Electronic Supplementary Information

Compact and efficient gas diffusion electrodes based on nanoporous alumina membranes for microfuel cells and gas sensors

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S1. Details on contact angle evaluation

Contact angle (θ) measurements were carried out by using a home-made instrument that employed a Hamilton syringe for dispensing 20-μL drops and a digital camera Point Grey model BFLY-PGE-05S2M-CS furnished with a magnification lens (6X) for image acquisition. The image processing for calculation of the drop θ values was carried out using the free software ImageJ with the Contact Angle plug-in, which allows to identify the drop shape and to calculate θ by the ADSA method based on the fitting of the Young-Laplace equation.[1] An example of the processed drop image is shown in Figure S1.

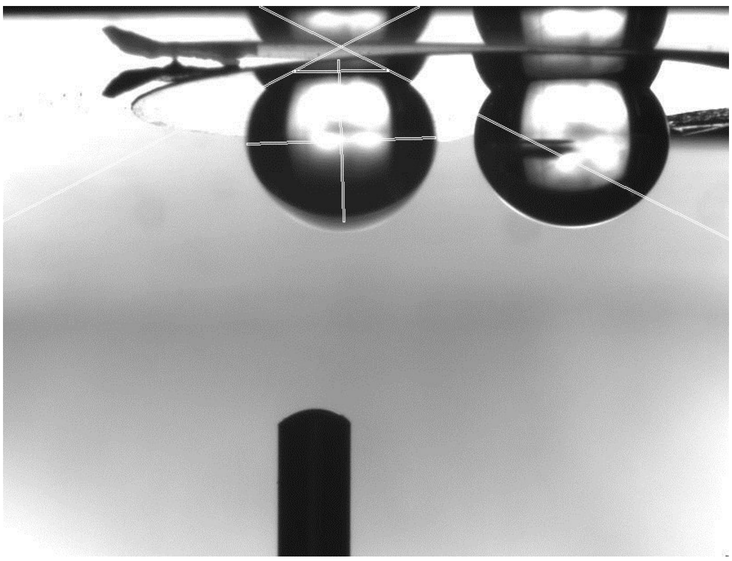


Figure S1. Details on contact angle identification and estimation from the drop images.

S2. Numerical simulations of single-pore gas diffusion electrodes

S2.a) *Introduction*

The mathematical model of a single-pore gas diffusion electrode for solving the mass transport of a dissolved species by diffusion coupled to its reaction under diffusion limiting conditions on the electrocatalytic surface is described. The conditions that were used to perform the numerical resolution of this model by the Finite Element Method using COMSOL Multiphysics® are also listed. These calculations were performed to obtain a semi-quantitative perception about the time-response of the electrode current and of the concentration profiles, and how the electrode configuration (allocation of the catalyst layer, partial pore flooding) affects these responses. The understanding of the physics of these phenomena would allow to design membrane-based gas diffusion electrodes that maximize the current densities and response times.

S2.b) *General model*

The model was built in a 2D cylindrical geometry with axial symmetry around the pore centre (at radius r = 0), where r and z are the radial and vertical (normal to the pore surface) coordinates. Thus, the gas/liquid interface at the pore opening was a circular surface centered at the coordinates (0,0), with a pore radius r_p. The electroactive surface was a ring surrounding the circular pore, which extended all the way to the radial boundary of the model (r_{max}). The electrolyte solution extended from z = 0 to the vertical boundary (z_{max}). In those cases where partial flooding of the pores was considered, the gas/liquid interface was placed at a z distance slightly below the electrode surface (z < 0). The general model is sketched in Figure S2.

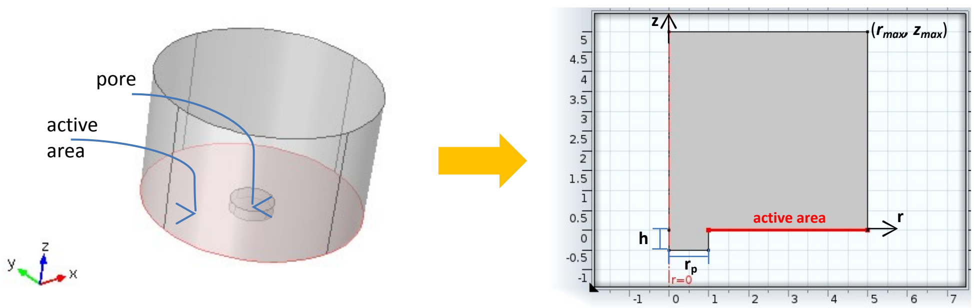


Figure S2. 3D representation of the simulated system (left) and its respective 2D model in cylindrical coordinates (right).

In the analyzed process, a reactive gas (which was H_2 in this work) is dissolved in the electrolyte at the gas/liquid interface located at the pore opening. Thus, assuming that the dissolution process ($H_{2(g)} \rightleftharpoons H_{2(dis)}$) is very fast, the concentration of dissolved species in the solution side of this interface (C^*) is in equilibrium with the gas phase through Henry Law ($C^* = p/k_H$, where p is the partial pressure and k_H is the Henry constant). Besides, the concentration of the dissolved species at any coordinate (r,z) of the solution and at any time (t), $C(r,z,t)$, changes due to the mass transport process into the solution. In the presence of a concentration gradient and in the absence of migration and convection, this mass transport is established by the Second Fick´s Law, which in cylindrical coordinates (r,z) is given by eq. (S1), where D is the diffusion coefficient.[2]

$$\frac{\partial C(r,z,t)}{\partial t} = D\left[\frac{\partial^2 C(r,z,t)}{\partial r^2} + \left(\frac{1}{r}\right)\frac{\partial C(r,z,t)}{\partial r} + \frac{\partial^2 C(r,z,t)}{\partial z^2}\right] \quad \text{(S1)}$$

In terms of the normalized parameters $R = r/r_p$, $Z = z/r_p$, $\tau = tD/r_p^2$, and $c = C/C^*$, the previous equation results in eq. (S2).

$$\frac{\partial c(R,Z,\tau)}{\partial \tau} = \left[\frac{\partial^2 c(R,Z,\tau)}{\partial R^2} + \left(\frac{1}{R}\right)\frac{\partial c(R,Z,\tau)}{\partial R} + \frac{\partial^2 c(R,Z,\tau)}{\partial Z^2}\right] \quad \text{(S2)}$$

As initially there is no dissolved species into the solution, the initial conditions for solving this differential equation are listed below:

$\tau = 0$;	$0 \leq R \leq R_{max}$; $0 < Z \leq Z_{max}$:	$c(R,Z,\tau = 0) = 0$	(S3-a)
	$0 \leq R \leq 1$; $-H < Z \leq 0$:	$c(R,Z,\tau = 0) = 0$	(S3-b)
	$0 \leq R \leq 1$; $Z = 0$:	$c(R,Z,\tau = 0) = 1$	(S4-a)
	$0 \leq R \leq 1$; $Z = -H$:	$c(R,Z,\tau = 0) = 1$	(S4-b)
	$1 < R \leq R_{max}$; $Z = 0$:	$c(R,Z,\tau = 0) = 0$	(S5)

The conditions (S3-a) and (S4-a) are applicable to the situation where the pore opening is exactly at the same level than the active surface ($Z = 0$), which is just a particular ideal situation that was analyzed in this work. In the partially flooded pore, condition (S3-b) also applies (where $H = h/r_p$ and h is the inundated pore height) in order to take into account the addition of the filled-pore volume, and condition (S4-b) applies at $Z = -H$ instead of condition (S4-a).

For $\tau > 0$, the boundary conditions that apply in each particular case are listed below:

$\tau > 0$;	$0 \leq R \leq R_{max}$; $Z = Z_{max}$:	$c(R,Z,\tau) = 0$	(S6)
	$R = R_{max}$; $0 < Z \leq Z_{max}$:	$c(R,Z,\tau) = 0$	(S7)
	$0 < R < R_{max}$; $0 < Z < Z_{max}$:	eq. (S2)	(S8-a)
	$0 < R < 1$; $-H < Z \leq 0$:	eq. (S2)	(S8-b)
	$0 \leq R \leq 1$; $Z = 0$:	$c(R,Z,\tau) = 1$	(S9-a)
	$0 \leq R \leq 1$; $Z = -H$:	$c(R,Z,\tau) = 1$	(S9-b)

Note that in the partially flooded pore, condition (S8-b) is added to (S8-a), while condition (S9-b) replaces (S9-a).

The analyzed reaction at the electroactive surface was the hydrogen oxidation reaction (*hor*), which in acid medium is given by eq. (S10).

$$\tfrac{1}{2}H_{2(dis)} \rightarrow H^+ + e^- \quad \text{(S10)}$$

It was assumed that this reaction operated under mass-transport limiting conditions, so the additional boundary condition (S11-a) was applied over the active surface. In some of the analyzed cases, this condition was also applied on both sides of a ring-shaped catalytic layer that extended over the pore opening with a negligible thickness (1/500) and an inner ring radius $R_o = r_o/r_p$ (i.e. over the range $R_o < R \leq 1$) at $Z = 0$ (condition (S11-b)), as will be detailed when describing this particular situation.

