA_ry*test(cTrPA_ry)+elan.dflux_cTrPA_rz*test(cTrPA_rz)	Material	Domains 2-3
elan.streamline*(isScalingSystemDomain==0)	Material	Domains 2-3
elan.crosswind*(isScalingSystemDomain==0)	Material	Domains 2-3

2.3.2 No Flux 1



No Flux 1

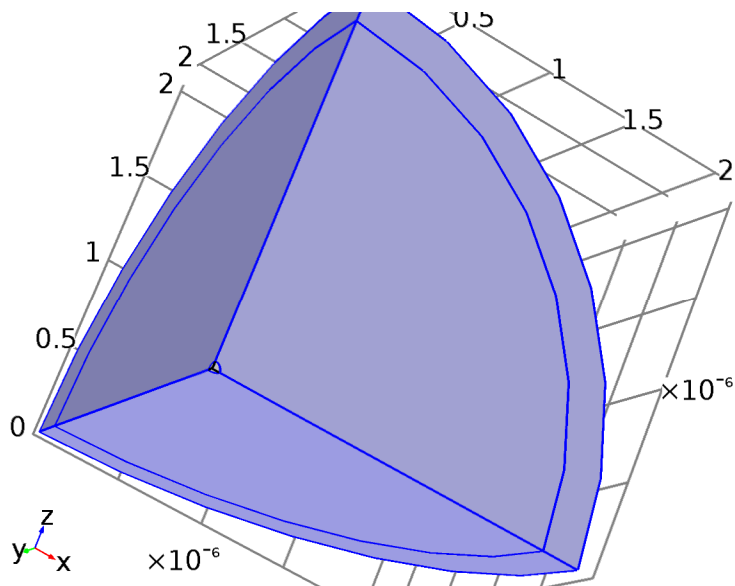
Selection

Geometric entity level	Boundary
Selection	No boundaries

Equations

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

2.3.3 Initial Values 1



Initial Values 1

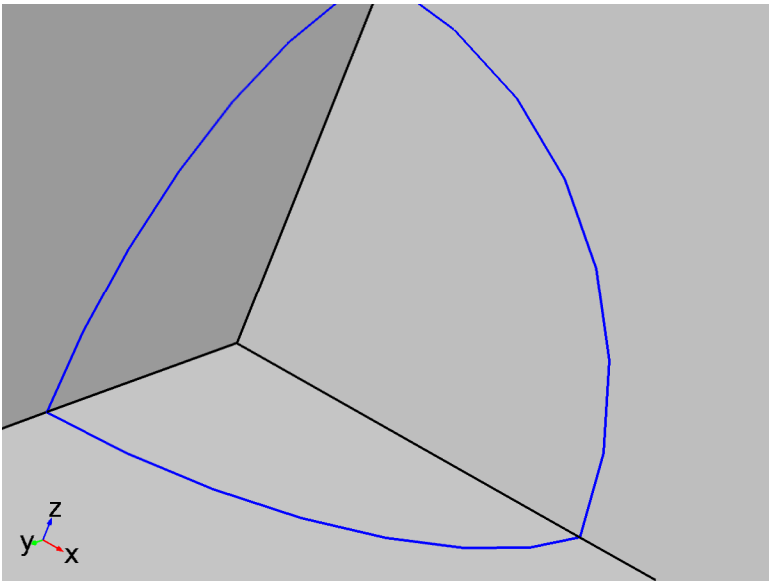
Selection

Geometric entity level	Domain
Selection	Domains 2-3

Settings

Description	Value
Concentration	{cRu_bulk, 0, 0, 0, 0, cTrPA_bulk, 0, 0}

2.3.4 Electrode Surface 1



Electrode Surface 1

Selection

Geometric entity level	Boundary
Selection	Boundary 6

Equations

$$i_{total} = \sum_m i_{loc,m} + i_{dl}$$
$$-\mathbf{n} \cdot \mathbf{N}_i = R_{i,tot}, \quad R_{i,tot} = \sum_{i,m, \dots} R_{i,m}$$

