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Determining Porosity and Permeability from AFM Images Using Image to Curve in COMSOL Multiphysics

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Abstract

In recent years, atomic force microscopy (AFM) has become a key technique for characterizing surface structures and materials at the microscopic level. An important part of the AFM image analysis is quantifying morphological properties such as porosity and permeability of the material. This paper focuses on the calculation of these parameters using the *Image to Curve* module of the COMSOL Multiphysics software, which allows digital images to be converted into analysable curves. The *Image to Curve* module is an efficient tool for obtaining quantitative data on the porosity and permeability of materials, allowing a better understanding of their structure and optimization of their properties for specific applications such as filtration, separation and fluid transport. The study shows how this module can be used to develop new materials with optimised properties, opening up new opportunities for innovation in materials engineering.

Keywords: Atomic force microscopy, porosity, permeability, *Image to Curve*

1 Introduction

Atomic Force Microscopy (AFM) has become a key tool for characterizing surface structures and materials at the microscopic level. This technology is particularly important for the study of biopolymers and hydrogels used in tissue engineering and other biotechnological applications. According to a study by J. Joshi and colleagues, AFM is one of the highest lateral resolution methods, allowing the study of samples in air and liquids, giving it an advantage over scanning electron microscopy, which requires a vacuum. The principle of AFM is to map the surface of the sample through interactions between the scanning tip and the sample surface, allowing the imaging of topography and the measurement of other physical properties, which is crucial for the study of biopolymers and hydrogels [1].

Hydrogels for biological applications were first described by Wichterle and Lim in the early 1960s [2]. These hydrogels are often defined as polymeric materials with a hydrophilic three-dimensional network capable of retaining significant amounts of water, up to a thousand times their dry weight. Due to ionic interactions and hydrogen bonds in the cross-linked structure, these hydrogels are insoluble, giving them the necessary mechanical strength and physical stability [3, 4].

The water content of the hydrogel is essential for its unique physicochemical properties, which are similar to those of living tissue. Pores in hydrogels can be formed during the synthesis process or can be present as smaller structures within the network. The size, distribution, and interconnection of these pores significantly influence the structural properties of the hydrogel and have a major impact on its functional properties, including its ability to transport and diffuse substances [5, 6, 7].

In this study, we have focused on the calculation of porosity and permeability based on the 2D geometry obtained from AFM images showing the surface of a 2% agarose-based hydrogel. These calculations were performed using the *Image to Curve* module and the *Creeping Flow* interface of the COMSOL Multiphysics software. The *Image to Curve* module allows the image to be used as a starting point for analysis by generating an interpolation curve from the contour of the imported image, which can then be used to generate the model geometry. After this conversion, it is necessary to remove unwanted regions that could affect the accuracy of the geometric model and subsequent calculations [8].

The Navier-Stokes equations, which are the basis for describing fluid motion, consider the viscous and compressive forces acting on the fluid. At very low Reynolds numbers, typical of microscopic scales and low velocities, the inertial forces are negligible compared to the viscous forces. This simplified model, known as Stokes flow, allows more efficient calculation and analysis. The *Creeping Flow* interface in COMSOL Multiphysics is specifically designed to simulate fluid flow at very low Reynolds numbers. Using this interface simplifies calculations and provides accurate simulations that are critical for determining material properties such as porosity and permeability, which are essential parameters for materials engineering and biomedical applications [9].

Using the *Image to Curve* module and the *Creeping Flow* interface, you can quantitatively analyse porosity and permeability based on the morphology and structure of materials. This allows you to not only design and optimise materials for specific applications, but also to continue your work using the additional modelling and simulation capabilities of COMSOL Multiphysics software.

2 Principles of AFM

An important aspect of atomic force microscopy (AFM) image analysis is the ability to accurately determine pore size and the degree of cross-linking in materials. The principle of operation is based on the interaction between a sharp tip at the end of a flexible beam and the surface of the sample. As the tip approaches the surface, it deforms due to the atomic forces acting on it. these changes in beam deflection are recorded and used to map the topography of the sample. the data obtained allows a detailed and magnified image of the surface to be produced, revealing fine structures and irregularities. this capability is particularly important in the analysis of materials such as hydrogels, where knowledge of pore size and degree of cross-linking significantly affects their functional size in applications. AFM thus provides the necessary information for the optimisation of these materials, thus contributing to the development of advanced technologies in the field of biomaterials [1].

3 COMSOL Implementation

The practical part of this study followed the procedures described in the COMSOL blog articles [8, 9].

