Calculating the permeability of model paper coating structures comprising incongruent particle shapes and sizes

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Abstract

The extent to which paper coating is permeable holds significance in a variety of operations related to coating and printing. Permeability is implicitly linked to the microstructural organisation of pore space and is further complicated by factors such as surface energetics and the properties of the permeating fluid. Relating the microstructural characteristics of coatings to permeability is a challenging yet essential objective. The research herein uses computational methods to generate anisotropic particulate microstructures, which are then used to statistically analyse pore space as well as for fluid dynamics simulations.

Particulate microstructures are generated using a voxel packing approach. Attempts are made to computationally mimic the microstructure for four different coatings made entirely of packed particle material. These include coatings consisting of kaolin, precipitated calcium carbonate (PCC), ground calcium carbonate (GCC) and plastic pigments (PP). Particle sizes were distributed within the packings as a function of volume percentages and are based upon experimentally determined data. Kaolin particles are modelled as hexagonal plates with a diametral size distribution ranging between 2.4 and 8.8µm. PCC particles are rod-like and represented using lengths ranging from 0.2 to 1.2µm with corresponding diameters from 0.05 to 0.3µm. The blocky construct of GCC particles are simulated using seven-face frustums with larger end diameters ranging between 0.5 and 2.5µm. Finally, plastic pigments are mimicked using spheres with diameters ranging from 0.12 to 0.29µm. The final porosities of kaolin, PCC, GCC and PP packings come to 34.9%, 48.1%, 35.9% and 39.8% respectively. These porosities vary in accuracy and are within 0.5%-9.2% of the reference packing porosities, as determined experimentally.

A modified Maximal Balls algorithm is used to statistically analyse and differentiate both, pore as well as neck space in the packing microstructure. Essentially, the algorithm assigns spheres to individual empty voxels in space allowing the ball to have extents no larger than from its centroid position to the nearest solid voxel. Pore or neck centres are consequently defined by local maxima and minima respectively. The interface defining pore from neck is defined by hierarchically structuring progressively smaller adjoining balls from the local maxima towards the local minima until the adjoining ball is the same size as the preceding ball.

Computational fluid dynamics simulations are conducted using a volume-of-fluid method for filled systems assuming no free surface influence. The simulations are driven by a pressure gradient and the packing permeability is calculated using the D'Arcy equation. The D'Arcy permeability values are compared with experimentally determined values and furthermore, a statistical variance of permeability is calculated within each packing structure. The permeability values are moreover compared between the different packings as a function of the different particle shapes used and the consequential pore-neck characteristics that are generated.