Settings

Description	Value
Film resistance	No film resistance

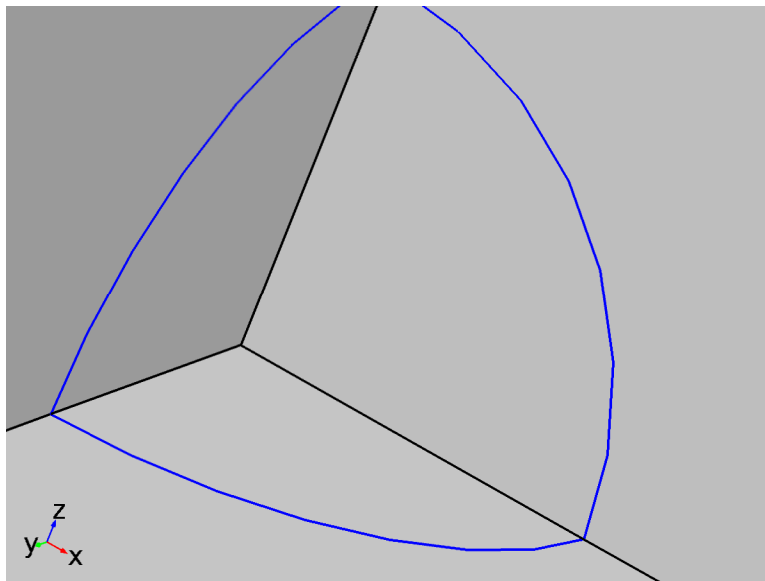
Description	Value
Boundary condition	Cyclic voltammetry
Linear sweep rate	v
Start potential	On
Start potential	0.8
Number of cycles	1
Vertex potential 1	E_vertex1
Vertex potential 2	E_vertex2
End potential	Off
End potential	0
Perturbation amplitude	0

Variables

Name	Expression	Unit	Description	Selection
elan.mulstopcond	$t > (\text{abs}(-0.8 + E_{\text{vertex1}}) + \text{elan.ncycle_els1} * \text{abs}(2 * (E_{\text{vertex1}} - E_{\text{vertex2}}))) / v$	1	Multiplicative stop condition	Global
elan.nil	elan.itot	A/m ²	Inward electrolyte current density	Boundary 6
elan.ncycle_els1	1	1	Number of cycles	Global
elan.Itot_els1	elan.els1.int(elan.itot*elan.dvolfactor)	A	Total current	Global
elan.phis_els1	elan.els1.int(elan.phisext*elan.dvolfactor)/elan.Area_els1	V	Electric potential	Global
elan.Ect	elan.phisext-elans.phil	V	Electrode potential	Boundary 6
elan.Area_els1	elan.els1.int(elan.dvolfactor)	m ²	Area	Global
elan.dvolfactor	1	1	Differential volume factor	Boundary 6

Name	Expression	Unit	Description	Selection
elan.itotavg_els1	elan.els1.int(elan.itot*elan.dvolfactor)/elan.Area_els1	A/m^2	Average total interface current density	Global
elan.Temp	model.input.mininput_temperature	K	Temperature	Boundary 6
elan.itot	0	A/m^2	Total interface current density	Boundary 6
elan.cycle_els1	max(round(0.5+(min(0,(abs(-0.8+E_vertex1)+(-1+elan.ncycle_els1)*abs(2*(E_vertex1-E_vertex2)))/v)-abs(-0.8+E_vertex1)/v)*v/abs(2*(E_vertex1-E_vertex2))),1)	1	Cycle number	Global
elan.phisext	elan.cv_els1(0)	V	External electric potential	Boundary 6

Electrode Reaction 1



Electrode Reaction 1

Selection

Geometric entity level	Boundary
Selection	Boundary 6

Equations

$$\eta_1 = \phi_{s,ext} - \phi_1 - E_{eq}$$

Settings

Description	Value
Equilibrium potential	User defined
Equilibrium potential	Ef1
Temperature derivative of equilibrium potential	User defined
Temperature derivative of equilibrium potential	0
Kinetics expression type	Concentration dependent kinetics
Limiting current density	Off
Exchange current density	1e2[A/m^2]
Anodic transfer coefficient	0.5
Cathodic transfer coefficient	0.5
Reduced species expression	cRuii
Oxidized species expression	cRuiii
Number of participating electrons	1
Stoichiometric coefficient	{1, 0, -1, 0, 0, 0, 0, 0}