3.1 Entering Parameters and Variables to Calculate Porosity and Permeability

Parameters and *Variables* are key to the parameterisation and organization of the model and can be found in the *Global Definitions* node of the COMSOL Multiphysics software. *Parameters* are used to define constant values that are applied throughout the model, making it easier to modify if necessary and improving clarity. Figure 1 shows the set of parameters used to calculate porosity and permeability in the model. This model, based on the AFM image, covers an area of 9 µm x 9 µm. The materials included in the model are water with a density of 1000 kg/m^3 and a dynamic viscosity of 0.001 Pa·s. The input pressure was set to 0.01 Pa, which serves as the initial condition for simulating flow in the porous structure.

Name	Expression	Value	Description
L	9 [um]	9E-6 m	Length
H	9 [um]	9E-6 m	Width
p0	0.01 [Pa]	0.01 Pa	Inlet pressure
rho0	1000 [kg/m^3]	1000 kg/m^3	Water density
mu0	0.001 [Pa*s]	0.001 Pa·s	Dynamic viscosity of water

Figure 1. Definition of the parameters that are used in the calculation of the porosity and permeability

Variables allow the calculation and application of expressions that can change dynamically in time or space, providing greater flexibility and the ability to handle complex relationships in the model. Figure 2 shows the definition of the variables used to calculate permeability and porosity. The pore space area and the porous matrix area must be calculated at the outset, as porosity is defined as the ratio of these two areas.
However, porosity alone is not sufficient to describe the ability of a porous medium to transmit flow. The shape and orientation of the pores also play an important role. According to Darcy's law, described by Eq:

$$\mathbf{u} = -\frac{k}{\mu}\nabla p$$

where **u** is the Darcy or surface velocity [m/s], k is the permeability [m^2], μ is the dynamic viscosity [Pa·s] and ∇p [Pa] is the pressure gradient. There are already predefined variables in the Creeping Flow interface that allow the calculation of the Darcy velocity. The volumetric flow rate is obtained by dividing the variable spf.out1.Mflow, which represents the mass flow rate across the outlet boundary, by a constant density. To take account of the 2D approximation and to obtain the Darcy velocity at the outlet per unit depth, the volumetric flow is further divided by the height.

Name	Expression	Unit	Description
por	A_por/A_tot		Porosity
A_por	intop1(1)	m^2	Pore area
A_tot	L*H	m^2	Membrane area
u_out	q_out/H/1[m]	m/s	Outflow velocity
q_out	spf.out1.Mflow/rho0	m^3/s	Flow rate
k0	u_out*mu0*L/p0	m^2	Permeability

Figure 2. Definition of the variables that are used in the calculation of the porosity and permeability

3.2 Image to Curve Add-In

Figure 3 shows an AFM image of the surface of a 2% agarose-based hydrogel sample, which serves as the starting point for the subsequent analysis. In [8], the *Image to Curve* module is described as a tool that allows the creation of an interpolation curve from the contour plot of an imported image. This curve is then integrated into the model geometry.

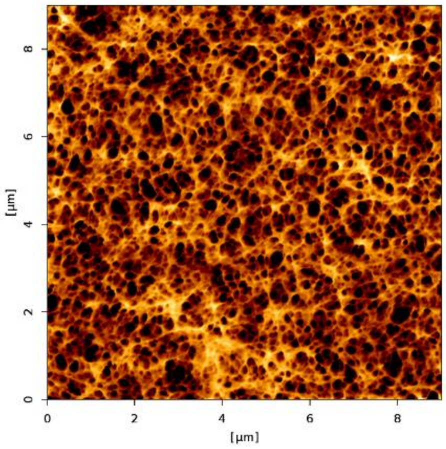

Figure 3. AFM image of the surface of a 2% agarose-based hydrogel sample

3.2.1 Adding the Image to Curve to the Model Builder

Figure 4 shows how to enable the *Image to Curve* add-on. In the *Developer Difference*, click *Add-in* Libraries and then tick the *Image to Curve* box. The add-in will then be added to the *Model Builder*.

