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Unified surface poromechanics theory capturing condensation-induced contraction of mesoporous materials

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The phenomenon of adsorption-induced deformation is prevalent in both natural materials such as wood and coal, as well as in engineered materials like cement, MOFs (Metal-Organic Frameworks), and porous polymers. As the partial pressure of adsorbate vapor rises, the strain isotherm of these materials can display intricate nonlinear and non-monotonic behaviors.

Under low partial pressures, most porous materials undergo volumetric expansion. This expansion can be attributed to the reduction of surface stress and the subsequent relaxation of adsorption stress experienced by the solid skeleton—a phenomenon commonly known as the “Bangham effect.” This effect is well-described by the surface poromechanics formulation proposed by Zhang (2018). For microporous materials, early adsorption can lead to a subtle shrinkage before the onset of swelling. This is linked to the development of negative disjoining pressures in nanopores, as explained by Eskandari-Ghadi and Zhang (2021).

Despite these advances, the current surface poromechanics formulation is only for a single-phase pore fluid and therefore, does not apply to partially saturated porous media nor capture the dynamics of phase transition of the pore fluids. For this reason, it is unable to model the sudden contraction of mesoporous media at intermediate vapor pressure levels induced by capillary condensation. This contribution outlines our progress toward developing a unified surface poromechanics formulation that meets the following criteria:

1. It takes into account the phase transition of pore fluid from vapor to liquid and the emergence of the liquid-vapor interface.
2. It accurately reproduces the water retention characteristic curve unique to each porous system.
3. It captures both the early Bangham expansion (without condensation) and the significant contraction resulting from condensation in a consistent manner.
4. The theory’s asymptotes at degrees of saturation equal to 0 and 1 align with the conventional poromechanics theory for single-phase pore fluid.

REFERENCES:

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References

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