Numerical Modeling of Sol-Gel Materials: An Aerogel Use-Case

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Abstract

The increasing demand for sustainable material development in various industries has led to a significant focus on computational algorithms to accelerate material design. Among these materials, aerogels - highly porous, low-density and thermally insulating structures - have gained attention for applications in insulation, energy storage and carbon capture. Despite extensive research, the synthesis of aerogels has historically relied on iterative experimental approaches. While over the years, there have been simulation-based approaches in understanding the gelation behavior, these studies often simplify the material behavior by often neglecting the physics of the formation of the primary particles themselves. This study presents a computational workflow for modeling aerogel formation, capturing the evolution from nucleation of primary particles to the gel network development. The presented workflow makes it possible to explore the interplay between sol-gel chemistry and the resulting microstructures, allowing a deeper understanding of the synthesis process. In addition, the computational model incorporates solvent exchange and drying effects both implicitly and explicitly. The finite Element Method is used to study drying-induced stresses, identifying critical load paths and potential damage mechanisms under high load conditions. By providing a fully digital approach to aerogel modelling, this workflow accelerates sustainable materials development and improves the understanding of aerogel‘s properties under varying synthesis conditions

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