Variables

Name	Expression	Unit	Description	Selection
elan.itot	elan.iloc_er1	A/m^2	Total interface current density	Boundary 6
elan.Qbfc	elan.Qrev_er1+elan.Qirrev_er1	W/m^2	Electrochemical reaction boundary heat source	Boundary 6
elan.Eeq_er1	Ef1	V	Equilibrium potential	Boundary 6
elan.dEeqdT_er1	0	V/K	Temperature derivative of equilibrium potential	Boundary 6
elan.i0_er1	100[A/m^2]	A/m^2	Exchange current density	Boundary 6

Name	Expression	Unit	Description	Selection
elan.alphaa_er1	0.5	1	Anodic transfer coefficient	Boundary 6
elan.alphac_er1	0.5	1	Cathodic transfer coefficient	Boundary 6
elan.CR_er1	cRuii	1	Reduced species expression	Boundary 6
elan.CO_er1	cRuiii	1	Oxidized species expression	Boundary 6
elan.iloc_er1	elan.i0_er1*(max(elan.CR_er1,eps^2)*exp(elan.alphaa_er1*F_const*elan.eta_er1/(R_const*model.input.mininput_temperature)))-max(elan.CO_er1,eps^2)*exp(-elan.alphac_er1*F_const*elan.eta_er1/(R_const*model.input.mininput_temperature))	A/m^2	Local current density	Boundary 6
elan.els1.er1.iloc	elan.iloc_er1	A/m^2	Local current density	Boundary 6
elan.els1.er1.Vi0_cRuii	1	1	Stoichiometric coefficient	Boundary 6
elan.els1.er1.Vi0_cRui	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er1.Vi0_cRuiii	-1	1	Stoichiometric coefficient	Boundary 6
elan.els1.er1.Vi0_cRuii_hv	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er1.Vi0_chv	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er1.Vi0_cTrPA	0	1	Stoichiometric coefficient	Boundary 6

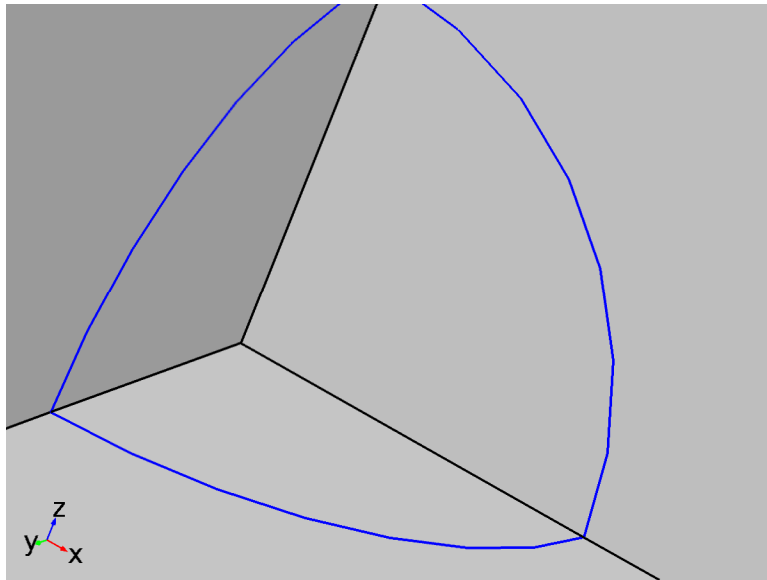
Name	Expression	Unit	Description	Selection
elan.els1.er1.Vi0_cTrPAH	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er1.Vi0_cTrPA_r	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er1.N0_cRuii	-elan.iloc_er1/F_const	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er1.N0_cRui	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er1.N0_cRuiii	elan.iloc_er1/F_const	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er1.N0_cRuii_hv	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er1.N0_chv	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er1.N0_cTrPA	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er1.N0_cTrPAH	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er1.N0_cTrPA_r	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.Qirrev_er1	elan.iloc_er1*elan.eta_er1	W/m ²	Irreversible heat flux	Boundary 6
elan.Qrev_er1	elan.iloc_er1*model.input.minput_temperature*elan.dEeqdT_er1	W/m ²	Reversible heat flux	Boundary 6
elan.eta_er1	elan.Ect-elan.Eeq_er1	V	Overpotential	Boundary 6

Weak expressions

Weak expression	Integration frame	Selection
elan.els1.er1.N0_cRuii*test(cRuii)	Material	Boundary 6
elan.els1.er1.N0_cRui*test(cRui)	Material	Boundary 6
elan.els1.er1.N0_cRuiii*test(cRuiii)	Material	Boundary 6
elan.els1.er1.N0_cRuii_hv*test(cRuii_hv)	Material	Boundary 6

