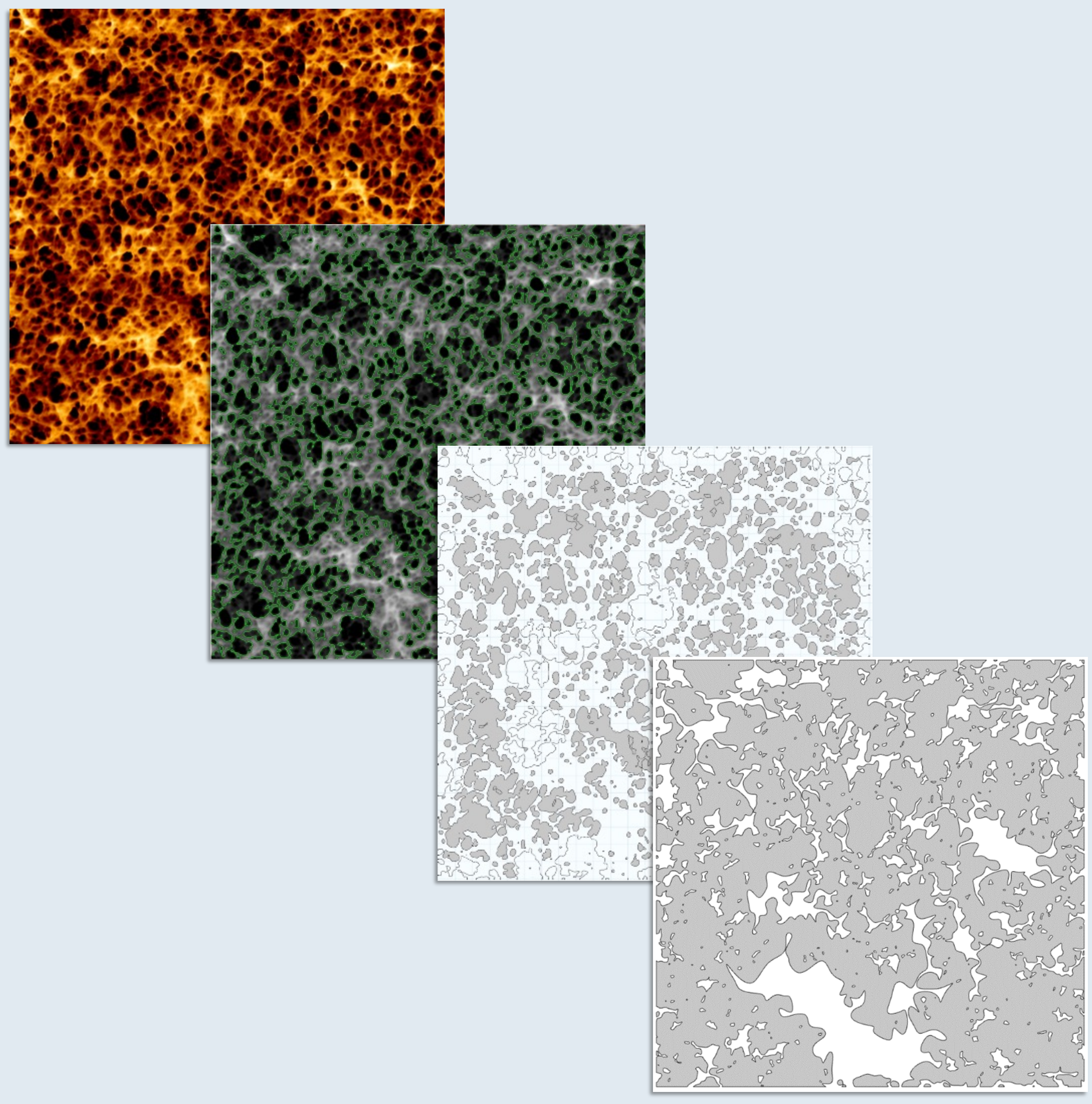

Determining Porosity and Permeability from AFM Images Using Image to Curve in COMSOL Multiphysics®

Generate geometry from AFM image with Image to Curve module for porosity and permeability calculation.

