Sensitivity Analysis of a Simulated Hydrogel

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Crosslinked polyelectrolytic polymers embedded in an aqueous solution, so-called hydrogels, show stimuli-responsive behaviour under various kinds of stimulation. These “smart” reactions can be triggered by e.g. chemical, electrical, mechanical or thermal stimuli. The hydrogels react via uptake or delivery of mobile ions and solvent, and show enormous swelling capabilities. This behaviour can be used for chemo-electro-mechanical energy converters or as an actuator or sensor.

The presented research investigates anionic hydrogels in the framework of a sensitivity analysis, by a design of experiment (DOE) with the use of ANSYS optiSLang. The hydrogel itself is modelled within a finite element code (Abaqus Unified FEA) as a user element. The applied stimuli are of different nature: chemical, electrical, mechanical and thermal.

On the one hand, the stimulus is applied by the change of boundary conditions, e.g. for chemical stimulation by a change of the concentrations of the constituents themselves ($\text{Na}^+$ and $\text{Cl}^-$). For electrically stimulated hydrogels, two electrodes are incorporated at the boundaries and the electric potential is changed. On the other hand, the mechanical stimulus is defined by prescribed displacements at a boundary of the fixed hydrogel. The thermal stimulus is applied over the whole domain in the form of transient temperature changes with temperature-dependent material parameters.

The reactions of the hydrogel differ – depending on the type of hydrogel and the stronger or weaker sensitivity – on the applied stimulus. The fully coupled three-field description of the chemo-electro-mechanical model enhanced with thermal dependencies is capable of giving local concentrations, electric potential and displacements.

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1 Introduction

Due to their polymer structure, hydrogels in aqueous solution respond to multiple stimuli, such as chemical, electrical, mechanical, thermal, optical or other. The mobile and bound ions lead to diffusive and migrative processes due to these stimuli. Mobile ions surrounded by hydration shells enter or leave the hydrogel due to the driving forces which leads to swelling or deswelling. This can be used for different applications, e.g. the use as sensors for pressure cf. [1] or concentrations (pH, medicine) cf. [2], or actuators and artificial muscles cf. [3] and [4].

Considering the sensitivities to the various stimuli Ehrenhofer et al. [5, 6] showed multisensitive swelling of these hydrogels and the sensitivity measure to different stimuli applying the $N$-field method and the trajectory method.

In the present research the sensitivity analysis is performed by the use of ANSYS optiSLang.

2 Modeling

The coupled three field approach – the chemo-electro-mechanical model with thermal dependencies – according to Attaran et al. [7] is applied. Only infinitesimal deformations are assumed. The hydrogel and its surrounding solution bath is modelled within the framework of the finite element method (FEM) by user defined elements in Abaqus. Different stimuli are applied, please refer to Keller et al. [8] and its references.

3 Numerical Results

Design of experiment (DOE) analyses of the hydrogel model with different types of stimulus are investigated in the following. First, the stimulation types are introduced, then the sensitivity analyses are performed.

3.1 Stimulation Types

The chemical stimulation is applied by prescribed, transient boundary conditions. The electrical stimulus is applied on two electrodes on the domain boundaries above and below the longer extents of the modelled hydrogel strip. The thermal stimulus is realized via prescribed temperature profiles for the whole domain. Due to their fabrication, hydrogels can show an extremely different behaviour to each type of stimulus, e.g. they can exhibit a degressive (or progressive) temperature behaviour, which means deswelling (or swelling) with increasing temperature [8].
3.2 Sensitivity Analyses

Due to former and actual studies the sensitivity analyses are performed using ANSYS optiSLang to incorporate Abaqus in a DOE environment, e.g. [9, 10]. In general 100 designs are calculated for the 1D and 2D models. Advanced Latin Hypercube sampling is used to cover the bandwidth of the design variables. The stimuli are applied separately or in a combined way. Coefficients of determination, correlation matrices, histograms or anthill plots are derived.

![Fig. 1](image)

**Fig. 1:** Sensitivity analysis – (a) linear correlation matrix, and anthill plots (b) concentration over displacement and (c) temperature over displacement for degressive temperature behaviour

Figure 1(a) shows a linear correlation matrix; all input and output parameters for a 2D DOE analysis are shown. Red and blue coloured fields show strong positive or negative correlations, respectively, which means increasing or decreasing responses with increasing stimulus [9]. Blue fields signal independent responses to the stimulus or input parameter. Figure 1(b) is an anthill plot of all designs. The input parameter is a prescribed concentration of \(0.5 \ldots 1.5\) mM at the boundary. The responses, depicted on the abscissa, are nodal displacements. As the initial concentration of \(Na^+\) and \(Cl^-\) is 1 mM, the displacement output for this input is zero. Increasing or decreasing the prescribed concentration leads to swelling – here negative displacements – or vice versa to deswelling – here positive displacements. Figure 1(c) shows another anthill plot. In this case a degressive temperature behaviour is modelled according to Shibayama and Tanaka [11]. With increasing temperatures the negative displacements are diminishing. The nearly horizontal course in the range of 308 K is due to the glass transition temperature.

4 Conclusions

A sensitivity analysis of polyelectrolyte gels in aqueous solution under various kinds of stimulation has been shown in the present research. Chemical, electrical, and thermal stimulation were investigated. The applied fully coupled multiphysics model is capable of calculation local deformations, concentration changes and electric potential of the investigated hydrogels. Concluding, the DOE is an excellent method to demonstrate the sensitivities due to the different stimuli in the investigated models.

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