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Pore scale flow modeling in Silica aerogel using scanning electron microscopy (SEM) image

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Abstract

Image-based pore scale modeling is a powerful computational tool for investigating transport in porous materials. The following is a finite element Stokes flow simulation of a Newtonian fluids through an advanced nanoporous material which is the Silica Aerogel. This type of non conventional pore scale modeling with COMSOL Multiphysics sheds new light on the movement of large particulates and colloids moving through the nanoporous geometries.

Keywords: SEM image, pore scale flow, advanced nanoporous material, Silica Aerogel, COMSOL Multiphysics.

1. Introduction

Silica Aerogel is receiving a lot of attention at this moment. It is a new kind of nanoporous advanced material composed of silica particles [1]. Due to its open mesoporous structure and huge specific surface area, Silica based aerogels have magnificent properties such as high porosity, low density, low thermal and electrical conductivities. It can be used as a heat insulating and energy saving materials. It can also be used in several other fields such as sound insulation, catalytic transport, aerospace, adsorption filtration and electronics [2-4]. Silica Aerogels possesses complicated microstructure. The modeling of the pore scale illuminate the understanding of the movement of large particulates and colloids moving through the nanoporous geometries. The swelling process of an aerogel and the deformation of the structure can be followed by titrating the solid sample with water or cyclohexane [5]. It is typical to represent fluid flow in the subsurface as a continuum process using average or "continuous" properties for the bulk rather than detailing the shape and orientation of each solid particle within a porous medium. Inserting the bulk properties into an equation, such as Darcy's law or Brinkman equations, gives an average flow rate for the total volume. While bulk approximations typically produce excellent estimates sufficient for considering flow over large areas, they might miss the between-grain nuances that a close-up Stokes flow analysis would give.

This study is aimed to provide a theoretical modeling of fluid flow through Silica aerogel using SEM image and solve for the flow velocity and pressure drop in the pore throats using the creeping flow interface.

2. Model description

The geometry is obtained using SEM image taking from the work of Peter Veres et al. [6] as it shows in figure1. At this resolution, we can clearly see the complexity of the pore space within the silica aerogel sample. For this simulation, the domain of simulation is reduced to a smaller rectangular section of the sample covering 750 nm by 1200 nm. A finite element fluid model is used to calculate the velocity field of the flow throughout the pore space.

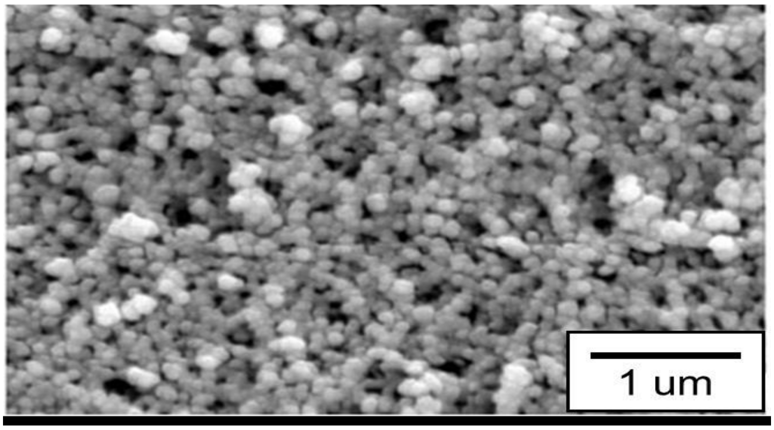

Fig 1. Scanning electron microscope image of Silica Aerogel[6].

3. Numerical model

The COMSOL Multiphysics software is used as an efficient tool of modeling and simulation of engineering and industrial applications involving several physics couplings. This tool is based on the finite elements approach and is employed to solve multiple physic problems via a set of elementary solvers that can be combined in different ways. In this study, the governing equations and initial and boundary conditions are numerically implemented by means of COMSOL Multiphysics.

3.1. Boundary conditions

The fluid adopted here is water. The fluid moves from left to right across the geometry. The flow in the pores does not penetrate the solid grains. The inlet and outlet fluid pressures are known. Assume no flow at the top and bottom boundaries. The primary zone of interest is the rectangular region with an upper left corner at (0, 0) nm (figure2). At the physical boundaries, the inlet pressure and the outlet pressure are known. Velocities are zero at the grain boundaries, which implies a no slip condition. The flow is symmetric about the top and bottom boundaries. The pressure drop is set to 0.715 Pa. The material properties are taken from the COMSOL Multiphysics 's library.

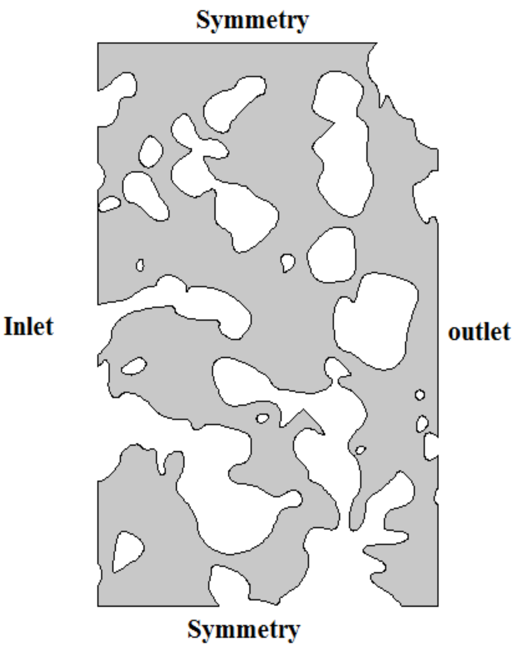

Fig 2. A 750 nm by 1200 nm geometry and boundary conditions.