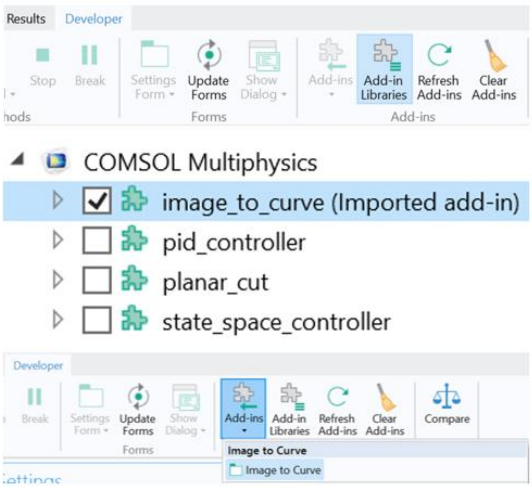

Figure 4. Adding the image to curve to the Model Builder

3.2.2 Image to Curve Setting

Before using *Image to Curve* it was first necessary to change the units in the *Geometry* node to micrometers (µm). An image in .png format was then imported into the Image section to represent the AFM image. After importing, the information displayed included the image size in pixels, the width of the image with the length unit defined by the *Geometry* node and set to 9µm, the file name and the filter used which remained at the default setting of Gaussian blur.

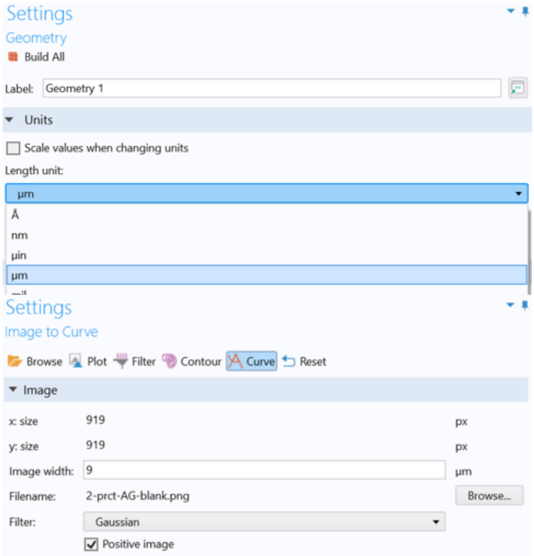

Figure 5. Image width setting

In the *Countour* section, by default a contour curve is automatically generated based on the average threshold of the pixel intensity in the filtered image. However, in our case it was necessary to adjust this setting manually, so we deselected the Automatic contour threshold option. We then entered a value of 0.24 in the *Contour* threshold field. After clicking the *Contour* button on the toolbar, the contour curves were displayed, as shown in Figure 6.

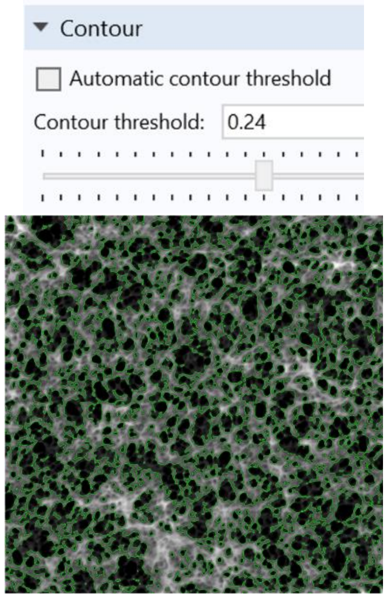

Figure 6. Contour settings and Image to contours (green)

In the *Curve* section, the default setting for the curve type is Open. In this case, this setting has been changed to Solid (closed curve) to ensure that a closed profile is created. The *Curve Tolerance* parameter has been set to 0.0013 in order to smooth the curves generated from *Contour*. This value determines how closely the generated curve should approximate the contours, which is important for maintaining the accuracy of the geometry in subsequent analysis and simulation.

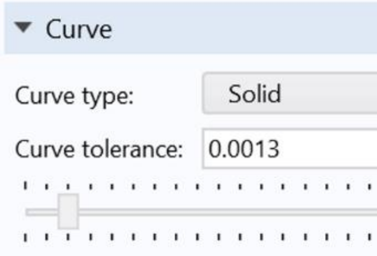

Figure 7. Curve settings

Click *Curve* to convert the imported image to geometry. This creates a basic curve that represents the shape of the image.