$\tau > 0$; $1 < R \leq R_{max}$; $Z = 0$: $c(R,Z,\tau) = 0$ (S11-a)

$\tau > 0$; $R_o < R \leq R_{max}$; $Z = 0$: $c(R,Z,\tau) = 0$ (S11-b)

Finally, the electrode current (i) can be obtained from the surface integral of the normal flux at the electrode surface, given by eq. (S12). In terms of normalized magnitudes, the normalized current (I) results from eq. (S13).

$$i = 2\pi F \int_{r_p}^{r_{max}} D \frac{\partial C(r,z,t)}{\partial z}\Big)_{z=0} r\,dr \quad \text{(S12)}$$

$$I = \frac{i}{FDC^* r_p} = 2\pi \int_{1}^{R_{max}} \frac{\partial c(R,Z,\tau)}{\partial Z}\Big)_{Z=0} R\,dR \quad \text{(S13)}$$

S2.c) *Analyzed cases*

Three different geometric situations were evaluated for the previously described diffusion/reaction system in cylindrical coordinates, which are schematized in Figure S3. The 2D simulation domain extended between the vertical boundaries (0,Z) and (R_{max},Z), and the horizontal boundaries (R,0) and (R,Z_{max}). Moreover, for the cases (b) and (c) involving a gas/liquid interface below $Z = 0$ (recessed gas inlet), an additional domain was introduced, which extended between the vertical boundaries (0,Z) and (1,Z), and the horizontal boundaries (R,0) and (R,-H). Eq. (S2) was applied all over these domains.

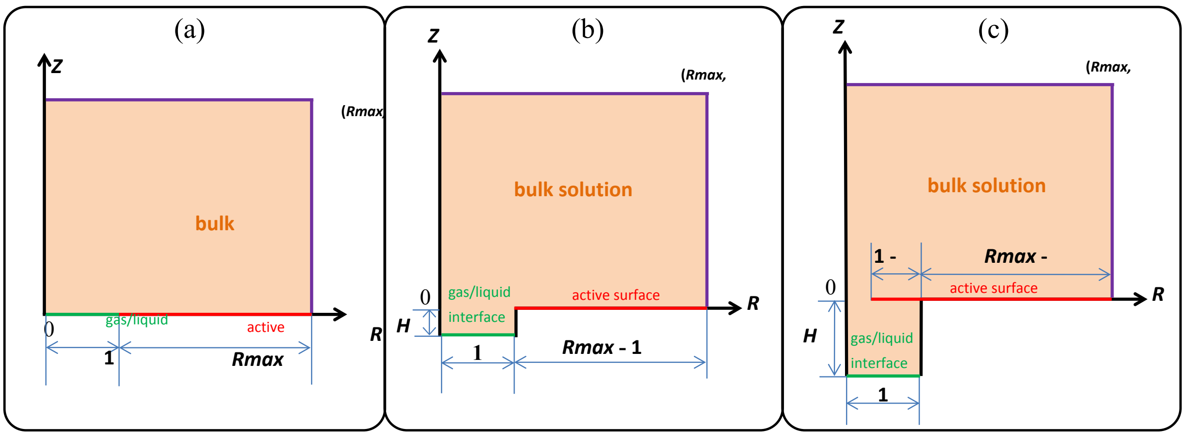


Figure S3. Schemes of the three analyzed simulation models. (a) Gas inlet leveled with the electrode surface at $Z = 0$. (b) Recessed gas inlet at $Z = -H$ ($Z < 0$). (c) Recessed gas inlet at $Z = -H$ with electrocatalytic ring layer at $Z = 0$ (ring opening radius: R_o).

The condition of isolated boundary was applied on the borders (0, $Z_{max} \leq Z \leq -H$) and (1, $0 \leq Z \leq -H$) (black lines in the schemes of Figure S2). For the lateral and top boundaries (violet lines in the schemes of Figure S3), which are located at (R_{max}, $Z_{max} \leq Z \leq 0$) and ($0 \leq R \leq R_{max}$, Z_{max}), the condition of null and invariable concentration was applied in order to accomplish boundary conditions (S6) and (S7). The simulation domain was large enough to assure that these boundaries are far enough from the concentration gradients, so they have no effects on the results. To guarantee this condition, simulations were performed with increasing values of R_{max} and Z_{max} up to an extent where no changes of the results were verified. The condition of null and invariable concentration was also applied on the "active surface" boundary (red line in the schemes of Figure S3), either over ($1 \leq R \leq R_{max}$, 0) or over ($R_o \leq R \leq R_{max}$, 0), in order to accomplish boundary conditions (S11-a) or (S11-b), respectively. Finally, the condition of invariable concentration (c = 1) was applied on the "gas/liquid interface" boundary (green line in the schemes of Figure S3) on the interval ($0 \leq R \leq 1$, 0) or ($0 \leq R \leq 1$, $-H$), for fulfillment of conditions (S9-a) or (S9-b), respectively.

S2.d) *Simulations in COMSOL Multiphysics®*

For performing simulations of the mass transport and electrode reaction in the described models, these systems were programmed in COMSOL Multiphysics® employing the module *Transport of Diluted Species (chds)*.[3,4] The time-dependent responses obtained from these models were the concentration profiles $c(R,Z,\tau)$, the normalized flux density at Z = 0 normal to the surface as a function of R, and the normalized current $I(\tau)$ calculated by numerically solving eq. (S13) both over the whole electrode surface and as a function of R. In fact, the long time responses of time-dependent calculations were compared with the results of calculations at steady state, where the condition given by eq. (S14) was applied. No differences were observed in the values calculated by both procedures, so steady-state calculations were carried out applying this last condition.

$$\frac{\partial c(R,Z,\tau)}{\partial \tau} = 0 = \left[\frac{\partial^2 c(R,Z,\tau)}{\partial R^2} + \left(\frac{1}{R}\right)\frac{\partial c(R,Z,\tau)}{\partial R} + \frac{\partial^2 c(R,Z,\tau)}{\partial Z^2}\right] \quad \text{(S14)}$$

Details on the definition of the geometric model, mesh design, equations and boundary conditions are described in the Appendix at the end of this document. The mesh was refined over the critical zones that involve diffusion and reaction, by choosing a number of elements that guarantee accurate-enough results using reasonable calculation times.[5,6] More precisely, a conventional "fine" mesh size was implemented over the whole simulations domain, excepting around the joint between the pore opening and the active surface, where a pre-defined "extremely fine" mesh domain was applied. Besides, as the flux density at the electrode surface was a target magnitude computed from these calculations, a "distribution meshing" was used over the whole active surface.

S3. References

1 A.F. Stalder, T. Melchior, M. Müller, D. Sage, T. Blu, M. Unser, *Colloids Surf. A*, 2010, **364**, 72.
2 A.J. Bard, L.R. Faulkner, *Electrochemical Methods – Fundamentals and Applications*, 2nd ed, Wiley, Hoboken, **2001**.

3 http://www.comsol.com
4 Voltammetry at a Microdisk Electrode, http://www.comsol.com/model/12877
5 I.J. Cutress, E.J.F. Dickinson, R.G. Compton, *J. Electroanal. Chem.*, 2010, **638**, 76.
6 A. Lavacchi, U. Bardi, C. Borri, S. Caporali, C. Fossati, I. Perissi, *J. Appl. Electrochem.*, 2009, **39**, 2159.

S4. Appendix

The program COMSOL 4.3a (License Number 2078045) was used for modeling and solving the systems with normalized parameters as described in Section S2. Two general models were designed to manage the three described cases. The first model was “Diffusion/reaction at an ideal and a fairly flooded pore”, which applied to cases (a) (ideal pore) and (b) (fairly flooded pore). The second model was “Recessed gas inlet with electrocatalytic ring layer”, which applied to case (c) (fairly flooded pore partially or totally covered by an electrocatalytic layer). The global definitions (for both models) and the particular settings for each case are listed below.

