Two-Scale Modeling Approach to Predict Permeability of Fibrous Media

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ABSTRACT

We previously demonstrated how one can develop a 3-D geometry to model the fibrous microstructure of a nonwoven fiberweb and use it to simulate its permeability at fiber level [1-6]. Developing 3-D models of most nonwoven fabrics (bonded fiberwebs), however, is cumbersome, as in the case of hydroentangled fabrics, for instance. In such cases, microscopic techniques are often used to generate 3-D images of the media's microstructures. Nevertheless, whether the microstructure is modeled or obtained from 3-D imaging, extensive computational resources are required to use them in fluid flow simulations [7]. To circumvent this problem, a two-scale modeling approach is proposed here that allows us to simulate the entire thickness of a commercial fabric/filter on a personal computer. In particular, the microscale permeability of a hydroentangled nonwoven is computed using 3-D reconstructed microstructures obtained from Digital Volumetric Imaging (DVI). The resulting microstructural permeability tensors are then used in a macroscale porous model to simulate the flow through the material's thickness and the calculation of its overall permeability.

INTRODUCTION

Nonwoven fabrics have been utilized in absorbency products, air and liquid filter, and composite materials among many others. Modeling fluid flow through fibrous media helps to develop a better understanding of behavior of these materials under operating condition. It is, therefore, not surprising that during the past decades, there have been many pioneering works aimed at understanding the parameters that influence the permeability of fibrous materials. Flow through 3-D models consisting of arrays of rods randomly oriented in all directions, were first solved by Spielman and Goren [8] via analytical techniques. Jackson and James [9] proposed new expressions for the 3-D structures made up of straight fibers. Most recently, further investigations on 3-D fibrous structures were undertaken by Clague et al. [10], Wang et al. [1] and Zoble et al. [3] who investigated the permeability of viscous flow through disordered fibrous microstructures.

An alternative approach to obtain microstructure permeability of fibrous media is serial sectioning-imaging [11]. The 2-D images obtained from sectioning can be used to virtually reconstruct the original 3-D microstructure [11]. Along with the above sectioning technique, X-ray-computed micro-tomography has also been developed and widely used in studying porous materials in general. Only a few works, however, are dedicated to fibrous materials [12-17]. In our previous work, an integrated approach using automated serial sectioning technique Digital Volumetric Imaging (DVI) and finite volume method were reported to predict the permeability of nonwoven fabrics [7]. In this paper, we couple our previous study with a dual-scale modeling to extend the range of its predictions to macroscales.

DIGITAL VOLUMETRIC IMAGING

Digital Volumetric Imaging (Micro-science Group Inc.), is a block-face fluorescence imaging technique [18]. In this technique, the material, embedded in a polymeric resin, is repeatedly sectioned and imaged. These 2-D cross-sectional images are then combined to construct a 3-D image. The resolution of images obtained from DVI ranges from 0.48 to $4.48\,\mu m/pixel$, with a field of view ranging from 0.45 to 4.4 mm [18].

For the current study, a hydroentangled nonwoven fabric made of nylon fibers with mean fiber diameters of 14.3 μm were produced in the pilot laboratory of the Nonwovens Cooperative Research Center (NCRC) at NC State University. The fibers used for making the fabric had a length of 3 cm and their webs were prepared via carding process.

FIGURE 1. 3-D image of the hydroentangled fabric considered in this study.

Hydroentanglement is a process used for mechanically bonding a web of loose fibers to form uniform entangled sheets of fibers [19, 20]. The impact of the waterjets with the fibers displaces and rotates them with respect to their neighbors. During these relative displacements, some of the fibers twist and entangle around others and inter-lock with them through fiber-to-fiber friction. The hydroentangled fabric used in this study has an average Solid Volume Fractions (SVF) of 11%.

Our fabric was stained using fluorescent dyes, and imaged. A total of 1200 cross-sectional images with a size of 1016×1024 pixels and a resolution of 1.77 $\mu m / \text{pixel}$ were obtained. *Figure 1* shows a reconstructed 3-D image of the fabric.

MICROSCALE PERMEABILITY MODELING

The complex fibrous geometry shown in *Figure 1* will be used here to compute the permeability of the fabric at microscales. In this paper, we used grid aligned version of Peskin's immersed boundary method implemented in Geodict software code [21]. Pressure drop was chosen in such a way that the flow velocity though the medium is kept below 0.05 m/s resulting in Reynolds Number < 1 (Stokes flow) and so the governing equations for conservation of mass and momentum are given below respectively:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0 \qquad (1)$$

$$\frac{\partial p}{\partial x} = \mu \left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right) \qquad (2)$$

$$\frac{\partial p}{\partial y} = \mu \left(\frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right) \qquad (3)$$