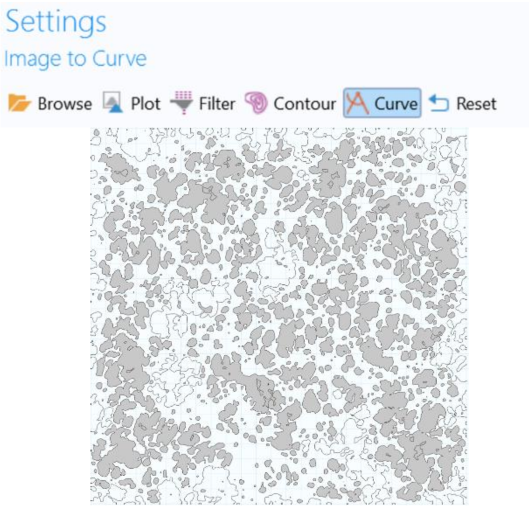

Figure 8. Conversion of imported image to geometry

3.2.3 Correction of geometry

The resulting geometry needs to be corrected. This correction involves removing extraneous or incorrect domains, smoothing out irregularities or adjusting contours to match as closely as possible the actual shape of the object being analysed. This step is necessary to achieve a correct representation of the geometry and accurate results in subsequent simulations and analyses.

The first step in the geometry adjustment was to create a square with the same dimensions as the imported image, i.e. 9 µm. This step was carried out using the *Square* tool where the appropriate dimensions were specified. The desired square was then created by clicking on *Build Selected*.

The *Convert to Solid* tool was then used in the *Conversions* section where all parts of the geometry were selected. After clicking *Build Selected*, all elements were converted to solid objects.

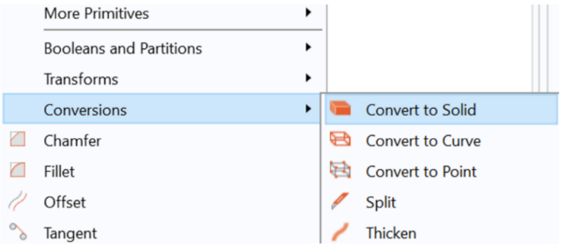

Figure 9. Convert to Solid

The next step was to remove the erroneous curves using the *Delete Entities* tool. Here the incorrect domains containing the erroneous curves were selected, the *Geometry* entity level was set to Boundary and once selected, *Build Selected* was clicked to remove them.

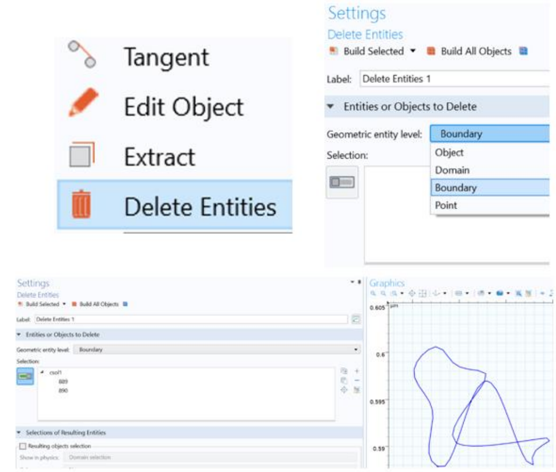

Figure 10. Delete Entities

The *Polygon* tool in the *Sketch* area was used to correct the area of crossed curves, allowing the area of crossing to be redrawn manually. Once the polygon was complete, it was confirmed by right-clicking and selecting *Finish Polygon*.

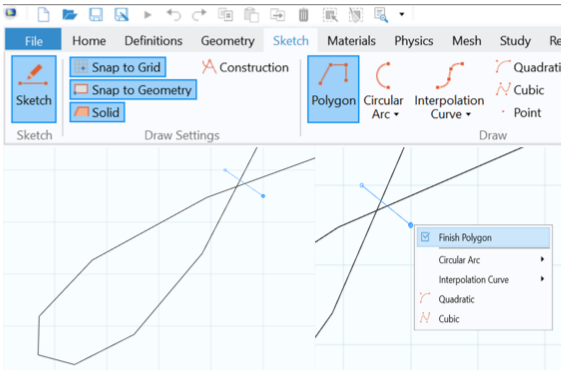

Figure 11. Polygon

The *Convert to Solid* tool was used again with the drawn polygon and curve selected in the *Input* section. After clicking *Build Selected* the polygon was converted to a solid object.

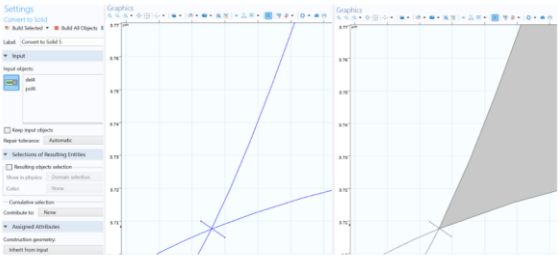

Figure 12. Convert to Solid

The polygon and curve in the *Entities or Objects to Delete* section were then selected and removed using the *Delete Entities* tool to fix the intersection point.