3.2. Meshing

Triangular elements are used to define the computational mesh with refinement near walls involving high properties gradients as presented in figure3.

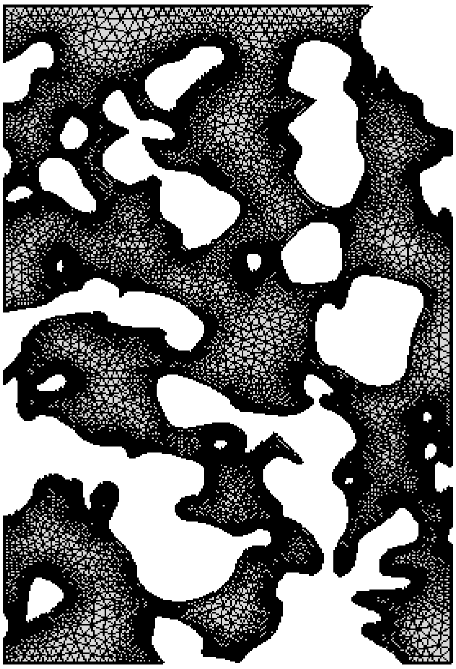

Fig 3. Mesh configuration.

4. Results

Figure 4 shows the COMSOL Multiphysics solution predicted with the creeping flow analysis for the fluid velocity field in the pore spaces of a micro-scale porous slice. The velocity magnitude is higher in the narrowest pores than at the inlet, tending to decrease in stretches where the channels' cross-sectional area increases. Illuminated streamlines were used to depict the continuous flow paths. The streamlines are colored according to the magnitude of the velocity field with the slower streams near the blue end of the spectrum and the faster streams near the red end. The porous material provides only a few complete pathways for transport in this domain. Therefore, the fluid tends to concentrate in flow along these pathways.

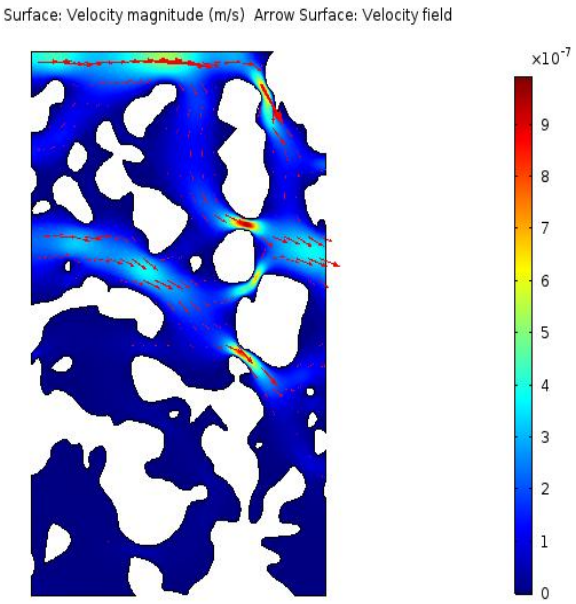

Fig 4. Surface and arrow plots of the velocity field calculated by the Creeping Flow interface.

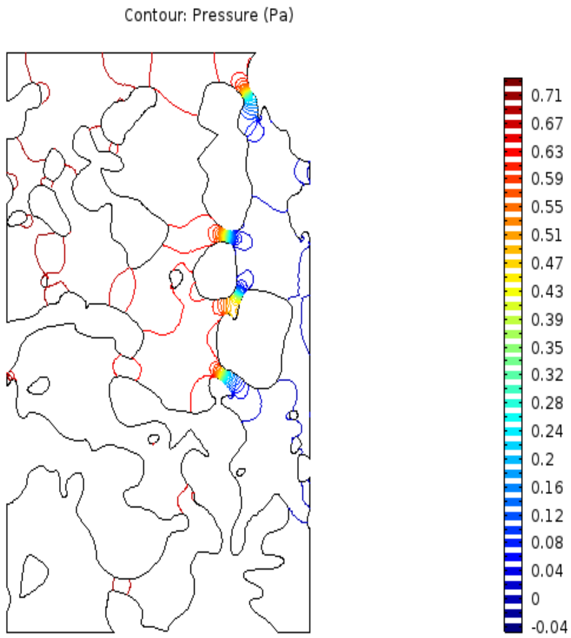

Fig 5. Pressure distribution.

5. Conclusion

In this paper, a pore scale flow modeling of Silica Aerogel using SEM image has been conducted. Through the microscopic eye of this simulation, we can look inside real nanoporous materials and explore the world in an entirely new resolution.

6. Acknowledgment

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