The Swelling Responsiveness of PH-Sensitive Hydrogels for 3D Arbitrary Shaped Geometry

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Abstract

The pH-sensitive hydrogels are responsive to the pH of surrounding solution, which often resemble to biomaterials. Recently, pH-sensitive hydrogels are widely used in various devices as sensing media. We present the simulation of swelling characteristic of 3D-arbitarary-geometry, pH-sensitive hydrogel in steady state conditions.

Three nonlinear partial-differential equations that are representing responsible physical phenomena namely- chemical, electrical and mechanical can describe the swelling responses to a chemical change in surrounding solution. Finite element analysis used for present study was carried out by full coupling of above three partial-differential equations with variable material properties in COMSOL Multiphysics®. Employing a moving mesh method for 3D geometry, the FEM simulation was performed to account for large-swelling of the pH-sensitive hydrogel.

Simulation of swelling of the hydrogel was carried out using COMSOL finite element software with the following multiphysics included in three different modules:
1. Nernst-Planck (NP) equation without electroneutrality
2. Conductive Media DC for Poisson's Equation
3. Plane Strain for Mechanical Field Equation

Within COMSOL, the three different modules were fully coupled to each other in the two reference frames. The Chemical Engineering Module and the AC/DC Module along with displaced mesh are considered in the moving mesh frame while the Structural Mechanics Module is used to evaluate the swelling in different conditions in the fixed mesh frame with large deformation. This was achieved by determining the new coordinates within the NP and Poisson's equations in a moving frame, while the deformation is calculated using the updated coordinates with the mechanical field equation in a fixed frame. [1-3]

Figure 1 shows the simulation results using above mentioned strategy has been validated for 2D geometry of hydrogel and results are in agreement with other published experimental results.

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Reference

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Figures used in the abstract

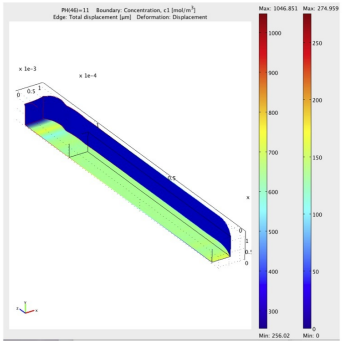

Figure 1: Simulation result of swelling characteristic of a pH-sensitive 3D hydrogel surrounded by pH-11 solution. The negatively charged hydrogel has 1800 mM of fixed charge with functional group pKa of 4.5.