Single-pore gas diffusion/reaction

1 Global Definitions

Global settings

Name	single-pore gas diffusion dimensionless.mph
Program	COMSOL 4.3a

Used products

COMSOL Multiphysics

1.1 Parameters

Parameters

Name	Expression	Description
R	5	Dimensionless maximum radial coordinate
Z	5	Dimensionless maximum vertical coordinate
a	1	Dimensionless pore radius
C_H2	1	Dimensionless concentration at the gas/liquid interface
D_ad	1	Dimensionless diffusion coefficient
h_p	0 to 2	Dimensionless pore penetration
top	0 to 1	Dimensionless width of catalyst layer on pore
h_top	1/500	Dimensionless height of catalyst layer

1.2 Variables

1.2.1 Variables

Selection

Geometric entity level	Entire model

Name	Expression	Description
I	mod1.intop1(intcpl_source_I)	

2 Model 1 for cases (a) and (b) – Diffusion/reaction at an ideal and a fairly flooded pore (mod1)

2.2 Definitions

2.2.1 Variables

2.2.1.1 Variables 2

Selection

Geometric entity level	Entire model

Name	Expression	Description
intcpl_source_I	2*pi*r*chds.dfluxz_cH2	

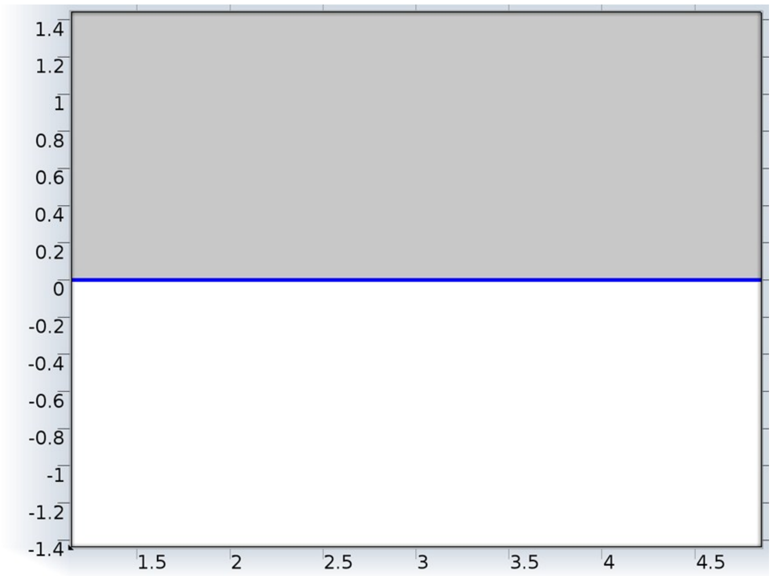
2.2.2 Model Couplings

2.2.2.1 Integration 1

Coupling type	Integration
Operator name	intop1

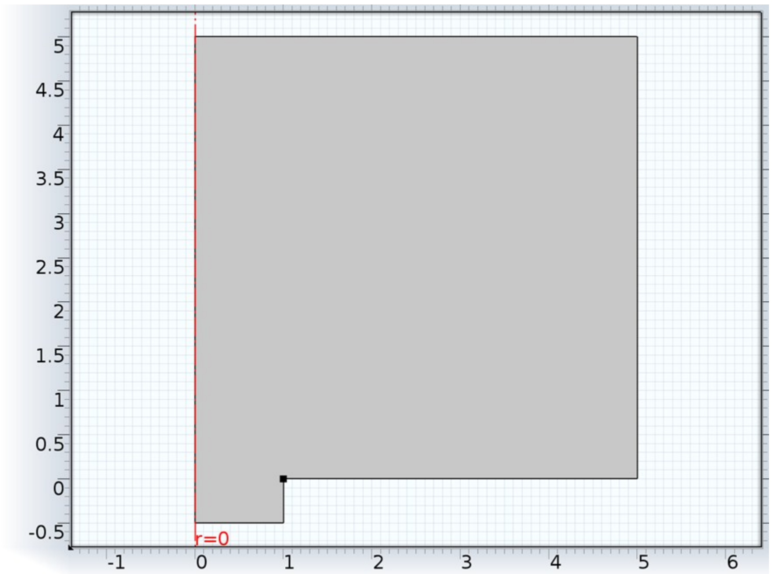
Source selection

Geometric entity level	Boundary
Selection	Boundary6



Source selection

2.3 Geometry 1



Geometry 1

Geometry statistics

Property	Value
Space dimension	2

Property	Value
Number of domains	1
Number of boundaries	5 for case (a) where –h_p = 0 7 for case (b)

2.3.1 Point 1 (pt1)

Selections of resulting entities

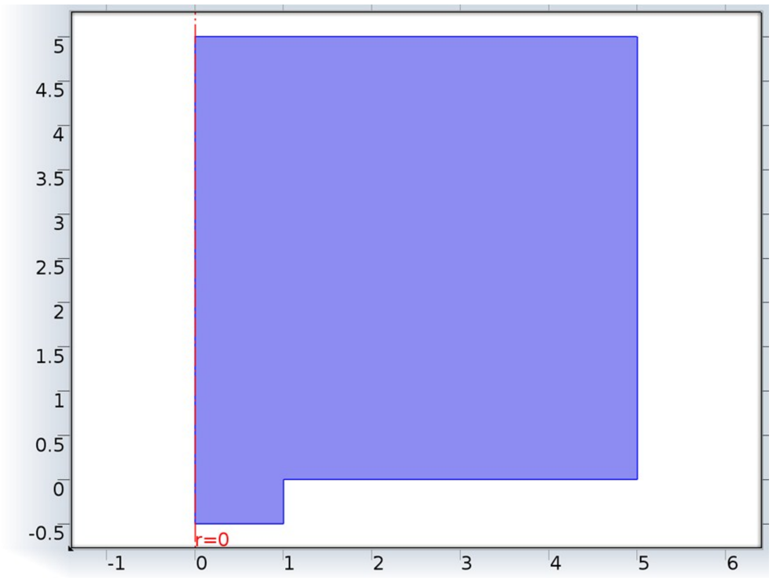
Name	Value
Point coordinate	{a, 0}

2.3.2 Bézier Polygon 1 (b1)

Polygon segments

Name	Value
Control points	{{0, 0, R, R, a, a, 0}, {0, Z, Z, 0, 0, -h_p, -h_p}}
Degree	{1, 1, 1, 1, 1, 1}
Weights	{1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1}
Valid vertex coordinates	{{0, 0}, {0, 5}, {5, 5}, {5, 0}, {1, 0}, {1, 0}, {0, 0}}

2.4 Transport of Diluted Species (chds)



Transport of Diluted Species

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

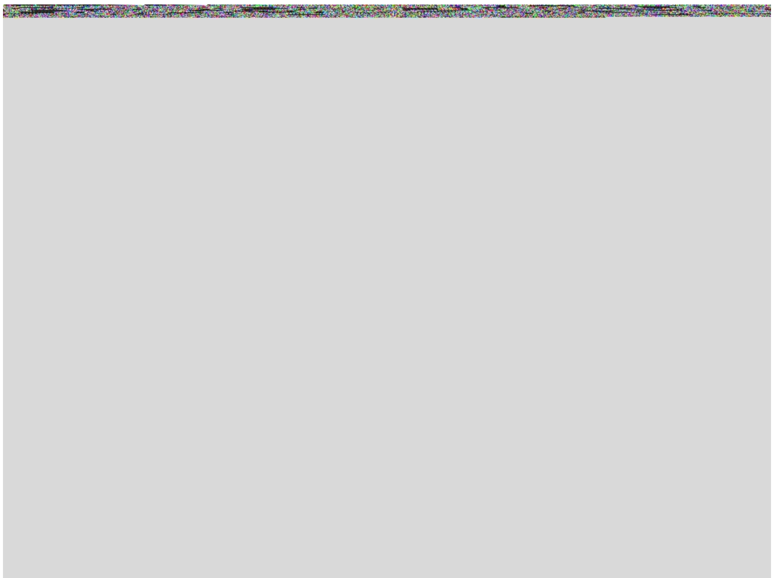
$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

Settings

Description	Value
Concentration	Linear
Compute boundary fluxes	1
Apply smoothing to boundary fluxes	1
Value type when using splitting of complex variables	Real
Equation form	Study controlled
Migration in electric field	0
Convection	0
Convective term	Non - conservative form
Equation residual	Approximate residual
Stream line diffusion	1
Cross wind diffusion	1
Cross wind diffusion type	Do Carmo and Galeão
Enable space-dependent physics interfaces	0
Show equation assuming	std1/time

2.4.1 Diffusion



Diffusion

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(-D_i \nabla c_i\right) = R_i$$

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

2.4.1.1 Settings

Settings

Description	Value
Velocity field	User defined
Velocity field	{0, 0, 0}

Description	Value
Electric potential	User defined
Electric potential	0
Diffusion coefficient	User defined
Diffusion coefficient	{{D_ad, 0, 0}, {0, D_ad, 0}, {0, 0, D_ad}}
Bulk material	None

