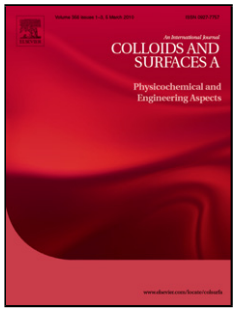

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Modelling of the microstructure of mesoporous alumina constrained by morphological simulation of nitrogen porosimetry

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Abstract

A procedure is proposed to simulate numerically experimental capillary condensation and evaporation isotherms in porous media, and to simulate random microstructures based on such isotherms. The present methodology is applied to a mesoporous material made of nanometric alumina "platelets". First, a numerical method is developed to compute the adsorption and desorption isotherms in digital porous media. The method, based on simple morphological operators, extends that of Münch and Holzer (2008) on mercury porosimetry. The meniscus of the vapour-liquid interface occurring during adsorption are simulated using a morphological closing (G. Matheron, 1967, J. Serra, 1982) of the solid phase by a sphere. The diameter of the sphere controls the radius of curvature of the vapour-liquid interface. To simulate desorption, a combination of morphological closing and hole-filling operators is used. For random media, the desorption curve is strongly sensitive to the volume of the computational domain. We overcome this effect by a percolation analysis of the gaseous phase during desorption. The present method allows one to predict the hysteresis and pore size distribution associated to porosimetry. To validate this approach, numerical results on simple geometries are compared with the work of Štěpánek et al. (2007) based on the Kelvin equation. The condensation and evaporation isotherms occurring in various ideal Boolean models simulating different types of porous media are also computed and interpreted. Second, nitrogen porosimetry data for mesoporous alumina is considered. Based on results obtained for multiscale microstructures, a random model is proposed for mesoporous alumina. To control both the size distribution and hysteresis, the porosity is made of a union of Boolean and hard-core models of spheres. The parameters of the model are identified and numerically adjusted to reproduce the experimental desorption isotherm. Finally, we develop a model of mesoporous alumina, consistent with both porosimetry data and Transmission Electron Microscopy images, made of aggregates of locally-aligned alumina platelets, as introduced in a previously-developed model (Wang et al., 2015). The model contains the following characteristic scales: the platelets's size, that of platelets aggregates, and the size-distribution of pores.

Keywords: Capillary condensation, Porosimetry, Adsorption, Random model, Pore size distribution, Microstructure modelling

1. Introduction

This work focuses on the modelling of the capillary condensation and evaporation phenomena, as described described by the Kelvin equation, in porous media. The Kelvin equation relates vapour/pressure equilibrium to the morphology of the pores: the more curved the local vapour/liquid interface is, the lower the equilibrium vapour pressure is. Accordingly, capillary condensation occurs first along highly curved interfaces. Porosimetry isotherm represents the amount of liquid (or equivalently, the remaining porosity filled by gas) as a function of pressure. When represented as a function of curvature radius, the isotherm is frequently interpreted as a cumulative size distribution for the porous phase [1]. Accordingly, the simulation of the capillary condensation and evaporation is important to study the relation between morphology of the material microstructure and experimental porosimetry data. Nevertheless, the question of determining the main microstructure parameters that influence the porosimetry remains open.