Characterization of Porous Media Using a Geometric Depiction of Fibrous Materials

Sumanth Swaminathan et. al., MPI Workshop 2014

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Executive Summary

   Over the course of the MPI 2014 Workshop, we advanced our understanding of different performance metrics of fibrous materials. We gained insight into the nature of fluid flow in cross-sections of porous media, mapped the geometry of meniscus movement around fibers, and successfully modeled the accumulation of individual particles on individual fibers. Moreover, we produced numerical computations of the effects of particle buildup both deterministically and stochastically on fluid flow in these cross-sections.

   The goals for Gore's involvement in this workshop were as follows:

   I. To understand and examine the current theory on air filtration,

   II. Study the accumulation of particles on a single fiber,

   III. Model single-particle trajectories fibrous materials stochastically.

   IV. Understand fluid meniscus movement through fibers,

   V. Characterize fibrous media in three dimensions.

As such, the MPI team of mathematicians broke into five groups, with each group examining each subject. Their findings are reported below:

Air Filtration Theory

   The single fiber efficiency E_Σ is obtained from the formula

$$E_\Sigma = 1 - (1 - E_D)(1 - E_I)(1 - E_R)(1 - E_{DR})(1 - E_G)$$

where E_D, E_I, E_R, E_{DR}, and E_G are single fiber efficiency due to diffusion, inertial impact, interception, combined diffusion and interception, and gravity respectively. We wrote a Matlab® script that calculates the efficiency of the filter given the input parameters above in addition to u_0, u_1, D, and C which are the air flow velocity in front of the filter, air flow velocity inside the filter, diffusion coefficient, and slip correction respectively. The script also uses one of three formulas to calculate E_I, depending on whether the Stokes number is a low, a medium, or a high value.

Particle Accumulation on Fiber

Taking a continuum mechanics approach, we assumed a Stokes flow and a Stefan condition at the interface and solved for concentration of particles in the flow and on the fiber. The aim here was to see what sort of shapes tended to build up as particles accumulated around the filter–that is, whether particles gather in a uniform manner, an oscillatory manner, or whether they tend to form dendrites stringing off of the particles.

Brownian Trajectories

We used a boundary element method to solve the Stokes equations for air flow in a channel. We assume that there are no-slip boundary conditions on the channel walls and on the surface of circular filters, and that there are Dirichlet conditions specifying constant velocities on both ends of the channel.

Our program calculates the fluid flow paths and then sends particles through our channel subject to Langevin dynamics one at a time. Each travels along the fluid flow being shifted by random movements perpendicular to the trajectory of the particle. We then model the trapping of the particles by the filter depending on the distance between the two.

Once a particle attaches to a filter, it then becomes part of the filter, and a new Stokes system is solved, and thus we account for the accumulation of particles in modeling the air flow.

Meniscus Movement

Three-Dimensional Fibril Model

During the previous MPI workshop (summer 2013), a two-dimension characterization of a network representing a porous medium was developed. One of our goals this year was to extend the previously developed code to obtain three-dimensional characterziations. For the 3D case, the domain was assumed to be a rectangular prism with periodic boundaries.

In our investigation of the previous code, we realized that the periodic boundary conditions were not always implemented correctly. We therefore first enhanced the 2D code to ensure periodic boundary conditions. There were a few different cases to considering when enforcing the periodic BCs. For most cases, only one shift was required to move a new node into the domain from where it was originally places. The more complicated cases correspond to when a new node was placed outside of the boundary close to one of the corners. Then two shifts were required to ensure that the new node and the line segment connecting the previous node to the new node ended up in the domain. After ensuring that the periodic boundary conditions were enforced, extending the two-dimensional code to three-dimensions was straightforward.