2.4.1.2 Variables

Name	Expression	Description	Selection
chds.Drr_cH2	D_ad	Diffusion coefficient, rr component	Domain 1
chds.Dphir_cH2	0	Diffusion coefficient, phir component	Domain 1
chds.Dzr_cH2	0	Diffusion coefficient, zr component	Domain 1
chds.Drphi_cH2	0	Diffusion coefficient, rphi component	Domain 1
chds.Dphiphi_cH2	D_ad	Diffusion coefficient, phiphi component	Domain 1
chds.Dzphi_cH2	0	Diffusion coefficient, zphi component	Domain 1
chds.Drz_cH2	0	Diffusion coefficient, rz component	Domain 1
chds.Dphiz_cH2	0	Diffusion coefficient, phiz component	Domain 1
chds.Dzz_cH2	D_ad	Diffusion coefficient, zz component	Domain 1
chds.Dav_cH2	0.5*(chds.Drr_cH2+chds.Dzz_cH2)	Average diffusion coefficient	Domain 1
chds.tfluxr_cH2	-chds.Drr_cH2*cH2r-chds.Drz_cH2*cH2z	Total flux, r component	Domain 1
chds.tfluxphi_cH2	-chds.Dphir_cH2*cH2r-chds.Dphiz_cH2*cH2z	Total flux, phi component	Domain 1
chds.tfluxz_cH2	-chds.Dzr_cH2*cH2r-chds.Dzz_cH2*cH2z	Total flux, z component	Domain 1
chds.dfluxr_cH2	-chds.Drr_cH2*cH2r-chds.Drz_cH2*cH2z	Diffusive flux, r component	Domain 1
chds.dfluxphi_cH2	-chds.Dphir_cH2*cH2r-chds.Dphiz_cH2*cH2z	Diffusive flux, phi component	Domain 1
chds.dfluxz_cH2	-chds.Dzr_cH2*cH2r-chds.Dzz_cH2*cH2z	Diffusive flux, z component	Domain 1
chds.gradr_cH2	cH2r	Concentration gradient, r component	Domain 1
chds.gradphi_cH2	0	Concentration gradient, phi component	Domain 1
chds.gradz_cH2	cH2z	Concentration gradient, z component	Domain 1
chds.ntflux_cH2	chds.bndFlux_cH2	Normal total flux	Boundaries 1–5
chds.ndflux_cH2	chds.bndFlux_cH2	Normal diffusive flux	Boundaries 1–5
chds.dfluxMag_cH2	sqrt(chds.dfluxr_cH2^2+chds.dfluxphi_	Diffusive flux	Domain 1

Name	Expression	Description	Selection
	cH2^2+chds.dfluxz_cH2^2)	magnitude	
chds.tfluxMag_cH2	sqrt(chds.tfluxr_cH2^2+chds.tfluxphi_cH2^2+chds.tfluxz_cH2^2)	Total flux magnitude	Domain 1
chds.Res_cH2	cH2t-chds.R_cH2	Equation residual	Domain 1
domflux.cH2r	chds.dfluxr_cH2	Domain flux	Domain 1
domflux.cH2z	chds.dfluxphi_cH2	Domain flux	Domain 1
chds.nrc	root.nrc/sqrt(root.nrc^2+root.nzc^2+eps)	Normal vector, r component	Boundaries 1–5
chds.nphic	0	Normal vector, phi component	Boundaries 1–5
chds.nzc	root.nzc/sqrt(root.nrc^2+root.nzc^2+eps)	Normal vector, z component	Boundaries 1–5
chds.bndFlux_cH2	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cH2)/(r*pi),NaN)	Boundary flux	Boundaries 1–5

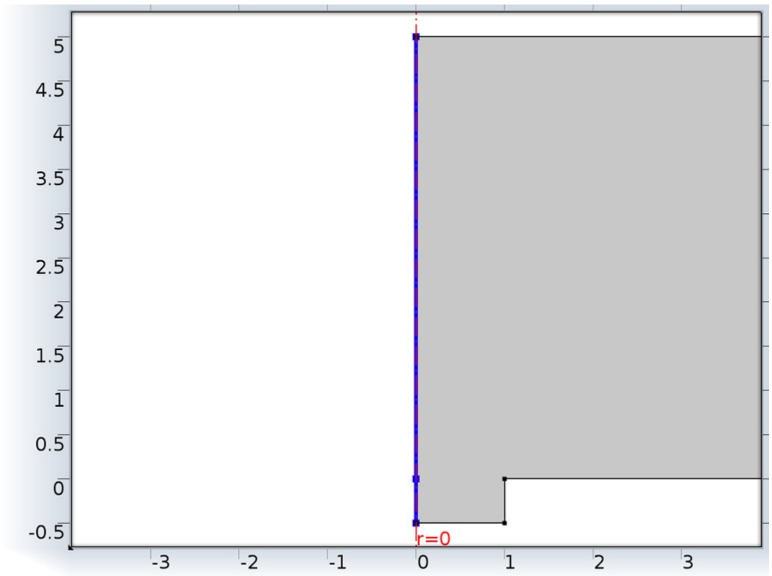
2.4.1.3 Shape functions

Name	Shapefunction	Unit	Description	Shapeframe	Selection
cH2	Lagrange (Linear)		Concentration	Material	Domain 1

2.4.1.4 Weak expressions

Weakexpression	Integrationframe	Selection
2*(-d(cH2,t)*test(cH2)-(chds.Drr_cH2*cH2r+chds.Drz_cH2*cH2z)*test(cH2r)-(chds.Dzr_cH2*cH2r+chds.Dzz_cH2*cH2z)*test(cH2z))*pi*r	Material	Domain 1
2*chds.streamline*pi*r	Material	Domain 1
2*chds.crosswind*pi*r	Material	Domain 1

2.4.2 Axial Symmetry 1

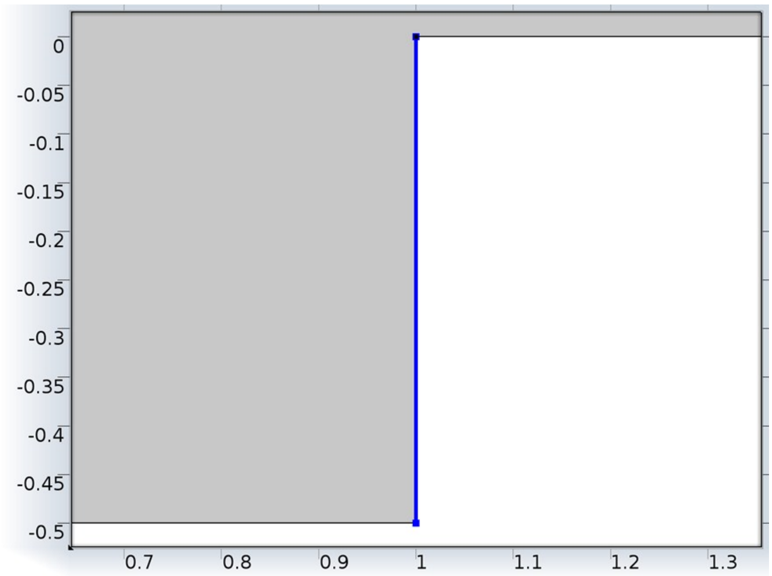


Axial Symmetry 1

Selection

Geometric entity level	Boundary
Selection	Boundary 1, 3

2.4.3 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundary 5

Equations

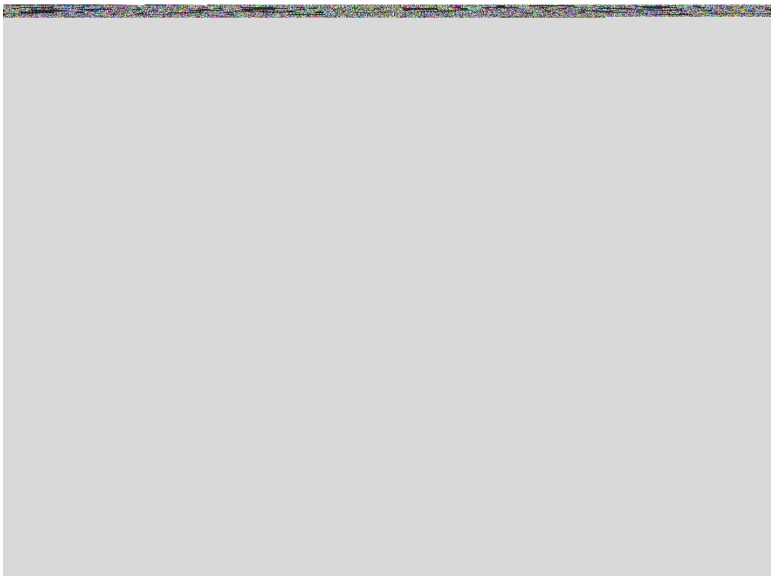
$$-\mathbf{n}\cdot\mathbf{N}_i = 0$$

2.4.3.1 Settings

Settings

Description	**Value**
Apply for all species	Apply for all species

2.4.4 Initial Values 1



Initial Values 1

Selection

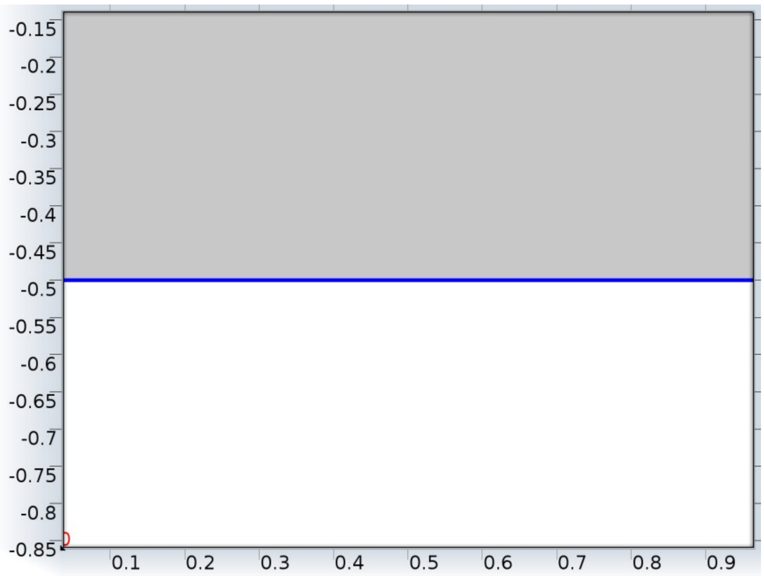
Geometric entity level	Domain
Selection	Domain 1

