Using MD simulations for the poromechanical formulation of a hygromechanical behavior of a nanoporous biological cellular composite

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ABSTRACT

Complementary to experimental analysis, computational modeling allows advancing the fundamental understanding of materials. Modeling provides the capability to determine material properties which cannot be directly determined from experiments and to explore new pathways for material development and technology innovation. To illustrate this, modeling at molecular scale using Molecular Dynamics is used to characterize the hygromechanical behavior at nanoscale of polymeric systems inspired by the biological composite that is wood. The work aims at elucidating the origin of the hygro-mechanical behavior of such complex polymeric materials. MD results are upscaled and used in continuum models, using a poromechanical framework thus full coupling of fluid transport and mechanical behavior. Upscaling to cellular scale and to timber scale is delineated, where the cellular scale is informed through accurate geometrical description using Xray CT at different relative humidity.

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