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Effect of air on water capillary flow in silica nanochannels HAR-VEY ZAMBRANO, Universidad de Concepcion, JENS WALTHER, Technical University of Denmark, ELTON OYARZUA, Universidad de Concepcion — Capillarity is a classical topic in fluid dynamics. The fundamental relationship between capillarity and surface tension is solidly established. Nevertheless, capillarity is an active research area especially as the miniaturization of devices is reaching the molecular scale. Currently, with the fabrication of microsystems integrated by nanochannels, a thorough understanding of the transport of fluids in nanoconfinement is required for a successful operation of the functional parts of such devices. In this work, Molecular Dynamics simulations are conducted to study the spontaneous imbibition of water in sub 10 nm silica channels. The capillary filling speed is computed in channels subjected to different air pressures. In order to describe the interactions between the species, an effective force field is developed, which is calibrated by reproducing the water contact angle. The results show that the capillary filling speed qualitatively follows the classical Washburn model, however, quantitatively it is lower than expected. Furthermore, it is observed that the deviations increase as air pressure is higher. We attribute the deviations to amounts of air trapped at the silica-water interface which leads to changes in the dynamics contact angle of the water meniscus.

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