2.4.4.1 Settings

Settings

Description	Value
Concentration	0

2.4.5 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 2

Equations

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

2.4.5.1 Settings

Settings

Description	Value
Concentration	1
Species cH2	1
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

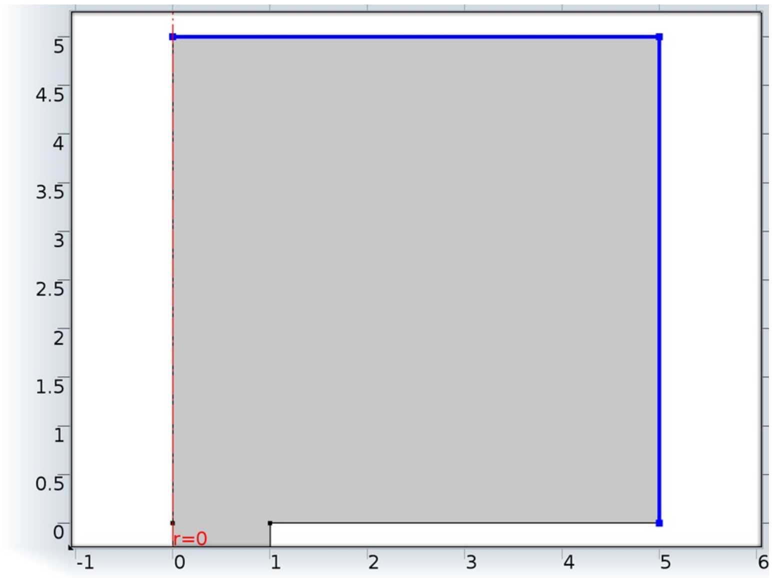
2.4.5.2 Variables

Name	Expression	Unit	Description	Selection
chds.c0_cH2	1		Concentration	Boundary 2

2.4.5.3 Constraints

Constraint	Constraint force	Shape function	Selection
-cH2+chds.c0_cH2	test(-cH2+chds.c0_cH2)	Lagrange (Linear)	Boundary 2

2.4.6 Concentration 2



Concentration 2

Selection

Geometric entity level	Boundary
Selection	Boundaries 4, 7

Equations

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

2.4.6.1 Settings

Settings

Description	Value
Concentration	0
Species cH2	1
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

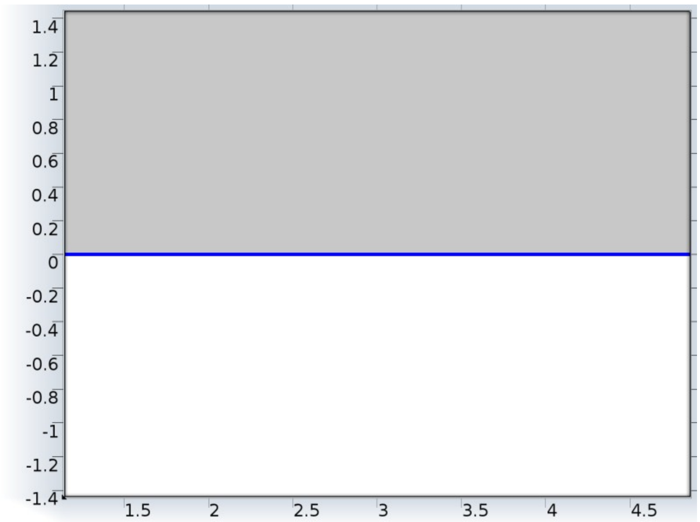
2.4.6.2 Variables

Name	Expression	Unit	Description	Selection
chds.c0_cH2	0		Concentration	Boundaries 4, 7

2.4.6.3 Constraints

Constraint	Constraint force	Shape function	Selection
-cH2+chds.c0_cH2	test(-cH2+chds.c0_cH2)	Lagrange (Linear)	Boundaries 4, 7

2.4.7 Concentration 3



Concentration 3

Selection

Geometric entity level	Boundary
Selection	Boundary6

Equations

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

2.4.7.1 Settings

Settings

Description	Value
Concentration	0
Species cH2	1
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

2.4.7.2 Variables

Name	Expression	Unit	Description	Selection
chds.c0_cH2	0		Concentration	Boundary 6

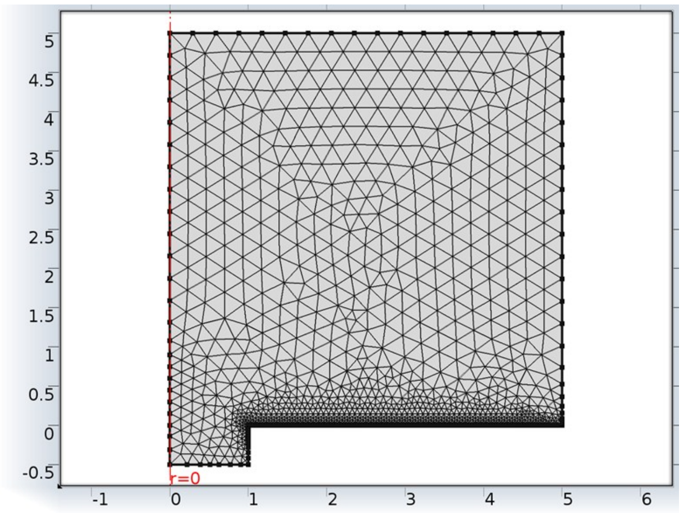
2.4.7.3 Constraints

Constraint	Constraint forcé	Shape function	Selection
-cH2+chds.c0_cH2	test(-cH2+chds.c0_cH2)	Lagrange (Linear)	Boundary 6

2.5 Mesh 1

Mesh statistics

Property	Value
Minimum element quality	0.724
Average element quality	0.9549
Triangular elements	2291
Edge elements	199
Vertex elements	7



Mesh 1

2.5.1 Size (size)

Settings

Name	Value
Maximum element size	0.292
Minimum element size	0.00165
Resolution of curvature	0.3
Maximum element growth rate	1.3
Predefined size	Fine

2.5.2 Free Triangular 1 (ftri1)

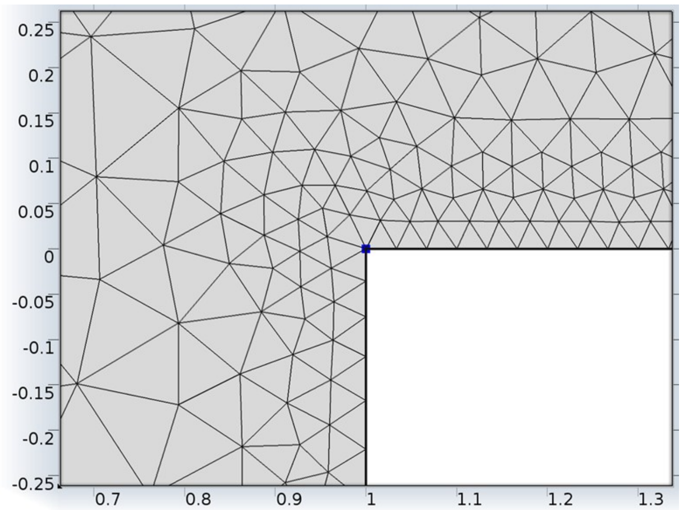
Selection

Geometric entity level	Domain
Selection	Remaining

2.5.2.1 Size 1 (size1)

Selection

Geometric entity level	Point
Selection	Point 5



Size 1

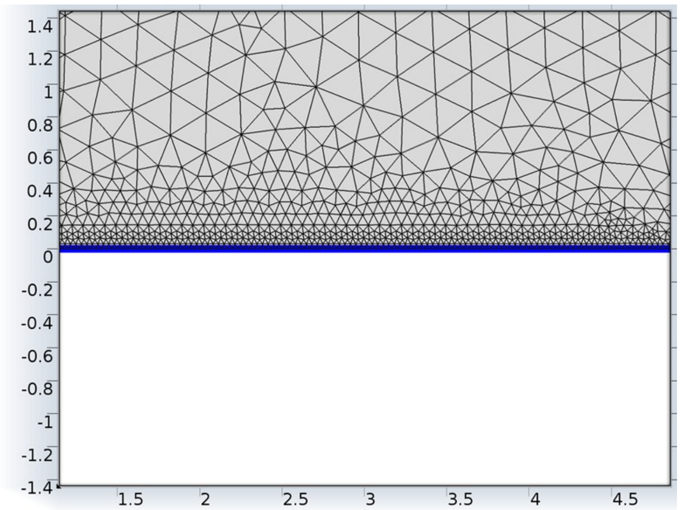
Settings

Name	Value
Maximum element size	0.055
Minimum element size	1.0E-4
Resolution of curvature	0.2
Predefined size	Extremely fine

2.5.2.2 Distribution 1 (dis1)

Selection

Geometric entity level	Boundary
Selection	Boundary6



Distribution 1

Settings

Name	Value
Distribution properties	Predefined distribution type
Number of elements	120
Distribution method	Geometric sequence

