6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 – 15 June 2018, Glasgow, UK

A MULTI-SCALE STUDY OF SORPTION-INDUCED SWELLING OF WOOD AND RELATED HYSTERESIS

Mingyang Chen[1], Benoit Coasne[2], Robert Guyer[3], Dominique Derome[4] and Jan Carmeliet[1,4]

[1] ETH Zurich, Swiss Federal University of Technology Zurich, Zürich, Switzerland.
[2] Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble, France.
[3] Department of Physics, University of Nevada, Reno, Nevada, United States.
[4] Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland.

Key Words: *Sorption-induced swelling; Hysteresis; Coupling; Multi-scale.*

Wood, as a hygroscopic material, undergoes changes in dimensions as well as in their mechanical and physical properties when exposed to moisture. Specifically, swelling and shrinkage have been observed respectively during adsorption and desorption process, with significant hysteresis with respect to relative humidity. As a great number of wooden structures serve in environmental conditions with significant humidity variations and undergo a large number of sorption cycles, it is thus important to figure out the mechanism behind this complex history-dependent behavior.

We study the hydro-mechanical behavior of amorphous cellulose, an important constituent of wood, with the help of Molecular Dynamics and grand canonical Monte Carlo method. The simulated sorption and strain isotherms show significant hysteresis, but no hysteresis is observed between moisture content and volumetric strain, which is in agreement with experiments. We find hysteresis of sorption directly related the sorption-induced swelling. An analysis of hydrogen bonds are conducted to reveal the microscopic mechanism behind this coupling behavior. We find that the sorption hysteresis relies on the creation of new adsorption sites. Specifically, during the adsorption process, hydrogen bonds between polymers are broken and new adsorption sites are exposed due to the moisture induced swelling. These sites bond to water, and the bonded water molecules become obstacles in the desorption phase. This difference in configurations, which are studied in detail, of water molecules results in the hysteresis of sorption and swelling/shrinkage.

Based on the microscopic mechanism unraveled, a dependent domain model is built by considering the influence of local strain on the porosity, modulus and critical chemical potential of filling. Implemented into Finite Element method, this model gives a good approximation of the coupling behavior between sorption and deformation of amorphous cellulose under the framework of continuum mechanics. Moreover, the hysteric behavior of amorphous cellulose, which includes non-congruence of sub-loops, is present. The influence of different external mechanical loadings on the sorption behavior is studied in details.

In summary, we reveal the mechanism of sorption-induced deformation of amorphous cellulose and related hysteresis and upscale it to the macroscopic level with the help of the dependent domain model.