Development of Permeability Models for Saturated Fluid Flow across Random and Aggregated Fiber Arrays

T.D. Papathanasiou¹ and Xiaoming Chen Department of Chemical Engineering University of South Carolina Columbia, SC 29208, USA

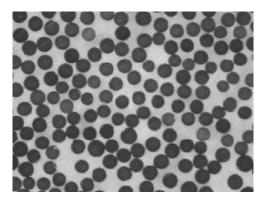
¹ Corresponding Author's e-mail: papathan@engr.sc.edu

SUMMARY We investigate computationally the effect of randomness as well as the effect of fiber aggregation on the hydraulic permeability (K_{eff}) of unidirectional fiber arrays. For this we carry out extensive viscous flow computations in various structured and unstructured fiber arrays using the Boundary Element Method (BEM) implemented on a 256-node Beowulf Intel cluster. Geometries are generated through a Monte-Carlo process, starting from uniform square arrays or from regular arrays of fiber clusters. Up to 196 individual fibers are included in each simulation Results demonstrate that at high values of (ϕ), deviations from the uniform array result in a decrease of K_{eff} . At lower porosity levels, the permeability shows a maximum at some intermediate value of the mean Nearest Neighbor Distance (\overline{d}_{nnd}). Finally, it is shown that fully clustered fiber arrays have higher K_{eff} than randomized ones; it is shown that for these systems (K_{eff}) scales with the deviation of Ripley's K-function for the given microstructure from that of the Poisson distribution.

KEYWORDS: permeability, fibrous media, liquid molding, composites manufacturing

BACKGROUND

Fibrous media are usually idealized as consisting of periodic or random arrays of fibers, which are typically represented as cylinders of circular cross section and constant radii [1,2]. In such representations, a unit cell can be identified; solution of the governing flow equations in this unit cell yields the flow rate (Q) and pressure drop (ΔP) from which the hydraulic permeability can be found using Darcy's law, $K_{eff} \approx \frac{Q}{\Delta P}$. However, regular fiber arrays are rarely encountered in real applications. Instead, fibers are either used in the form of bundles or in the form of preforms in which individual filaments assume random positions (Fig. 1). The permeability of structured arrays of fiber bundles was studied by Papathanasiou and co-workers [3-5] as well as by Advani and co-workers [6-8]. The permeability in random or quasi-random fiber arrays was also studied [9-10]. However, little work has been done to distinguish between random fiber distributions and correlate them with permeability data.



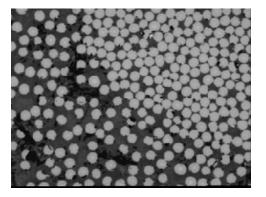


Fig. 1: Typical microstructures of unidirectional laminates. The image to the left is a technically flawless micrograph. The image to the right (showing the transition from a cluster to a resin-rich region) illustrates some problems commonly found in micrographs obtained from polished cross-sections. Both images obtained in our Laboratory using a BX50 Olympus microscope at 200x magnification.

MODEL SYSTEMS

Microstructures such as those of Fig. 1 can undoubtedly be used in a computational study. However, use of micrographs in computational work poses certain practical difficulties, such as fluctuation of fiber volume fraction in different image frames, existence of damaged (Fig. 1, right) or mis-oriented fibers or other 'edge' effects. As an alternative, computer simulation allows both, flexibility and exact control of the generated microstructures. In this work, fiber distributions were generated using a Monte Carlo perturbation method. This is a variant of the method described by Torquato [11] the difference being that the acceptance or rejection of a microstructural configuration is governed by a 'non-overlap' rule. To generate a fiber distribution, the model requires inputs such as the porosity (ϕ) , the number of fibers (N_f) , a minimum allowable inter-fiber distance (d_{min}) , the number of perturbation steps (N_p) , the maximum displacement of fiber during a move (δ) and an initial fiber distribution. Given a sufficient number of randomizing steps, this model produces fiber distributions possessing similar spatial characteristics (as evidenced by the corresponding pair-correlation function); additionally, these distributions are independent of the initial configuration. Due to the finite fiber size and the imposition of d_{min}, the simulated fiber distribution can never be completely random (that is, Poisson). Actually, the model employed in this study may be viewed as one of the self-inhibiting (or hard-core) models [12]. The minimum inter-fiber distance (d_{min}) is a key parameter affecting the spatial statistics of the generated microstructures. Fig. 2 shows two fiber distributions generated with different minimum inter-fiber distances and ϕ =0.7. It is clear that small values of d_{min} result in microstructures characterized by small fiber aggregates randomly placed throughout the domain. As d_{min} increases, the pattern becomes more regular. Additionally, the patterns generated through the MC process become more regular as the porosity gets smaller. It is known that the K(r) of patterns generated by a self-inhibiting model will fall below that corresponding to a Poisson pattern.

