# A Coarse-Grained Model for Microscale Multiphase Interactions and Its Applications in Dynamic Wetting

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## Abstract

Understanding the response of unsaturated porous media under various loading conditions and multiphase flows at the microscale is crucial in civil and geotechnical engineering. This work demonstrates the ability of our recently developed coarse-grained molecular dynamics framework to reproduce the physical and mechanical properties of the microscale liquid-vapour, solid and liquid-vapour-solid systems. In particular, the coarse-grained model can reproduce: (1) the experimental density and surface tension of water in the water-vapour system, and (2) the experimental density, tensile strength and Young's modulus of silica in the silica model after the calibration of the particle-particle interaction parameters. The wettability of the liquid-vapour-solid system can be controlled by adjusting the parameters of the solid-liquid particle interactions. We further extend our coarse-grained model to the study of the dynamic contact angle of a $CO_2$-water-silica system as a function of the contact line velocity at different water pressures. The preliminary results show that the $CO_2$ contact angle increases with an increase in the contact line velocity.

**Keywords:** coarse-grained molecular dynamics, contact angle, multiphase interactions, microscale.