3 Model 2 for case (c) - Recessed gas inlet with electrocatalytic ring layer (mod1)

3.1 Definitions

3.1.1 Variables

3.1.1.1 Variables 2

Selection

Geometric entity level	Entire model

Name	Expression	Description
intcpl_source_I	2*pi*r*chds.dfluxz_cH2	

3.1.2 Model Couplings

3.1.2.1 Integration 1

Coupling type	Integration
Operator name	intop1

Source selection

Geometric entity level	Boundary
Selection	Boundary 10

3.1.3 Coordinate Systems

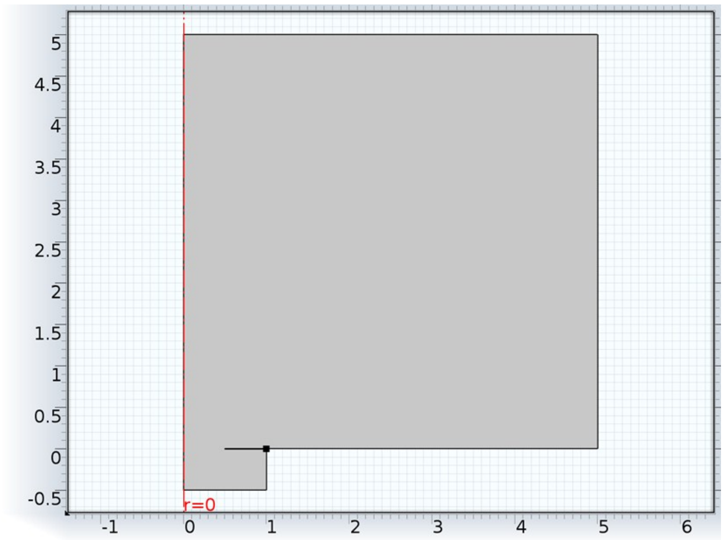
3.1.3.1 Boundary System 1

Coordinate system type	Boundary system
Identifier	sys1

Settings

Name	Value
Coordinate names	{t1, to, n}
Create first tangent direction from	Global Cartesian

3.2 Geometry 1



Geometry 1

Geometry statistics

Property	Value
Space dimension	2
Number of domains	2
Number of boundaries	11

3.2.1 Point 1 (pt1)

Selections of resulting entities

Name	Value
Point coordinate	{a, 0}

3.2.2 Bézier Polygon 1 (b1)

Polygon segments

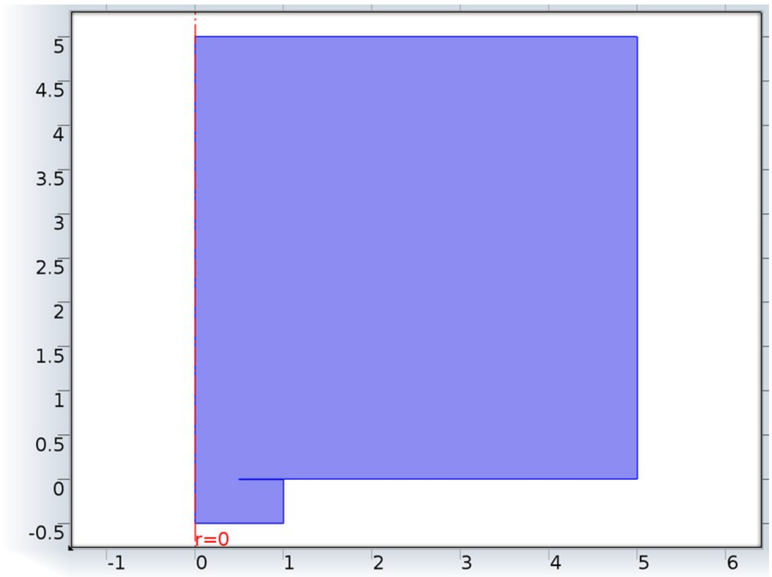
Name	Value
Control points	{{0, 0, R, R, a, a, 0}, {0, Z, Z, 0, 0, -h_p, -h_p}}
Degree	{1, 1, 1, 1, 1, 1}
Weights	{1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1}
Valid vertex coordinates	{{0, 0}, {0, 5}, {5, 5}, {5, 0}, {1, 0}, {1, -0.5}, {0, -0.5}, {0, 0}}

3.2.3 Bézier Polygon 2 (b2)

Polygon segments

Name	Value
Control points	{{a, top, top, a}, {0, 0, -h_top*3, -h_top*3}}
Degree	{1, 1, 1}
Weights	{1, 1, 1, 1, 1, 1}
Valid vertex coordinates	{{1, 0}, {0.5, 0}, {0.5, -0.0060}, {1, -0.0060}, {1, 0}}

3.3 Transport of Diluted Species (chds)



Transport of Diluted Species

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

Settings

Description	Value
Concentration	Linear
Compute boundary fluxes	1
Apply smoothing to boundary fluxes	1
Value type when using splitting of complex variables	Real

Description	Value
Equation form	Study controlled
Migration in electric field	0
Convection	0
Convective term	Non - conservative form
Equation residual	Approximate residual
Streamline diffusion	1
Crosswind diffusion	1
Crosswind diffusion type	Do Carmo and Galeão
Enable space-dependent physics interfaces	0
Show equation assuming	std1/time

3.3.1 Diffusion

Diffusion

Selection

Geometric entity level	Domain
Selection	Domain 1

Equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) = R_i$$

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

3.3.1.1 Settings

Settings

Description	Value
Velocity field	User defined
Velocity field	{0, 0, 0}
Electric potential	User defined
Electric potential	0
Diffusion coefficient	User defined
Diffusion coefficient	{{D_ad, 0, 0}, {0, D_ad, 0}, {0, 0, D_ad}}
Bulk material	None

3.3.1.2 Variables

Name	Expression	Description	Selection
chds.Drr_cH2	D_ad	Diffusion coefficient, rr component	Domain 1
chds.Dphir_cH2	0	Diffusion coefficient, phir component	Domain 1
chds.Dzr_cH2	0	Diffusion coefficient, zr component	Domain 1
chds.Drphi_cH2	0	Diffusion coefficient, rphi component	Domain 1
chds.Dphiphi_cH2	D_ad	Diffusion coefficient, phiphi component	Domain 1
chds.Dzphi_cH2	0	Diffusion coefficient, zphi component	Domain 1
chds.Drz_cH2	0	Diffusion coefficient, rz component	Domain 1
chds.Dphiz_cH2	0	Diffusion coefficient, phiz component	Domain 1
chds.Dzz_cH2	D_ad	Diffusion coefficient, zz component	Domain 1
chds.Dav_cH2	0.5*(chds.Drr_cH2+chds.Dzz_cH2)	Average diffusion coefficient	Domain 1
chds.tfluxr_cH2	-chds.Drr_cH2*cH2r-chds.Drz_cH2*cH2z	Total flux, r component	Domain 1
chds.tfluxphi_cH2	-chds.Dphir_cH2*cH2r-chds.Dphiz_cH2*cH2z	Total flux, phi component	Domain 1
chds.tfluxz_cH2	-chds.Dzr_cH2*cH2r-chds.Dzz_cH2*cH2z	Total flux, z component	Domain 1
chds.dfluxr_cH2	-chds.Drr_cH2*cH2r-chds.Drz_cH2*cH2z	Diffusive flux, r component	Domain 1
chds.dfluxphi_cH2	-chds.Dphir_cH2*cH2r-chds.Dphiz_cH2*cH2z	Diffusive flux, phi component	Domain 1
chds.dfluxz_cH2	-chds.Dzr_cH2*cH2r-chds.Dzz_cH2*cH2z	Diffusive flux, z component	Domain 1
chds.gradr_cH2	cH2r	Concentration gradient, r component	Domain 1
chds.gradphi_cH2	0	Concentration gradient, phi component	Domain 1
chds.gradz_cH2	cH2z	Concentration gradient, z component	Domain 1
chds.ntflux_cH2	chds.bndFlux_cH2	Normal total flux	Boundaries 1–8, 10–11
chds.ndflux_cH2	chds.bndFlux_cH2	Normal diffusive flux	Boundaries 1–8, 10–11
chds.dfluxMag_cH2	sqrt(chds.dfluxr_cH2^2+chds.dfluxphi_cH2^2+chds.dfluxz_cH2^2)	Diffusive flux magnitude	Domain 1
chds.tfluxMag_cH2	sqrt(chds.tfluxr_cH2^2+chds.tfluxphi_cH2^2+chds.tfluxz_cH2^2)	Total flux magnitude	Domain 1
chds.Res_cH2	-chds.R_cH2	Equation residual	Domain 1
domflux.cH2r	chds.dfluxr_cH2	Domain flux	Domain 1
domflux.cH2z	chds.dfluxphi_cH2	Domain flux	Domain 1
chds.nrc	root.nrc/sqrt(root.nrc^2+root.nzc^2+eps)	Normal vector, r component	Boundaries 1–8, 10–11
chds.nphic	0	Normal vector, phi component	Boundaries 1–8, 10–11
chds.nzc	root.nzc/sqrt(root.nrc^2+root.nzc^	Normal vector, z	Boundaries

