Mechanics of cellulose gels to aerogels

Nina Borzecka*[1] and Ameya Rege[1,2]

[1]German Aerospace Center – Germany
[2]University of Twente – Netherlands

Abstract

Cellulose aerogels are novel, biodegradable alternatives to state-of-the-art plastic-based porous materials, particularly interesting for thermal insulation and mechanical stability. Moreover, with increasing demand of sustainable processes and materials, biopolymer-based aerogels are attracting a considerable attention. The key to their exceptional properties, such as low density, well-developed surface area, high sorption capacity and excellent insulating properties is their high porosity. To obtain that porosity, the aerogel synthesis requires application of supercritical drying – transition of the liquid filling the gel network to gas state without causing significant volume shrinkage. The fundamental understanding of the correlation between gel structure, drying conditions and the final porosity is crucial for better understanding of the system on fundamental level, but also for process and product optimization in the future.

Cellulose gels synthesis steps and mechanical behavior were simulated with discrete element method (DEM) extended with bonded particle model (BPM). The diffusion and aggregation of cellulose chains is represented with a coarse-grained Langevin dynamics with consideration of hydrogen-bonding formation due to van der Waals forces. The computationally obtained gel undergoes the postprocessing steps corresponding to the actual experimental procedure: washing, solvent exchange and supercritical drying. The mechanical behavior of the structure depending on its structural properties was examined with uniaxial tests and the supercritical drying was represented by applying hydrostatic compression mimicking the pressure subjected within the autoclave on the gel network.

The parameters sensitivity analysis results provide a fundamental understanding of the influence of the polymer-polymer interaction on the structure formation process and final pore structure. The developed approach was validated with experimental data and it indicates a high potential for prediction of cellulose aerogels' properties with high accuracy. The proposed model is a significant step towards creation of a digital twin for cellulose aerogels, but also has a great potential to be extended for systems based on other polymers.

*Speaker