Engineering Analysis with Boundary Elements
Volume 151, June 2023, Pages 1-7

Investigation of the mechanical stability of polyethylene glycol hydrogel reinforced with cellulose nanofibrils for wound healing: Molecular dynamics simulation

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https://doi.org/10.1016/j.enganabound.2023.02.055

Abstract

Wound healing can be improved via various materials in clinical cases. Today, nanocomposites are regarded as promising structures for this purpose. In the current computational study, we introduced Polyethylene glycol (PEG) hydrogel-cellulose nanocomposite to improve wound healing. For this purpose, molecular dynamics (MD) simulations were used to analyze hydrogel-cellulose nanocomposite at standard conditions. Therefore, the present paper investigates the mechanical stability of PEG hydrogel reinforced with cellulose nanofibrils. MD simulations were done in two main phases: equilibrium and deformation process as initial and final phases, respectively. Our simulation results show the defined samples' physical stability at 300K and 1bar. This procedure predicted from temperature and total energy convergence after 10ns. The results of the mechanical test outputs show that inserting cellulose into pure PEG hydrogel leads to improving their mechanical performance. Numerically, the ultimate strength and Young's modulus of the designed nanocomposite increased to 0.26MPa and 0.39MPa (respectively) in the presence of 3% cellulose nanofibrils. The increased mechanical strength shows hydrogel-cellulose nanocomposite can be used for wound healing in clinical applications.