Name	Expression	Description	Selection
	2+eps)	component	1–8, 10–11
chds.bndFlux_cH2	-uflux_spatial(cH2)	Boundary flux	Boundaries 5–7
chds.bndFlux_cH2	if(r>0.0010/sqrt(sqrt(mean(emetric2))),-0.5*dflux_spatial(cH2)/(r*pi),NaN)	Boundary flux	Boundaries 1–4, 8, 10–11

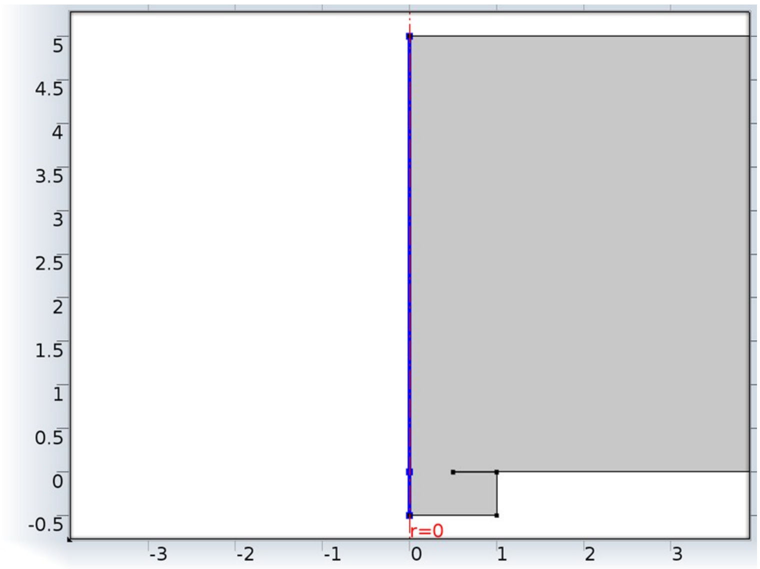
3.3.1.3 Shape functions

Name	Shape function	Unit	Description	Shape frame	Selection
cH2	Lagrange (Linear)		Concentration	Material	Domain 1

3.3.1.4 Weak expressions

Weak expression	Integration frame	Selection
2*(-d(cH2,t)*test(cH2)-(chds.Drr_cH2*cH2r+chds.Drz_cH2*cH2z)*test(cH2r)-(chds.Dzr_cH2*cH2r+chds.Dzz_cH2*cH2z)*test(cH2z))*pi*r	Material	Domain 1
2*chds.streamline*pi*r	Material	Domain 1
2*chds.crosswind*pi*r	Material	Domain 1

3.3.2 Axial Symmetry 1

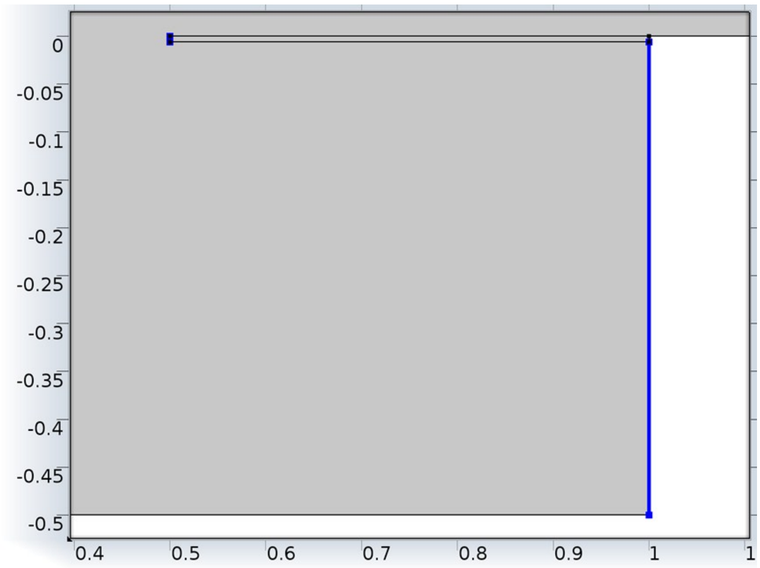


Axial Symmetry 1

Selection

Geometricentitylevel	Boundary
Selection	Boundaries 1, 3

3.3.3 No Flux 1



No Flux 1

Selection

Geometric entity level	Boundary
Selection	Boundaries 5, 8

Equations

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

3.3.3.1 Settings

Settings

Description	Value
Apply for all species	Apply for all species

3.3.4 Initial Values 1

Initial Values 1

Selection

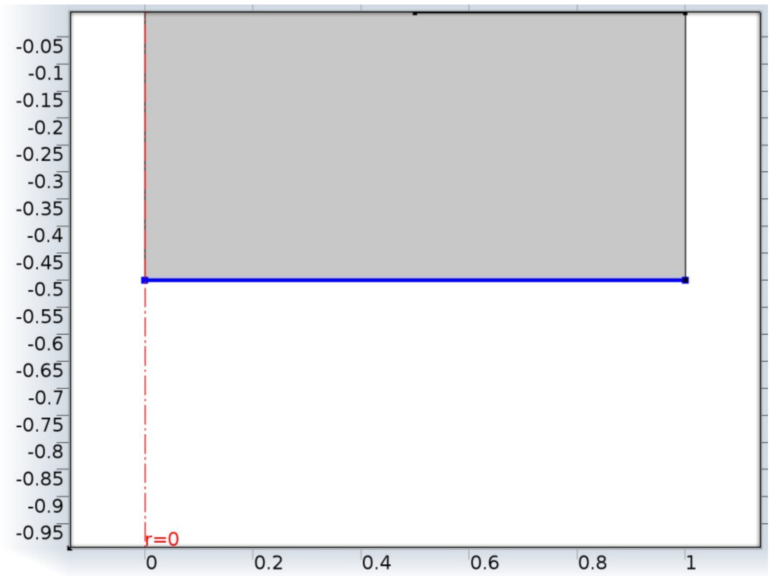
Geometric entity level	Domain
Selection	Domain 1

3.3.4.1 *Settings*

Settings

Description	Value
Concentration	0

3.3.5 Concentration 1



Concentration 1

Selection

Geometric entity level	Boundary
Selection	Boundary 2

Equations

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

3.3.5.1 *Settings*

Settings

Description	Value
Concentration	1
Species cH2	1
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

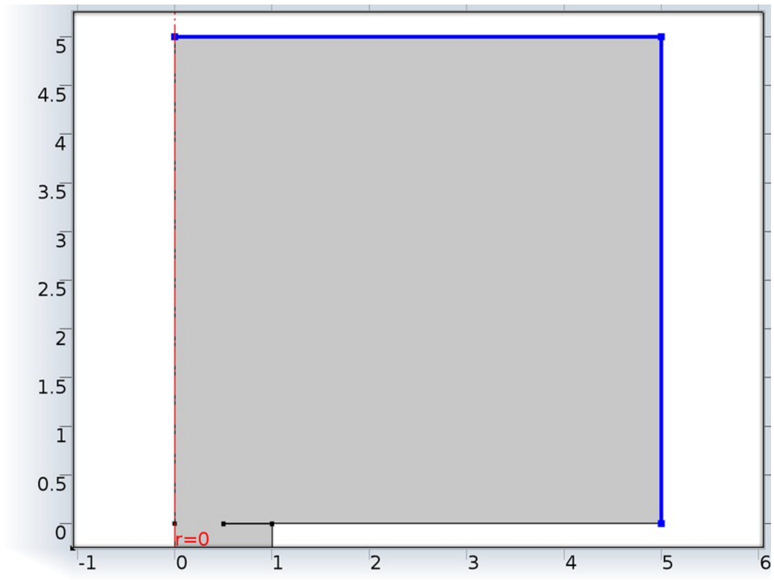
3.3.5.2 *Variables*

Name	Expression	Unit	Description	Selection
chds.c0_cH2	1		Concentration	Boundary 2

3.3.5.3 *Constraints*

Constraint	Constraint force	Shape function	Selection
-cH2+chds.c0_cH2	test(-cH2+chds.c0_cH2)	Lagrange (Linear)	Boundary 2

3.3.6 Concentration 2



Concentration 2

Selection

Geometric entity level	Boundary
Selection	Boundaries 4, 11

Equations

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

3.3.6.1 Settings

Settings

Description	Value
Concentration	0
Species cH2	1
Apply reaction terms on	All physics (symmetric)
Use weak constraints	0