Weak expression	Integration frame	Selection
elan.els1.er1.N0_chv*test(chv)	Material	Boundary 6
elan.els1.er1.N0_cTrPA*test(cTrPA)	Material	Boundary 6
elan.els1.er1.N0_cTrPAH*test(cTrPAH)	Material	Boundary 6
elan.els1.er1.N0_cTrPA_r*test(cTrPA_r)	Material	Boundary 6

Electrode Reaction 2



Electrode Reaction 2

Selection

Geometric entity level	Boundary
Selection	Boundary 6

Equations

$$i_1 = \phi_{s,ext} - \phi_1 - E_{eq}$$

Settings

Description	Value
Equilibrium potential	User defined
Equilibrium potential	Ef2
Temperature derivative of equilibrium potential	User defined
Temperature derivative of equilibrium potential	0

Description	Value
Kinetics expression type	Concentration dependent kinetics
Limiting current density	Off
Exchange current density	1e2[A/m ²]
Anodic transfer coefficient	0.5
Cathodic transfer coefficient	0.5
Reduced species expression	cTrPA
Oxidized species expression	cTrPAH
Number of participating electrons	1
Stoichiometric coefficient	{0, 0, 0, 0, 0, 1, -1, 0}

Variables

Name	Expression	Unit	Description	Selection
elan.itot	elan.iloc_er2	A/m ²	Total interface current density	Boundary 6
elan.Qbfc	elan.Qrev_er2+elan.Qirrev_er2	W/m ²	Electrochemical reaction boundary heat source	Boundary 6
elan.Eeq_er2	Ef2	V	Equilibrium potential	Boundary 6
elan.dEeqdT_er2	0	V/K	Temperature derivative of equilibrium potential	Boundary 6
elan.i0_er2	100[A/m ²]	A/m ²	Exchange current density	Boundary 6
elan.alphaa_er2	0.5	1	Anodic transfer coefficient	Boundary 6
elan.alphac_er2	0.5	1	Cathodic transfer coefficient	Boundary 6
elan.CR_er2	cTrPA	1	Reduced species expression	Boundary 6
elan.CO_er2	cTrPAH	1	Oxidized species expression	Boundary 6

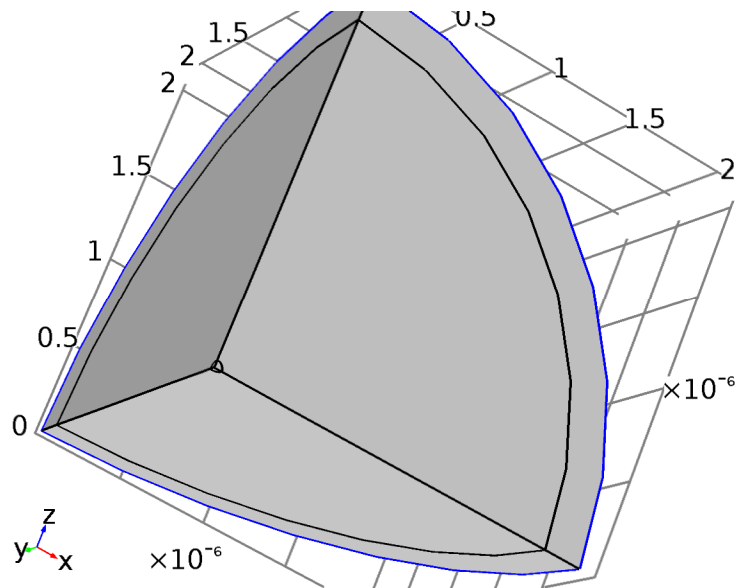
Name	Expression	Unit	Description	Selection
elan.iloc_er2	$\text{elan.i0_er2} * (\max(\text{elan.CR_er2}, \epsilon^2) * \exp(\text{elan.alphaa_er2} * F_{\text{const}} * \text{elan.eta_er2} / (R_{\text{const}} * \text{model.input.mininput_temperature}))) - \max(\text{elan.CO_er2}, \epsilon^2) * \exp(-\text{elan.alphac_er2} * F_{\text{const}} * \text{elan.eta_er2} / (R_{\text{const}} * \text{model.input.mininput_temperature})))$	A/m ²	Local current density	Boundary 6
elan.els1.er2.iloc	elan.iloc_er2	A/m ²	Local current density	Boundary 6
elan.els1.er2.Vi0_cRuii	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.Vi0_cRui	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.Vi0_cRuiii	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.Vi0_cRuii_hv	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.Vi0_chv	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.Vi0_cTrPA	1	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.Vi0_cTrPAH	-1	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.Vi0_cTrPA_r	0	1	Stoichiometric coefficient	Boundary 6
elan.els1.er2.N0_cRuii	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er2.N0_cRui	0	mol/(m ² *s)	Inward flux	Boundary 6

