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Tortuosity Computations of Porous Materials using the Direct Simulation Monte Carlo

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Low-density carbon fiber preforms, used as thermal protection systems (TPS) materials for planetary entry systems, have permeable, highly porous microstructures consisting of interlaced fibers. Internal gas transport in TPS is important in modeling the penetration of hot boundary-layer gases and the in-depth transport of pyrolysis and ablation products. The gas effective diffusion coefficient of a porous material must be known before the gas transport can be modeled in material response solvers; however, there are very little available data for rigid fibrous insulators used in heritage TPS.

The tortuosity factor, which reflects the efficiency of the percolation paths, can be computed from the effective diffusion coefficient of a gas inside a porous material and is based on the micro-structure of the material. It is well known [1,2], that the tortuosity factor is a strong function of the Knudsen number. Due to the small characteristic scales of porous media used in TPS applications (typical pore size of the order of 50 micron), the transport of gases can occur in the rarefied and transitional regimes, at Knudsen numbers above 1. A proper way to model the gas dynamics at these conditions consists in solving the Boltzmann equation using particle-based methods that account for movement and collisions of atoms and molecules.

In this work we adopt, for the first time, the Direct Simulation Monte Carlo (DSMC) method to compute the tortuosity factor of fibrous media in the rarefied regime. To enable realistic simulations of the actual transport of gases in the porous medium, digitized computational grids are obtained from X-ray micro-tomography imaging of real TPS materials. The SPARTA DSMC solver [3] is used for simulations. Effective diffusion coefficients and tortuosity factors are obtained by computing the mean-square displacement of diffusing particles.

We first apply the method to compute the tortuosity factors as a function of the Knudsen number for computationally designed materials such as random cylindrical fibers and packed bed of spheres with prescribed porosity. Results are compared to literature values obtained using random walk methods in the rarefied and transitional regime and a finite-volume method [1,2] for the continuum regime [4,5]. We then compute tortuosity factors for a real carbon fiber material with a transverse isotropic structure (FiberForm [5]), quantifying differences between through-thickness and in-plain tortuosities at various Knudsen regimes.

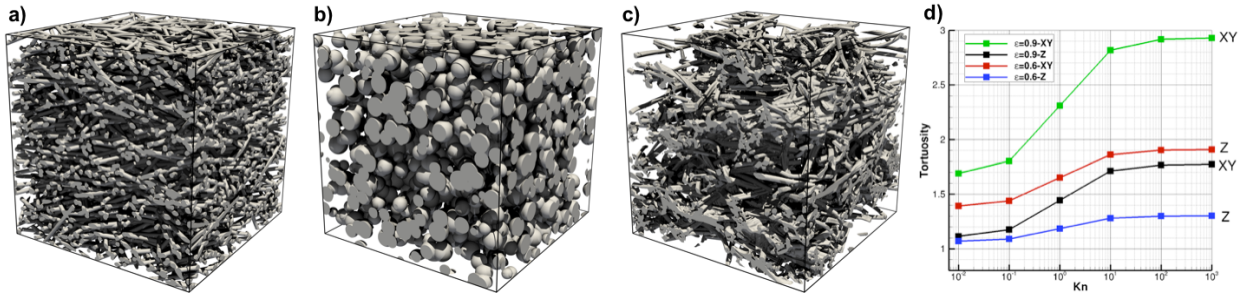

Figure 1. Volume rendering of materials studied in DSMC. a) Randomly overlapping cylindrical fibers, 0.9 porosity, b) randomly packed bed of spheres, 0.9 porosity, c) FiberForm, 0.87 porosity. d) Tortuosity factor as a function of the Knudsen number for volume a) and for a similar volume of 0.9 porosity.

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