$$\frac{\partial p}{\partial z} = \mu \left(\frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right) \qquad (4)$$

where v_x, v_y, and v_z are velocity in the *x*, *y*, and *z* directions, respectively, and p and μ are pressure and viscosity respectively. Periodic boundary conditions were used in the simulation. Permeability tensors were computed using Darcy's law:

$$v_x = \frac{1}{\mu} \left(k_{xx} \frac{\partial p}{\partial x} + k_{xy} \frac{\partial p}{\partial y} + k_{xz} \frac{\partial p}{\partial z} \right) \qquad (5)$$

$$v_y = \frac{1}{\mu} \left(k_{yx} \frac{\partial p}{\partial x} + k_{yy} \frac{\partial p}{\partial y} + k_{yz} \frac{\partial p}{\partial z} \right) \qquad (6)$$

$$v_z = \frac{1}{\mu} \left(k_{zx} \frac{\partial p}{\partial x} + k_{zy} \frac{\partial p}{\partial y} + k_{zz} \frac{\partial p}{\partial z} \right) \qquad (7)$$

where here $k_{ij}\ (i, j = x, y, z)$ is the full permeability tensor of the subdomain. Microstructural permeability of the hydroentangled fabric was found by simulating the flow through a series of subsamples (see *Figure 2*) taken from the original DVI image shown in *Figure 1*.

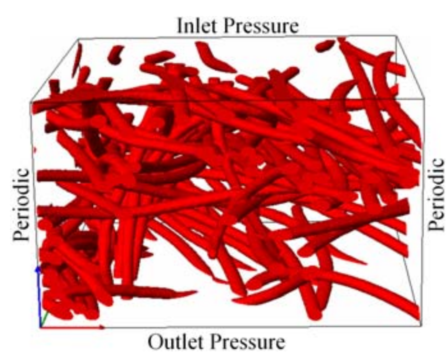


FIGURE 2. Computational domain along with the boundary conditions.

Local (microscale) permeability constants of the specimen shown in *Figure 1* can be found by taking series of subdomains from the original 3-D image and solving the flow equations using the GeoDict code.

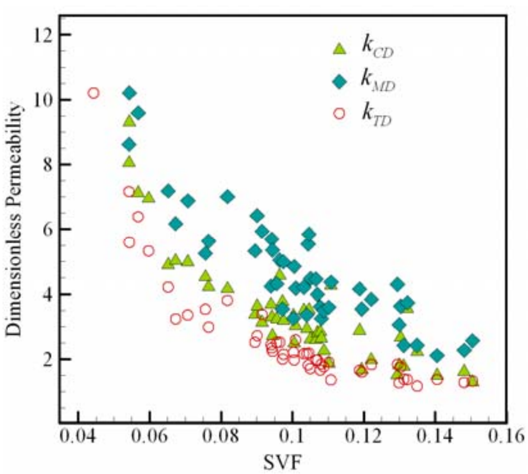


FIGURE 3. Subdomain permeability predictions in different directions versus SVF

In order to find an appropriate size for the simulation domain, we used the Brinkman screening length. A simulation domain greater than the Brinkman length, $\sqrt{k}$ (where k is permeability of the medium), by a factor of 14 is sufficiently large to smooth out the effect of local inhomogeneities [10]. We considered a series of sub-domains with a size of 200×200×200 voxels. This is large enough to represent the microscale properties of our fibrous media and, at the same time, small enough to allow the computations to be carried out on a personal computer.

In *Figure 3*, the local permeability constants obtained form simulating a series of subdomains in the machine (k_{MD}), cross-machine (k_{CD}), and thickness (k_{TD}) directions are shown versus the SVF. It may be observed that the local SVF considerably changes from one region to another within the specimen resulting in different local permeability values.

In *Figure 3*, note that k_{TD} is smaller than k_{CD} and k_{MD}. Interestingly, it can also be seen that k_{MD} is smaller than k_{CD} indicating that there is some degree of in-plane directionality in the material.

The abovementioned subdomains can also be imported to the Computational Fluid Dynamics (CFD) code from Fluent Inc.