Name	Expression	Unit	Description	Selection
elan.els1.er2.N0_cRuiii	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er2.N0_cRuii_hv	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er2.N0_chv	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er2.N0_cTrPA	-elan.iloc_er2/F_const	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er2.N0_cTrPAH	elan.iloc_er2/F_const	mol/(m ² *s)	Inward flux	Boundary 6
elan.els1.er2.N0_cTrPA_r	0	mol/(m ² *s)	Inward flux	Boundary 6
elan.Qirrev_er2	elan.iloc_er2*elan.eta_er2	W/m ²	Irreversible heat flux	Boundary 6
elan.Qrev_er2	elan.iloc_er2*model.input.minput_temperature*elan.dEeqdT_er2	W/m ²	Reversible heat flux	Boundary 6
elan.eta_er2	elan.Ect-elan.Eeq_er2	V	Overpotential	Boundary 6

Weak expressions

Weak expression	Integration frame	Selection
elan.els1.er2.N0_cRuii*test(cRuii)	Material	Boundary 6
elan.els1.er2.N0_cRui*test(cRui)	Material	Boundary 6
elan.els1.er2.N0_cRuiii*test(cRuiii)	Material	Boundary 6
elan.els1.er2.N0_cRuii_hv*test(cRuii_hv)	Material	Boundary 6
elan.els1.er2.N0_chv*test(chv)	Material	Boundary 6
elan.els1.er2.N0_cTrPA*test(cTrPA)	Material	Boundary 6
elan.els1.er2.N0_cTrPAH*test(cTrPAH)	Material	Boundary 6
elan.els1.er2.N0_cTrPA_r*test(cTrPA_r)	Material	Boundary 6

2.3.5 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 10

Equations

$$c_i = c_{0,i}$$

Settings

Description	Value
Species cRu _{ii}	On
Species cRu _i	On
Species cRu _{iii}	On
Species cRu _{ii} _hv	On
Species chv	On
Species cTrPA	On
Species cTrPAH	On
Species cTrPA_r	On
Concentration	{cRu_bulk, 0, 0, 0, 0, cTrPA_bulk, 0, 0}
Apply reaction terms on	All physics (symmetric)