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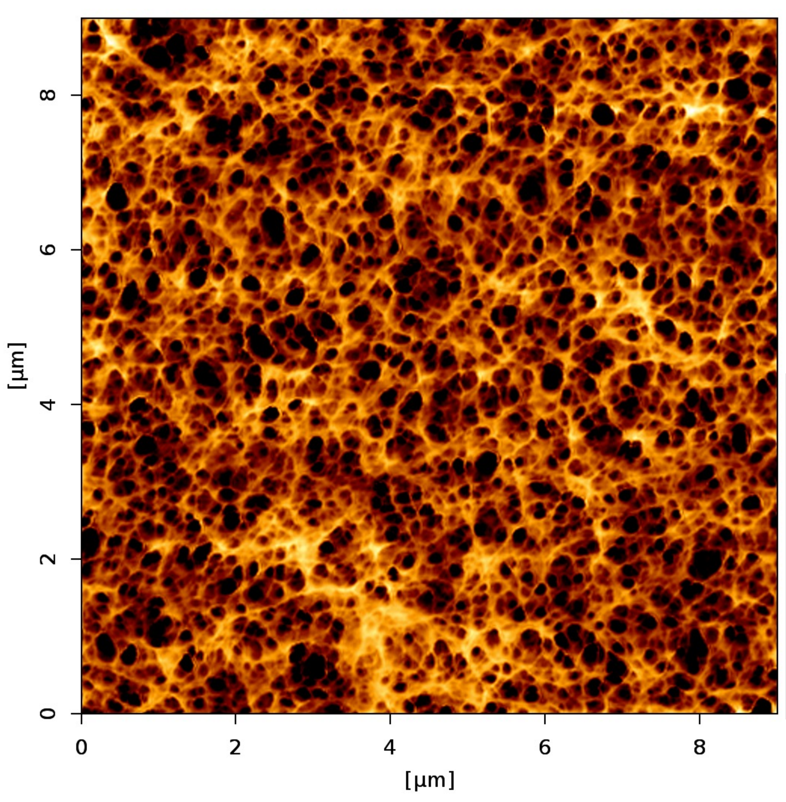
Abstract

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 analysis of AFM images is the quantification of 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 analyzable 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 optimized properties, opening up new opportunities for innovation in materials engineering.



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/m³	Water density
mu0	0.001 [Pa*s]	0.001 Pa·s	Dynamic viscosity of water

Name	Expression	Unit	Description
por	A_por/A_tot		Porosity
A_por	intop1(1)	m²	Pore area
A_tot	L*H	m²	Membrane area
u_out	q_out/H/1[m]	m/s	Outflow velocity
q_out	spf.out1.Mflow/rho0	m³/s	Flow rate
k0	u_out*mu0*L/p0	m²	Permeability

FIGURE 1: AFM image of the surface of a 2% agarose-based hydrogel sample (left) and definition of the parameters and the variables (right)

Methodology

Parameters and variables were used in the COMSOL Multiphysics software to calculate permeability and porosity, allowing dynamic adjustments to the model based on the AFM image. Porosity was calculated as the ratio of the pore area to the area of the porous matric, with Darcy's Law describing the flow through the medium. The AFM image was processed using the Image to Curve add-on, which converted the image contours into a closed curve that was then integrated into the model geometry. Subsequent geometry correction involved removing erroneous curves and adjusting intersections using the polygon tool. Creeping flow physics was used to simulate the flow with defined boundary conditions based on a known pressure differential. The water material was selected from the library, a finer physically controlled mesh was used and the simulation were performer using a stationary study.

Results

Permeability analysis from AFM images helps to evaluate material effectiveness for specific applications. The Image to Curve add-in and the Creeping Flow interface in COMSOL Multiphysics allows quantitative analysis of porosity and permeability, providing insight for optimizing material properties.