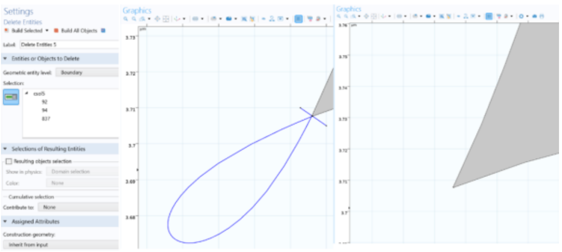

Figure 13. Entities or Objects to Delete

Finally, a second quad was added with the appropriate dimensions using the *Square* tool, and after clicking *Build Selected*, the quad was created. In the last step, the *Difference* tool in the *Booleans and Partitions* section was used to add the second square, successfully completing the geometry and making it ready for simulation.

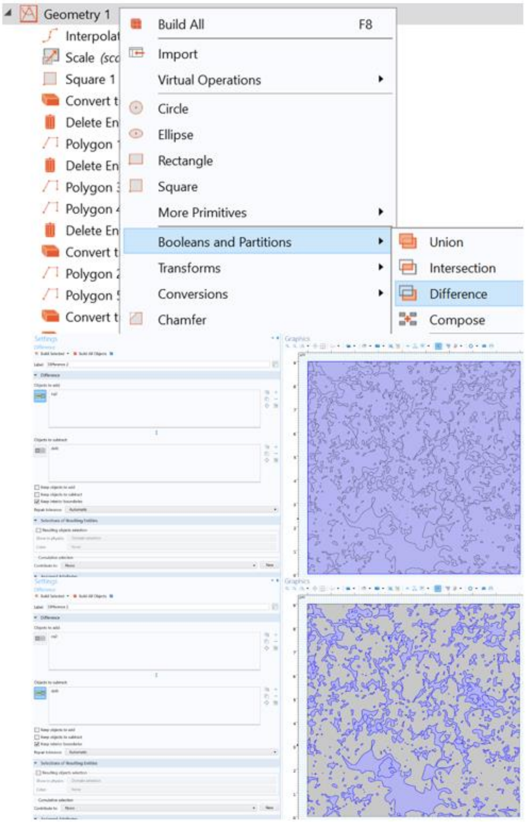

Figure 14. Difference

The resulting AFM image geometry is shown in Figure 15.

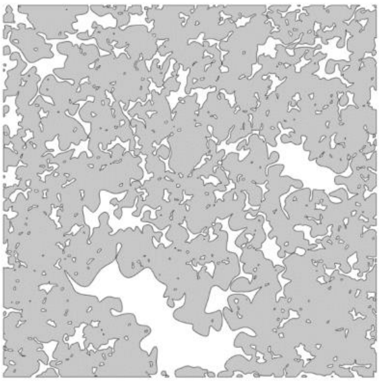

Figure 15. The resulting geometry of the AFM image

3.3 „Creeping Flow“ Physics Setting

The *Creeping Flow* interface is used to treat flow in the crevices of a porous medium. This interface solves the Stokes equations in channels.

$$0 = -\nabla \mathrm{p} + \nabla \cdot \mu(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

$$\nabla \cdot \mathbf{u} = 0$$

where p is the pressure [Pa], u is the velocity field [m/s] and μ is the dynamic viscosity of the fluid [Pa·s].

3.3.1 Boundary Condition

In this model, the inlet and outlet pressures of the fluid are known and we also assume that there is no flow at the upper and lower boundaries. This means that a no flow condition is set at the upper and lower boundaries, ensuring that no fluid flows through these boundaries.
The pressure drop in the system is therefore simulated by setting the pressure conditions between the left (inlet) and right (outlet) sides of the geometry. The inlet pressure of the fluid is set on the left side, while the outlet pressure is defined on the right side. These boundary conditions define the direction of fluid flow in the system and simulate a smooth pressure drop from left to right. This makes it possible to analyse the fluid flow within the model, in particular to calculate permeability or determine flow patterns.
Figure 16 shows the flow simulation procedure for a known pressure difference between the inlet and outlet.