Description	Value
Use weak constraints	Off
Constraint method	Elemental

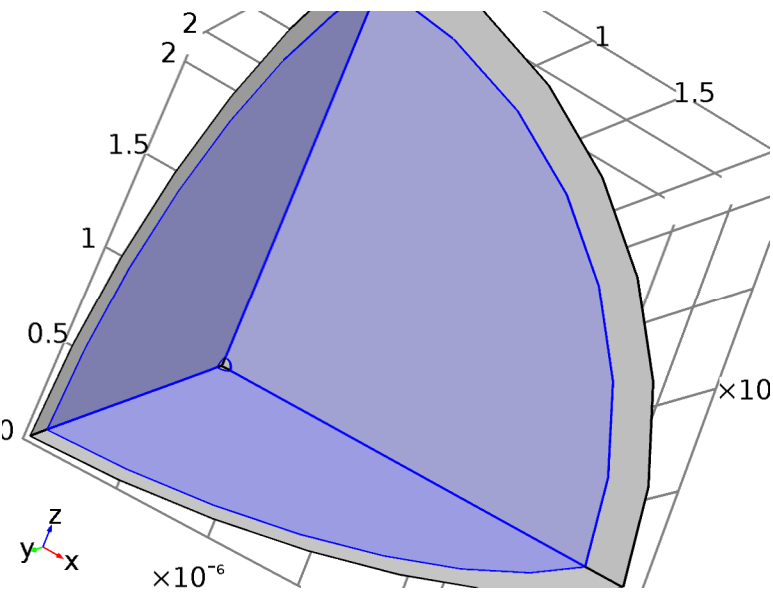
Variables

Name	Expression	Unit	Description	Selection
elan.c0_cRuii	cRu_bulk	mol/m ³	Concentration	Boundary 10
elan.c0_cRui	0	mol/m ³	Concentration	Boundary 10
elan.c0_cRuiii	0	mol/m ³	Concentration	Boundary 10
elan.c0_cRuii_hv	0	mol/m ³	Concentration	Boundary 10
elan.c0_chv	0	mol/m ³	Concentration	Boundary 10
elan.c0_cTrPA	cTrPA_bulk	mol/m ³	Concentration	Boundary 10
elan.c0_cTrPAH	0	mol/m ³	Concentration	Boundary 10
elan.c0_cTrPA_r	0	mol/m ³	Concentration	Boundary 10

Shape functions

Constraint	Constraint force	Shape function	Selection
-cRuii+elan.c0_cRuii	test(-cRuii+elan.c0_cRuii)	Lagrange (Linear)	Boundary 10
-cRui+elan.c0_cRui	test(-cRui+elan.c0_cRui)	Lagrange (Linear)	Boundary 10
-cRuiii+elan.c0_cRuiii	test(-cRuiii+elan.c0_cRuiii)	Lagrange (Linear)	Boundary 10
-cRuii_hv+elan.c0_cRuii_hv	test(-cRuii_hv+elan.c0_cRuii_hv)	Lagrange (Linear)	Boundary 10
-chv+elan.c0_chv	test(-chv+elan.c0_chv)	Lagrange (Linear)	Boundary 10
-cTrPA+elan.c0_cTrPA	test(-cTrPA+elan.c0_cTrPA)	Lagrange (Linear)	Boundary 10
-cTrPAH+elan.c0_cTrPAH	test(-cTrPAH+elan.c0_cTrPAH)	Lagrange (Linear)	Boundary 10
-cTrPA_r+elan.c0_cTrPA_r	test(-cTrPA_r+elan.c0_cTrPA_r)	Lagrange (Linear)	Boundary 10

2.3.6 Reactions 1



Reactions 1

Selection

Geometric entity level	Domain
Selection	Domain 2

Equations

$$\frac{dc_i}{dt} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

Settings

Description	Value
Total rate expression	User defined
Total rate expression	-537*cTrPAH + 1e10*cRui*cRuiii
Total rate expression	User defined
Total rate expression	537*cTrPAH - 1e10*cRui*cRuiii
Total rate expression	User defined
Total rate expression	-1e10*cRui*cRuiii
Total rate expression	User defined
Total rate expression	1e10*cRui*cRuiii - 15848 *cRuii_hv
Total rate expression	User defined

Description	Value
Total rate expression	15848 *cRuii_hv
Total rate expression	User defined
Total rate expression	0
Total rate expression	User defined
Total rate expression	-537*cTrPAH
Total rate expression	User defined
Total rate expression	0

Variables

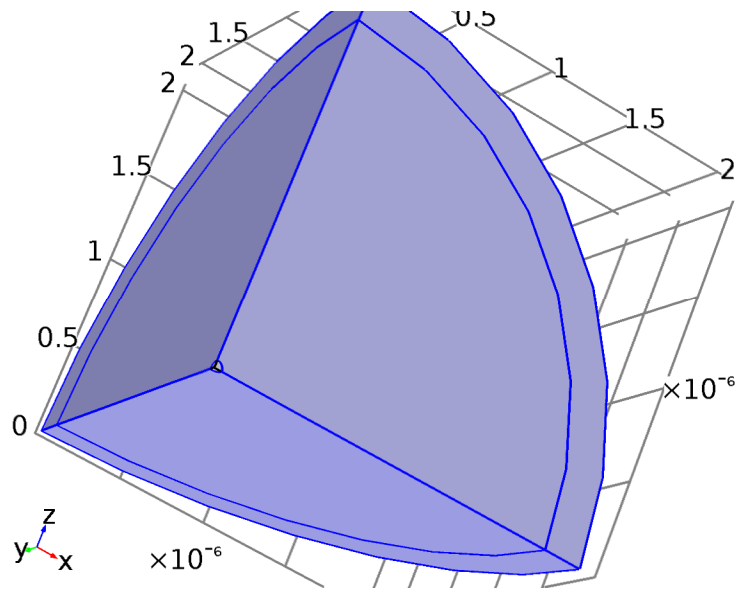
Name	Expression	Unit	Description	Selection
elan.R_cRuii	elan.reac1.R_cRuii	mol/(m ³ *s)	Total rate expression	Domain 2
elan.R_cRui	elan.reac1.R_cRui	mol/(m ³ *s)	Total rate expression	Domain 2
elan.R_cRuiii	elan.reac1.R_cRuiii	mol/(m ³ *s)	Total rate expression	Domain 2
elan.R_cRuii_hv	elan.reac1.R_cRuii_hv	mol/(m ³ *s)	Total rate expression	Domain 2
elan.R_chv	elan.reac1.R_chv	mol/(m ³ *s)	Total rate expression	Domain 2
elan.R_cTrPA	elan.reac1.R_cTrPA	mol/(m ³ *s)	Total rate expression	Domain 2
elan.R_cTrPAH	elan.reac1.R_cTrPAH	mol/(m ³ *s)	Total rate expression	Domain 2
elan.R_cTrPA_r	elan.reac1.R_cTrPA_r	mol/(m ³ *s)	Total rate expression	Domain 2
elan.reac1.R_cRuii	model.input.R_cRuii	mol/(m ³ *s)	Total rate expression	Domain 2
elan.reac1.R_cRui	model.input.R_cRui	mol/(m ³ *s)	Total rate expression	Domain 2
elan.reac1.R_cRuiii	model.input.R_cRuiii	mol/(m ³ *s)	Total rate expression	Domain 2