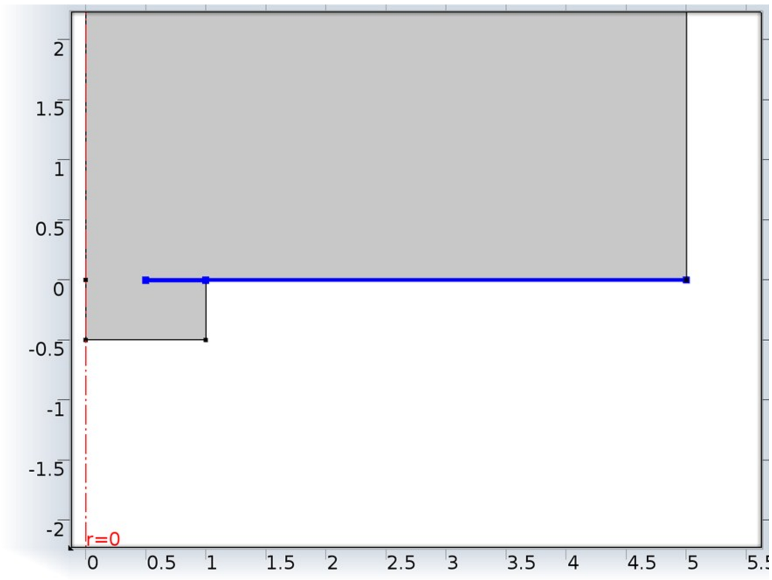
3.3.6.2 Variables

Name	Expression	Unit	Description	Selection
chds.c0_cH2	0		Concentration	Boundaries 4, 11

3.3.6.3 Constraints

Constraint	Constraint force	Shape function	Selection
-cH2+chds.c0_cH2	test(-cH2+chds.c0_cH2)	Lagrange (Linear)	Boundaries 4, 11

3.3.7 Concentration 3



Concentration 3

Selection

Geometric entity level	Boundary
Selection	Boundaries 6–7, 10

Equations

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

3.3.7.1 Settings

Settings

Description	Value
Concentration	0
Species cH2	1
Apply reaction terms on	All physics (symmetric)
Use weakconstraints	0

3.3.7.2 Variables

Name	Expression	Unit	Description	Selection
chds.c0_cH2	0		Concentration	Boundaries 6–7, 10

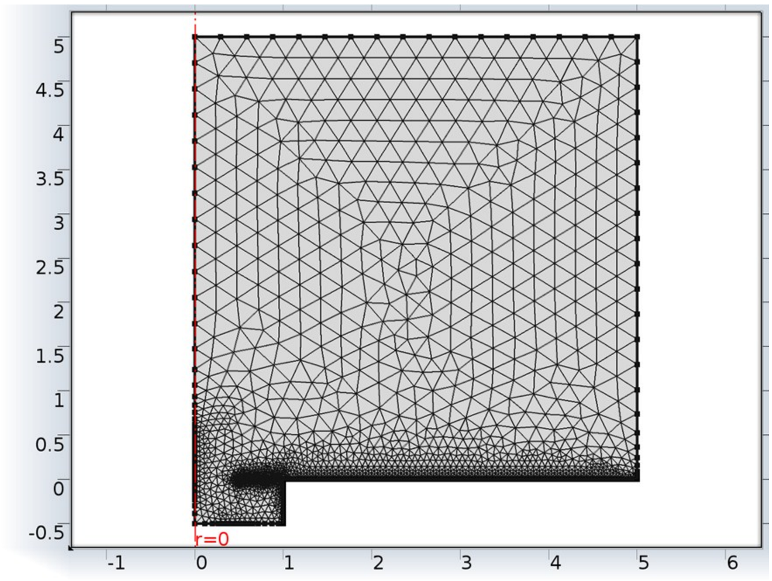
3.3.7.3 Constraints

Constraint	Constraint force	Shape function	Selection
-cH2+chds.c0_cH2	test(-cH2+chds.c0_cH2)	Lagrange (Linear)	Boundaries 6–7, 10

3.4 Mesh 1

Mesh statistics

Property	Value
Minimum element quality	0.6981
Average element quality	0.9453
Triangular elements	4445
Edge elements	358
Vertex elements	10



Mesh 1

3.4.1 Size (size)

Settings

Name	Value
Maximum element size	0.292
Minimum element size	0.00165
Resolution of curvature	0.3
Maximum element growth rate	1.3
Predefined size	Fine

3.4.2 Free Triangular 1 (ftri1)

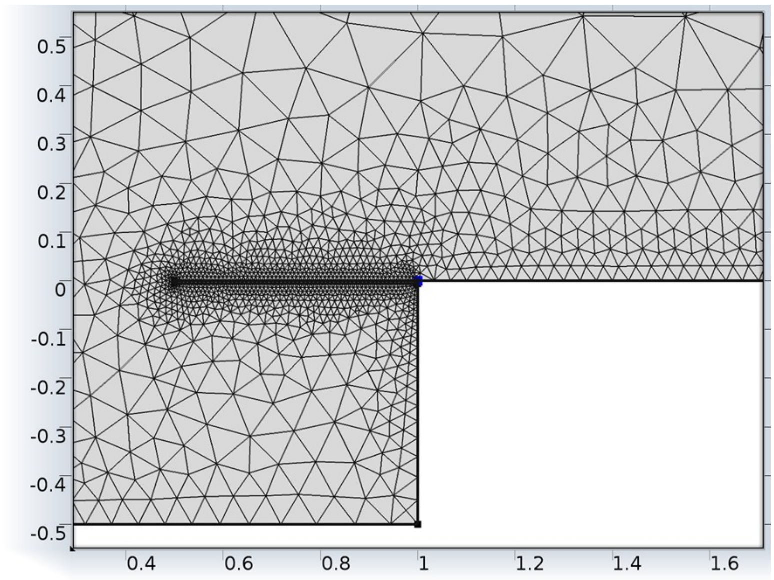
Selection

Geometric entity level	Domain
Selection	Remaining

3.4.2.1 Size 1 (size1)

Selection

Geometricentitylevel	Point
Selection	Point 8



Size 1

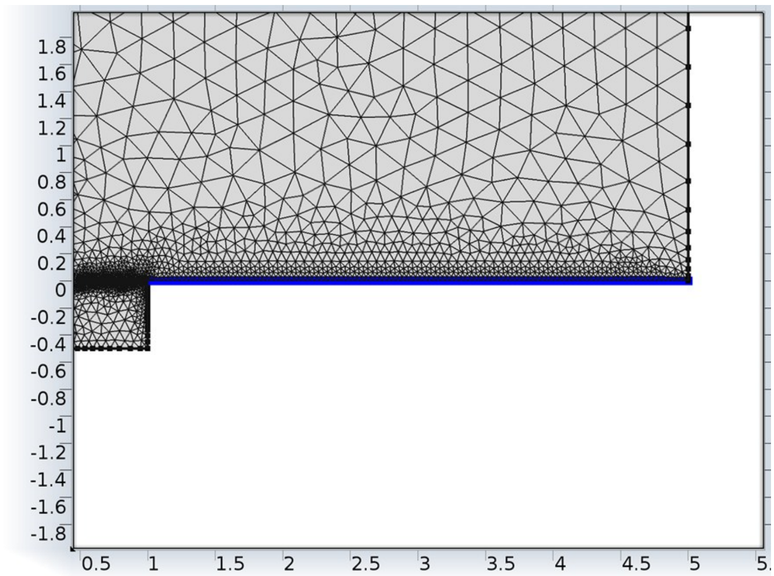
Settings

Name	Value
Maximum element size	0.055
Minimum element size	1.1E-4
Resolution of curvature	0.2
Predefined size	Extremely fine

3.4.2.2 Distribution 1 (dis1)

Selection

Geometric entity level	Boundary
Selection	Boundary 10



Distribution 1

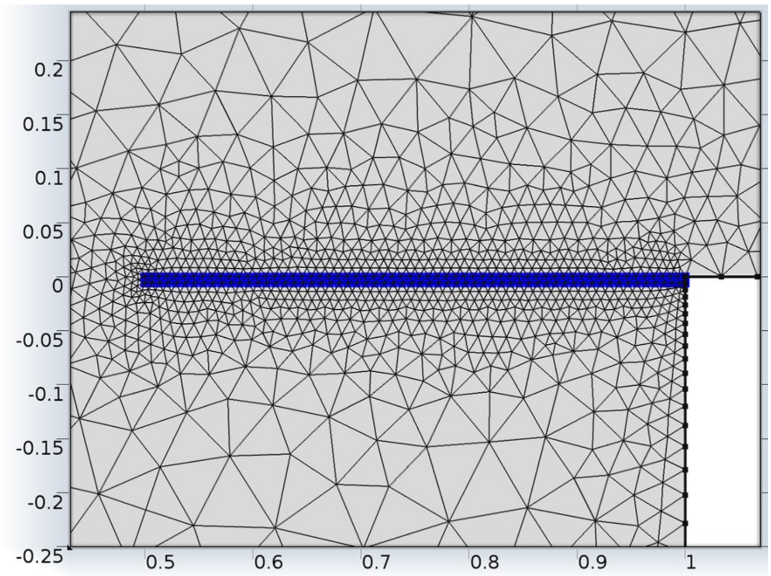
Settings

Name	Value
Distribution properties	Predefined distribution type
Number of elements	120
Distribution method	Geometric sequence

3.4.2.3 Size 2 (size2)

Selection

Geometric entity level	Boundary
Selection	Boundaries 6–7



Size 2

Settings

Name	Value
Maximum element size	0.055
Minimum element size	1.1E-4
Resolution of curvature	0.2
Predefined size	Extremely fine