Multiphysics Simulation Of The Swelling Kinetics Of PH-Responsive Anionic Hydrogels

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Abstract

pH-responsive hydrogels have over the years drawn research interest in applications such as microfluidic control and separation, chemo-mechanical sensing systems and controlled drug delivery, owing to their ability to undergo significant volume changes in response to changes in pH of the surroundings. To dynamically control the characteristic swelling property of pH-sensitive hydrogels, understanding of their conformational changes is required. To achieve this, mathematical modelling and simulation can offer insights that complement empirical studies. The Poisson-Nernst-Planck (PNP) equations, coupled with mechanical balance equations, can model the interplay of chemo-electro-mechanical fields for hydrogels exposed to ionic environments and consequent swelling phenomena. Analytical solutions for this continuum model exist for one-dimensional cases but are not feasible generally.
In this work, a cylindrical anionic hydrogel immersed in a buffer solution has been modelled on a two-dimensional axisymmetric domain using COMSOL Multiphysics software. In the software, the transport of diluted species interface solves the Nernst Planck equation (for the distribution of ionic concentrations of the species in solution), while the electrostatics interface under AC/DC module solves the Poisson equation (for the distribution of the electrical potential in the subdomains) and the solid mechanics interface which solves the mechanical balance equation (for the deformation/displacement of the hydrogel) were all fully coupled and solved using the Direct-PARADISO linear system solver. To be able to compare computational results with experimentally published data (for the case where hydrogels were confined in a microchannel to allow for deformation in the radial direction only), roller boundary conditions were imposed at the top and bottom of the hydrogel to constrain displacement in the axial direction.
Parametric studies for transient and equilibrium simulations were performed on the model to determine the effects that varying material properties (such as concentration of the initial fixed charge group at the backbone of the hydrogel and modulus of elasticity of the hydrogel), and the surrounding external conditions (such as ionic strength and pH value of the buffer solution) all have on the size of the pH responsive hydrogel.
The main results of swelling ratio as a function of pH value obtained from the simulation compare favourably (R^2=0.9878) with experimental work conducted in the literature for Polyhydroxyethylmethacrylate hydrogels. In addition, the results show that, increasing the initial fixed charge concentration of the cations in solution, increases the swelling ratio of the hydrogel. The plots are in good agreement with those in the published literature. Hence, these results provide some validation for the model, which has the potential to offer predictions for volume variation as a function of pH changes in the environment.

Figures used in the abstract

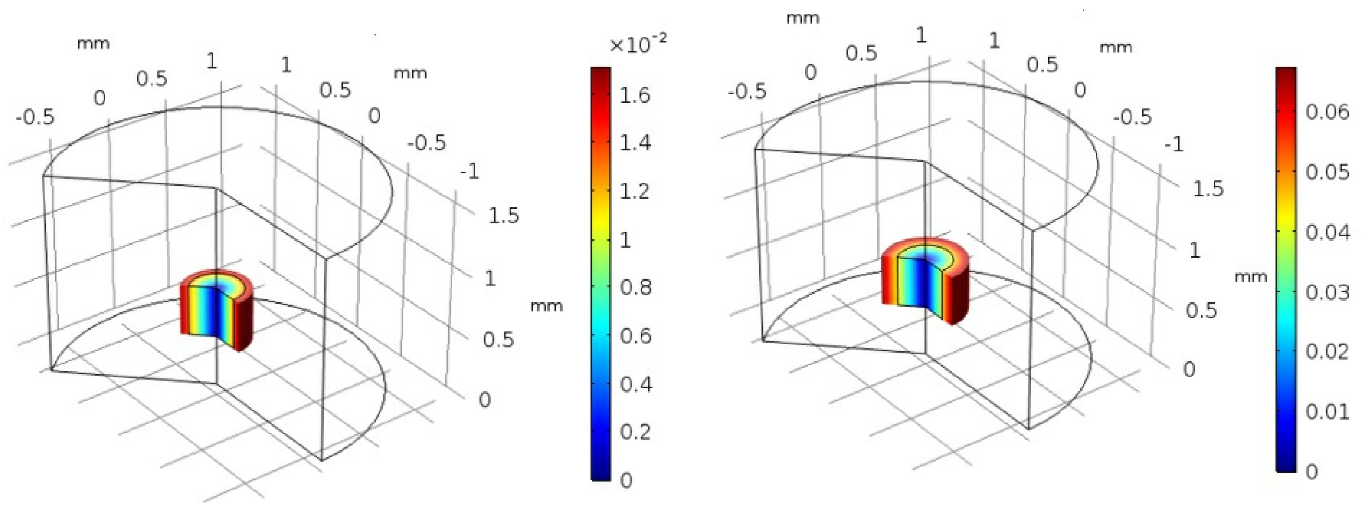

Figure 1 : Deformation at pH = 2 (Left) and Deformation at pH = 8 (Right)

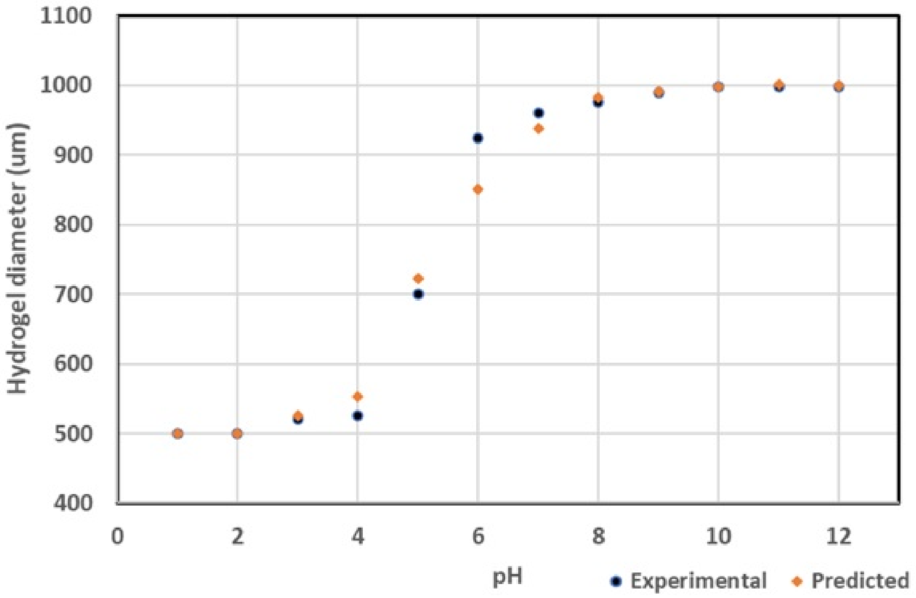

Figure 2 : Validation of experimental swelling data against simulation data