Name	Expression	Unit	Description	Selection
elan.reac1.R_cRuii_hv	model.input.R_cRuii_hv	mol/(m ³ *s)	Total rate expression	Domain 2
elan.reac1.R_chv	model.input.R_chv	mol/(m ³ *s)	Total rate expression	Domain 2
elan.reac1.R_cTrPA	model.input.R_cTrPA	mol/(m ³ *s)	Total rate expression	Domain 2
elan.reac1.R_cTrPAH	model.input.R_cTrPAH	mol/(m ³ *s)	Total rate expression	Domain 2
elan.reac1.R_cTrPA_r	model.input.R_cTrPA_r	mol/(m ³ *s)	Total rate expression	Domain 2

Weak expressions

Weak expression	Integration frame	Selection
elan.reac1.R_cRuii*test(cRuii)	Material	Domain 2
elan.reac1.R_cRui*test(cRui)	Material	Domain 2
elan.reac1.R_cRuii*test(cRuii)	Material	Domain 2
elan.reac1.R_cRuii_hv*test(cRuii_hv)	Material	Domain 2
elan.reac1.R_chv*test(chv)	Material	Domain 2
elan.reac1.R_cTrPA*test(cTrPA)	Material	Domain 2
elan.reac1.R_cTrPAH*test(cTrPAH)	Material	Domain 2
elan.reac1.R_cTrPA_r*test(cTrPA_r)	Material	Domain 2

2.3.7 Symmetry 1



Symmetry 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 4-5, 7-8, 11-12

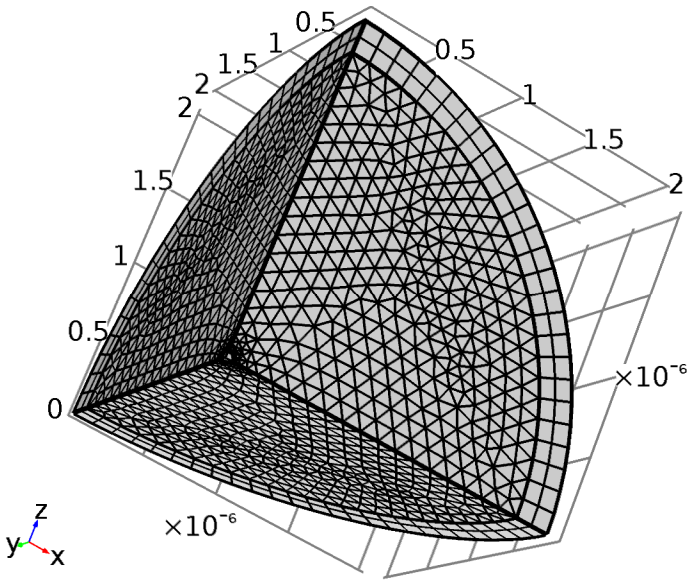
Equations

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

2.4 Mesh 1

Mesh statistics

Description	Value
Minimum element quality	0.1706
Average element quality	0.7783
Tetrahedral elements	38692
Prism elements	2100
Triangular elements	3934
Quadrilateral elements	156
Edge elements	231
Vertex elements	9