Global Evaluation was used to calculate porosity (por), total membrane area (A_tot), pore area (A_por) and permeability (k0) as shown in FIGURE 2. The experimentally determined porosity was found to be 0.813. Minor deviations may occur due to image to curve conversion where contour adjustments and geometry corrections were necessary. However, the module remains effective and further refinement may improve accuracy.

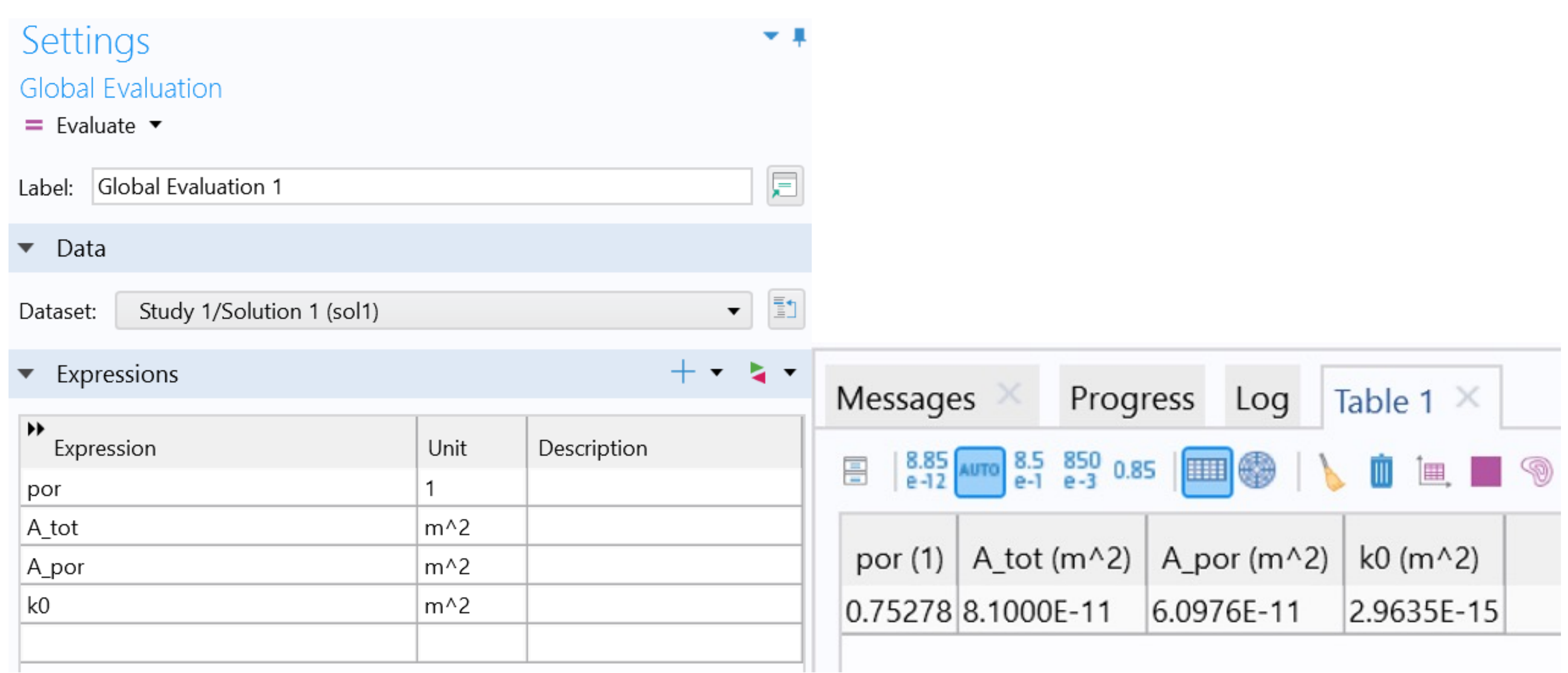


FIGURE 2. Global Evaluation settings and the obtained result

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2. Young A., Computing Porosity and Permeability in Porous Media with a Submodel, *COMSOL Blog*, September, 2017

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