

TWO-SCALE COMPUTATIONAL MODELS FOR THE DISJOINING PRESSURE BASED ON A NON-LOCAL ANISOTROPIC HYPERNETTED CHAIN CLOSURE INCLUDING ION FLUCTUATION AND CORRELATION EFFECTS

C. MOYNE^{*}, T. DUNG. LE^{*}, M. A. MURAD^{**} AND SIDARTA LIMA ^{***}

^{*}Universite de Lorraine
Laboratoire d'Energetique et de Mecanique Theorique et Appliquee France
e-mail: Christian.Moyne@ensem.inpl-nancy.fr Dung.Le@ensem.inpl-nancy.fr

^{**} Laboratorio Nacional de Computação Científica LNCC Brazil
e-mail: murad@lncc.br

^{***} Dept of Mathematics Federal University of Rio Grande do Norte Brazil
email sidarta@lncc.br

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Abstract. A new homogenization method is proposed to compute the disjoining pressure in electrically charged porous media. The pore-scale model is based on the Poisson problem for the electric potential coupled with the integral Ornstein-Zernike equation supplemented by a anisotropic hypernetted chain closure to describe the ion-ion correlation functions along with a general representation for the chemical potential of the ions including a non-local excess component which captures the effects of the finite size of the ions. The non-local pore-scale model arises from the Statistical Mechanics framework and, in contrast to the classical electrical double layer theory based on the local Poisson-Boltzmann problem, does not assume point charge ions but rather charged hard spheres with charge located at their center. Numerical results are obtained for stratified micro-structure of parallel particles using collocation schemes. Such results show that for higher valence ions the effects of ion-ion correlation forces give rise to attraction between the particles for some values of particle separation characterized by negative values of the disjoining pressure.