It is also known that, in the absence of strong clustering, K(r) is not a sensitive measure at longer length scales. In this situation, it is meaningful to use the Nearest Neighbor Distance (NND) as the measure to characterize the microstructure. For each fiber, one nearest neighbor distance can be found. While in a regular pattern the NNDs take the same value, a distribution of NNDs exists in a random pattern. Apparently, the distribution of NNDs corresponds to the distribution of narrowest pore spacing in the studied fibrous porous media and the allowable minimum value of NND is just the minimum inter-fiber distance specified by the model. The histograms of distributions of NNDs for the selected patterns in Fig.2a-b are plotted in Fig.2c. The skewed and steep shape of the distribution of NNDs is typical for the hard-core model [13].

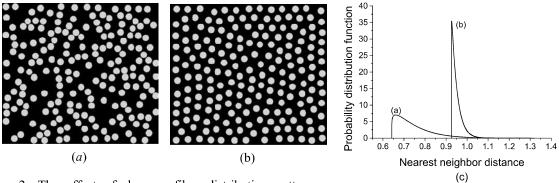


Fig. 2: The effect of d_{min} on fiber distribution patterns generated through a Monte-Carlo algorithm, starting from a square array. $\phi = 0.7$, $N_f = 196$. (a): $d_{min} = 0.05D$; (b): $d_{min} = 0.5D$. (D) is the fiber diameter

RESULTS AND DISCUSSION

Simulations were carried out using a parallel BEM code developed in-house, in microstructures generated at four different porosities ($\phi = 0.7, 0.6, 0.5, 0.45$) and with different minimum inter-fiber distances. In all models, N_f =196. There is a small but measurable size effect that is currently being investigated in detail. However, this does not change the trends discovered in this study. The mean nearest neighbor distance is used to correlate the microstructure to the dimensionless permeability K_{eff}/R². Lower values of \bar{d}_{mnd} correspond to fiber arrays that deviate the most from the uniform square array. The results of a large number of simulations are plotted in Fig.3. Open symbols represent the corresponding permeability data for regular square packing arrangements at ϕ =0.7, 0.6, 0.5 and 0.45 respectively, as obtained by numerical simulation. The permeability of different microstructural realizations (at the same level of porosity) can vary significantly, particularly at relatively low porosity. For this reason several realizations are studied at each level of (ϕ , \bar{d}_{nnd}) and averages along with the corresponding error bars are shown in Fig. 3. For low porosities, the computational results show that K_{eff} decreases as the extent of randomness of the fiber distribution (manifested by lower \bar{d}_{nnd}) increases.

This behavior is much more pronounced at lower porosities and suggests that extensive deviation from the uniform array results in the formation of many narrow gaps which effectively block the flow while not forming any easy flow path. This observation agrees with the recent finding by Bechtold et al.[10]. It does not contradict the common view that clustering will increase the permeability, since there is no significant clustering observed in such random microstructures. At high porosity (ϕ =0.7), there is a trend for the permeability to increase as \overline{d}_{nnd} decreases further down to less than about half the fiber radius. This is likely due to the fact that the chance to form easy flow path is bigger in random structure of high porosities. It is also noticed that permeability in a fiber array with large \overline{d}_{nnd} actually exceeds that of the square array. This is because the model tends to form a hexagonal array which has a larger permeability than that of a square array when the porosity is smaller than a certain value.

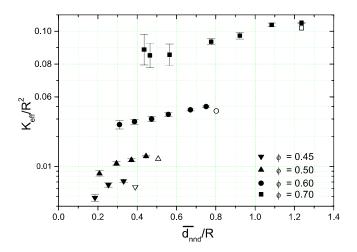


Fig. 3. Correlation of permeability with the mean nearest neighbor distance. Each filled data point represents the average of 10 simulations. The size of the error bars is 2σ , (σ) being the standard deviation.

