

3-d modeling of biopolymer aerogels

Rajesh Chandrasekaran¹, Markus Hillgärtner¹, Ameya Rege², Barbara Milow², Mikhail Itskov¹

¹ *Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany*

² *Department of Aerogels and Aerogel Composites, Institute of Materials Research, German Aerospace Center, Cologne, Germany*

E-mail: chandrasekaran@km.rwth-aachen.de

Biopolymer aerogels have gained more attention in the research areas due to their sustainability, ease of functionalization and tunable properties. Due to their biocompatibility and biodegradability, they are intensively used for food packaging and drug delivery applications. These demand the study of the mechanical properties of biopolymer aerogels to characterize the loading bearing capacity. The mechanical properties of aerogels generally depend on their microstructural properties which can be tailored by different synthesis and drying methods. In this work, a 3-d geometrical model representing the heterogeneous cellular morphology of biopolymer aerogels is described based on the experimental pore-size distribution (PSD) data, using random packing of spheres and the Laguerre-Voronoi tessellations (LVT). The PSD data obtained from experiments accounts for the random cell sizes within the aerogel network. The cell edges of the generated 3-d Voronoi tessellation are meshed as beam elements with a circular cross section corresponding to cell wall fibers in the aerogel network and used as a periodic representative volume element (RVE) to simulate the mechanical properties under deformation and investigate the effect of microstructural properties on the bulk behavior of aerogels. This work is an extension of our previous Voronoi tessellation based 2-d description of biopolymer aerogels [1].

References

[1] A. Rege, M. Hillgärtner, M. Itskov, *The Journal of Supercritical Fluids* 151: 24-29 (2019)