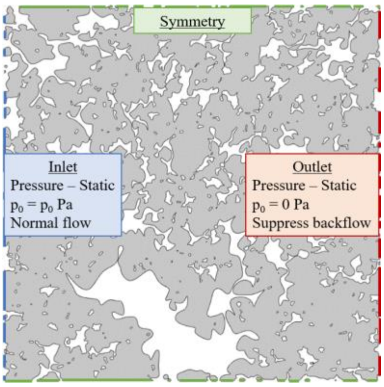

Figure 16. Geometry and Boundary Condition settings - inlet (blue), outlet (red), symmetry (green)

3.4 Material, Mesh and Study

In the practical part of the modelling in the COMSOL Multiphysics software, the following steps were taken to set up the material, the mesh and the study.
The integrated material library in COMSOL was used in the *Materials* node. Water was selected as the material according to the model requirements. Within the *Geometric Entity Selection*, the entire geometry was selected for the material application to ensure that the material properties were correctly assigned to all relevant parts of the model.
In the *Mesh* node, *Physically Controlled Mesh* was selected. This mesh type was selected to ensure that the mesh parameters were automatically set based on the physical properties of the model. The mesh element size was set to *Finer*, which allowed a finer and more detailed mesh to be created for more accurate simulations.
For the study selection, *Stationary* study was chosen based on its suitability for analysing problems where the solution is not expected to change with time. Thus, the simulation searches for a static, time-independent solution to the problem that satisfies the specified conditions.

4 Results and Discussion

The *Global Evaluation* function was used in the simulations to calculate important parameters such as porosity (por), total membrane area (A_tot), pore area (A_por) and permeability (k0). The results presented in Figure 18 show that the model value of porosity was 0.75278 and permeability was calculated to be $2.9635 \cdot 10^{-15}$ m^2. However, the experimentally determined porosity was found to be 0.813, which represents some deviation from the model results.

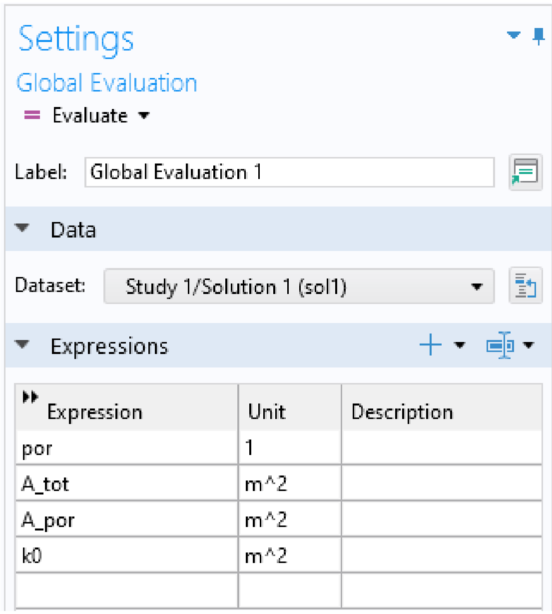

Figure 17. Global Evaluation settings

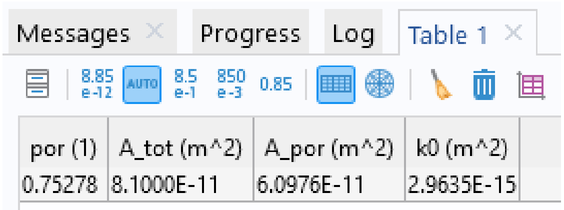

Figure 18. The obtained result

This deviation can be caused by several factors. One of the most important is the image-to-curve conversion performed during data analysis. During this step it was necessary to adjust the contours and correct the geometry of the model, which may have resulted in minor inaccuracies and a consequent difference in the comparison values. Despite these deviations, the *Image to Curve* module is still an effective tool for morphological analysis. Its results can be improved by more precise adjustments and calibration of the geometry, which would allow an even better agreement with the experimental data.

5 Conclusions

Porosity is a key parameter in the characterisation of materials as it significantly affects their mechanical, electrical and physical properties. In addition, permeability is another key factor that determines the ability of a material to transport liquids or gases. For example, high permeability increases the suitability of a material for applications such as filtration, separation or fluid transport.

Permeability analysis using atomic force microscopy images can determine the effectiveness of materials for specific applications. The *Image to Curve* module and the *Creeping Flow* interface in COMSOL Multiphysics software can be used to quantitatively evaluate the porosity and permeability of a material. These tools provide a deeper insight into the structure of materials, enabling a more accurate understanding of their behaviour and the optimisation of their properties for desired applications, whether in biotechnology, engineering or other fields.

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