To verify that clustering results in increased K_{eff} , we carried out simulations in clustered microstructures. The models used in this were generated by the same Monte Carlo method, starting from a regular pattern containing four clusters. To quantify the deviation of the clustered pattern from randomness, the following statistic measure was used:

clustered pattern from randomness, the following statistic measure was used:
$$L = \frac{1}{N} \sum_{i} K(r_i) / \pi r_i^2 \qquad r_i \le r_0 \tag{1}$$

where r_i is the distance at which K(r) is evaluated and πr^2 is the theoretical value for the Poisson distribution. If the pattern is clustered, L is larger than one. If the pattern is regular, L is less than one. Fig. 4 shows the correlation between L and $K_{\rm eff}$. It is evident that clustering does increase the permeability dramatically because of the formation of wide flow path. As the fiber distribution becomes randomized, it is expected that the constriction effect by the narrow pore spacing will again become the dominant factor. It is noted that L fails to correlate with $K_{\rm eff}$ when there is no strong clustering.

CONCLUSIONS

We have shown that deviation of the microstructure of a fibrous medium from the uniform square array results in permeability changes that can be correlated to the mean Nearest Neighbor Distance (\bar{d}_{nnd}) of the random microstructure. It is also shown that fully clustered fiber arrays have higher permeability than random ones; for such clustered systems it is shown that permeability scales with the deviation of Ripley's K-function from the Poisson distribution.

REFERENCES

- 1 Bruschke, M. V. and Advani, S. G., 1993, "Flow of Generalized Newtonian Fluids across a Periodic Array of Cylinders", *J.Rheol.*, Vol. <u>37</u>, pp. 479-498.
- 2 Gebart, B. R., 1992, "Permeability of Unidirectional Reinforcements for RTM", *J. Comp. Mat.*, Vol. <u>26</u>, pp. 1100-1133.
- 3 Papathanasiou, T.D., 1997, "On the Effective Permeability of Square Arrays of Permeable Fiber Tows", *Int. J. Multiphase Flow*, Vol. <u>23</u>, pp. 81-92.
- 4 B. Markicevic and T.D. Papathanasiou, "A model for the transverse permeability of bi-material layered fibrous preforms", Polymer Composites, **24**(1), 68-82, 2003
- 5 T.D. Papathanasiou, E. Gravel, S.C. Barwick and E.D. Dendy, "Non-isotropic structured fibrous media: The permeability of regular arrays of fiber bundles of elliptical cross-section", Polymer Composites, **23**(4), 520-529, 2002
- 6 Sadiq, T. A.K., Advani, S. G. and Parnas, R. S., 1995, "Experimental Investigation of Transverse Flow through Aligned Cylinders", *Int. J. Multiphase Flow*, Vol. <u>21</u>, pp755-774.
- 7 Pillai, K. M. and Advani, S. G., 1995, "Numerical and Analytical Study to Estimate the Effect of Two Lengths Scales upon the Permeability of a Fibrous Porous Medium", *Transport in Porous Media*, Vol. **21**, pp. 1-17.
- 8 Ranganathan, S., Phelan, F. R. Jr. and Advani, S. G., 1996, "A Generalized Model for the Transverse Fluid Permeability in Unidirectional Fibrous Media", *Polymer Composites*, Vol. 17, pp. 222-231.
- 9 Ghaddar C. K., 1995, "On the permeability of unidirectional fibrous media: A parallel computational approach", Phys. Fluids, Vol. 7, pp. 2563-2585.
- Bechtold G. and Ye Lin, 2003, "Influence of fiber distribution on the transverse permeability in fiber bundles", *Comp. Sci. and Technol.*, Vol. <u>63</u>, pp. 2069-2079.
- 11 Torquato S., 2001, Chapt. 12 in: Random Heterogeneous Material, Springer-Verlag.
- 12Ripley B. D., 1977, "Modeling Spatial Patterns", *Journal of Royal Statistical Society, Series B*, Vol.**39**, pp. 172-212.
- Pyrz R., 1994, "Quantitative Description of the Microstructure of Composites. Part I: Morphology of Unidirectional Composite Systems", *Comp. Sci. and Technol.*, Vol. <u>50</u>, pp. 197-208.

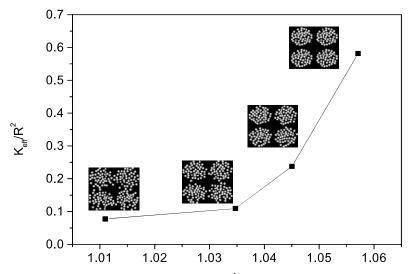


Fig. 4: Correlation of permeability in clustered patterns with L (Eqn. 1). ϕ = 0.7, $N_{\rm f}$ = 196.