# Fluids in porous media: a morphometric approach to structure-property relations


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Predicting the relationship between the morphology of porous media and their physical properties, e.g, the conductivity, elasticity and permeability, is a long-standing problem and important to a range of applications from geophysics to materials science [1]. Here, a set of four morphological measures, so-called Minkowski functionals, is defined which allows one to quantitatively characterize the shape of spatial structures, to optimally reconstruct porous media, and to accurately predict material properties [2]. The method is based on integral geometry and Kac's theorem which relates the spectrum of the Laplace operator to the four Minkowski functionals. Analytic expressions for mean values of Minkowski functionals in Boolean models lead to the definition of an effective shape of a grain in a system made up of a distribution of arbitrarily shaped constituents. Reconstructing the microstructure using this effective grain shape yields an excellent match to the percolation thresholds and to the mechanical and transport properties across all phase fractions [3]. Additionally, the use of the effective shape in effective medium formulations leads to good explicit predictions of bulk moduli. The method is verified for several model systems and sedimentary rock samples, demonstrating that a single tomographic image is sufficient to estimate the morphology and physical properties such as permeabilities and elastic moduli for a range of porosities.

Also the thermodynamic behavior of fluids in porous media, i.e., the shape dependence of the grand canonical potential and of surface energies of a fluid bounded by an arbitrarily shaped convex pore can be calculated in the thermodynamic limit fully from the knowledge of the Minkowski functionals, i.e., of only four morphometric measures [4]. This remarkable result is based on Hadwiger's theorem on the completeness of the additive Minkowski functionals and the assumption that a thermodynamic potential is an additiv functional which can be understood as a more precise definition for the conventional term extensive. As a consequence, the surface energy and other thermodynamic quantities contain in the thermodynamic limit, beside a constant term, only contributions linear in the mean and Gaussian curvature of the pore and not an infinite number of curvature terms. Finally, starting from a microscopic density functional for an inhomogeneous fluid in a porous medium the phase coexistence (capillary condensation) and the critical point of the fluid is determined in terms of structure functions and morphological measures of the pore space and calculated explicitly for specific random porous structures using results from integral geometry.


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