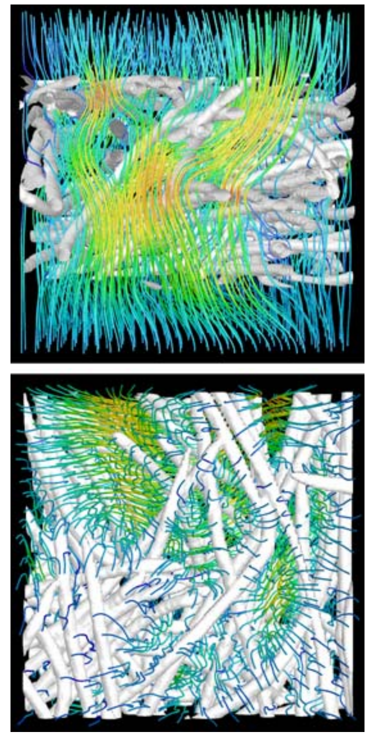


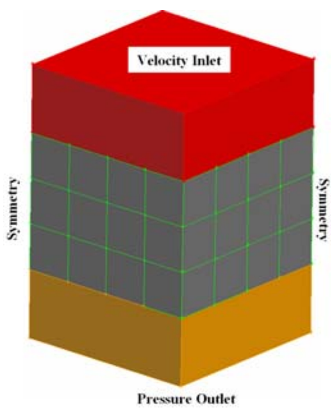
FIGURE 4. Flow path lines through the medium colored by velocity magnitudes a) side view, and b) bottom view.

Fluent code takes advantage of the finite volume method of Patankar [22] and can similarly be used to calculate the microscale permeability, or many other properties, of the subdomains. *Figure 4* shows an example of a subdomain simulated in Fluent code together with the flow path lines colored by velocity field throughout the medium.

MACROSCALE PERMEABILITY MODELING

From a practical point of view local permeability constants need to be converted to a single representative value i.e., effective permeability in order to be used in practical applications. Obviously, the effective permeability would be obtained if one could simulate the entire thickness of the fabric (see *Figure 1*). However, as mentioned earlier, such a simulation is requires excessive computational power. We, therefore, used the local permeability tensors obtained from our microscale modeling a macroscale porous media model implemented in the Fluent CFD code to compute the effective permeability of the material.

A porous medium in Fluent is modeled by the addition of a momentum sink term to the fluid flow equation in a specified region of the solution domain. This momentum sink term is a viscous resistance which we found from our sub-domain modeling. These local permeability constants contribute to a pressure gradient in each porous region creating an overall pressure drop for the whole domain. Boundary conditions considered for the simulations are shown in *Figure 5*. Symmetry boundary condition is considered for all the sides of the computational box. A fluid entry and exit zone was placed over the nonwoven material in a distance $L = 0.5t$ where t here is the thickness of the fibrous medium in the simulation box. This is to ensure that the pressure drop calculation is carried out in the regions far from any flow gradients. Note that if the sample size is large enough, the choice of symmetry boundary conditions will not affect the simulation results. This is because flow is mainly in the through-plane direction and lateral flows are negligible.



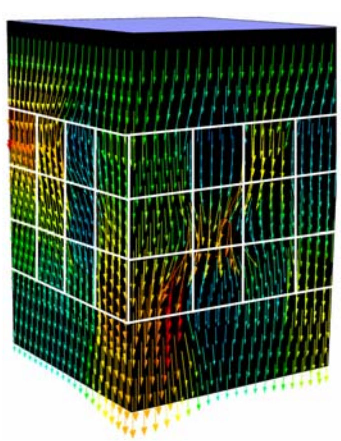


FIGURE 5. a) Simulation domain together with boundary conditions used in calculating effective permeability, b) velocity field throughout the thickness

The CPU time needed for running each of our 48 sub-domain simulations was around 90 minutes. Our lumped model simulation, on the other hand, required less than 2 GB of RAM and took only about 30 minutes to converge. The dimensionless effective permeability obtained from this simulation was found to be 2.12.

COMPARISION WITH EXPERIMENT

In order to further validate our simulations, we measured the through-plane permeability of our fabric using a Frazier air permeability tester. A constant pressure drop of 0.5 inches of water was used in the experiment. A total of 30 tests were conducted which resulted in an average dimensionless permeability of about 2.19 with a Standard Deviation of 0.07. Obviously, simulations are in good agreement with our experimental measurement. This hybrid technique of finding effective permeability based on realistic data obtained from the high resolution microstructure of fibrous structure together with porous media lumped models seems promising in regard to efficiency and time consumption.

CONCLUSIONS

In this work, we proposed a two-scale approach for calculating effective permeability of fibrous materials. Two-scale modeling, generally, is a relevant approach for simulating the flow through porous media with different length-scales. Here at microscales, we solved the flow field at the fiber level and obtained the materials microstructural permeability. At macroscales, we used the results of microscale modeling and obtained the total effective permeability of the material. We demonstrated that two-scale modeling allows one to simulate the entire thickness of a commercial fabric/filter on a personal computer with a reasonable CPU time – a task that would require a supercomputer otherwise. We also compared our two-scale permeability simulations with experimental data and observed good agreement.

Our microscale simulations revealed that for a carded hydroentangled fabric permeability is lowest in the Thickness Direction (TD) and highest in the Machine Direction (MD).

ACKNOWLEDGEMENT

The current work is supported by the Nonwovens Cooperative Research Center (NCRC). Their support is gratefully acknowledged.

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