Mesh 1

2.4.1 Size (size)

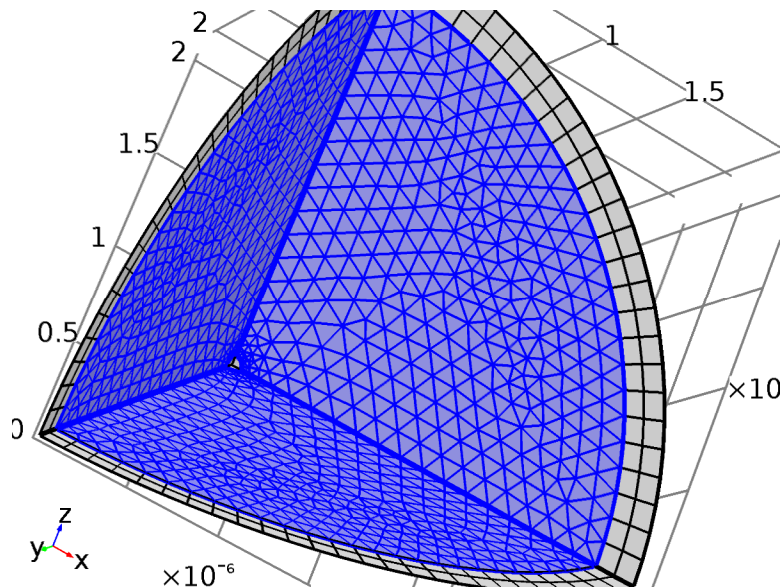
Settings

Description	Value
Maximum element size	1.12E-7
Minimum element size	8.16E-9
Curvature factor	0.4
Resolution of narrow regions	0.7
Maximum element growth rate	1.4
Predefined size	Finer

2.4.2 Free Tetrahedral 1 (ftet1)

Selection

Geometric entity level	Domain
Selection	Domain 2

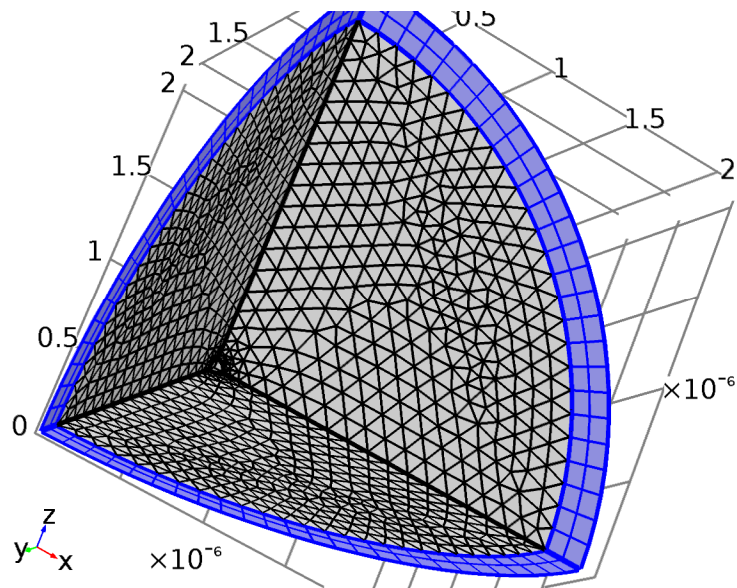


Free Tetrahedral 1

2.4.3 Swept 1 (swe1)

Selection

Geometric entity level	Domain
Selection	Domain 3



Swept 1

3 Study 1

Computation information

Computation time	41 min 2 s
CPU	2 cores
Operating system	Mac OS X

3.1 Cyclic Voltammetry

Study settings

Description	Value
Include geometric nonlinearity	Off

Physics and variables selection

Physics interface	Discretization
Electroanalysis (elan)	physics

Mesh selection

Geometry	Mesh
Geometry 1 (geom1)	mesh1

3.2 Solver Configurations

3.2.1 Solver 1

4 Results

4.1 Data Sets

4.1.1 Data Set 1

4.2 Plot Groups

4.2.1 Plot Group 1

4.2.2 Plot Group 1

4.2.3 Plot Group 1

4.2.4 Plot Group 1

4.2.5 Plot Group 1