

Numerical Simulation of PH Sensitive Hydrogel Response in Different Solutions

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Abstract

The understanding of hydrogel swelling response in different environments is essential for its use in different practical applications. This necessitates its simulation in steady state and transient conditions. This paper mainly deals with the details of the numerical simulation performed by developing coupled formulation of chemo-electro-mechanical behavior of the hydrogel in response to changing pH of the surrounding solution. Simulations were performed to determine the response of hydrogel with varying pH of the surrounding solution in a wide range of pH (2-12), mainly representing its response for different solutions. The investigation of the responsiveness of the hydrogels is focused mainly on the chemical composition of the immersed solution and to change in the solvent. The methodology used for this finite element based simulation is presented. The swelling characteristics of the hydrogel (of arbitrary geometry) with different functional group (PKa) are compared in steady state and transient conditions. This analysis is carried out using COMSOL and the effects of fixed charge density, buffer solution concentration and solution pH on the swelling were studied in different simulations. The mobile ion and fixed charge concentrations showed to take around an hour before they stabilize in response to a given change in pH. Swelling as well as deswelling responses showed similar variation in the transient conditions. These simulation results are compared with available experimental evidence to show the accuracy of the model.