Supplementary material for

Swelling of a hemi-ellipsoidal ionic hydrogel for determination of material properties of deposited thin polymer films: an inverse finite element approach

Victorien Prot[1], Hrafn Mar Sveinsson[2], Kamila Gawel[2], Ming Gao[2], Bjørn Skallerud[1] and Bjørn Torger Stokke[2*]

[1]Biomechanics Division, Department of Structural Engineering, The Norwegian University of Science and Technology, NTNU, NO-7491 Trondheim, Norway
[2]Biophysics and Medical Technology, Department of Physics, The Norwegian University of Science and Technology, NTNU, NO-7491 Trondheim, Norway
[*]Corresponding author

A Mixing of the solvent with the multilayer shell

In order to take into account the mixing of the solvent with the multilayers, a mixing term is added to eq.(35) leading to the strain energy function $\overline{W}$ to model the multilayer shell assumed to be a neutral gel insensitive to the mobile ions in the external solution:

$$\begin{aligned}\overline{W} &= \frac{C_0}{4}\Omega\left(\frac{1}{1-\Lambda\sqrt{I_1/3}}-\Lambda\left(\sqrt{\frac{I_1}{3}}-2\Lambda\frac{I_1}{3}+\Lambda^2\left(\frac{I_1}{3}\right)^{3/2}\right)\right)+\overline{W}_0 \\ &\quad +\frac{k_BT}{v_s}\left((J-1)\ln\left(1-\frac{1}{\mathrm{J}}\right)+\chi\left(1-\frac{1}{\mathrm{J}}\right)\right), \qquad \text{(A.1)}\end{aligned}$$

$$\text{with} \quad \Omega=\frac{L}{l_p}, \quad \Lambda=\frac{r_0}{L} \quad \text{and} \quad r_0^2=2l_p^2\left(\frac{L}{l_p}-1+e^{-L/l_p}.\right), \qquad \text{(A.2)}$$

The initial swelling of the multilayer shell in Ω_1 represented by the isotropic state of strain $\mathbf{F}_0=\lambda_{0s}\mathbf{1}$ (see Figure 2) is determined solving $\frac{\partial\overline{W}}{\partial\mathbf{C}}(\lambda_{0s})=0$. Therefore, the end-to-end distance in Ω_1 is $\lambda_{0s}r_0$.
The identified parameters obtained with the FE constrained model the deposited shells with 4 and 8 bilayers (Chitosan-alginate) using eq.(A.1) are reported in Table A.1. Additionally, comparisons between experiments and numerical simulations using the identified parameters of Table A.1 are shown in Figure A.1.
The values of the parameter C_0 obtained with eq.(A.1) are in the same range but slightly lower than those obtained with eq.(35), i.e when the shell is modeled as fully incompressible.
Finally, we also provide a calibration plot (see Figure A.2) where χ in eq.(A.1) is assumed to be equal to 1.

Table A.1: Elastic parameter C_0 (eq.(A.1))for the deposited shells with 4 and 8 bilayers (Chitosan-alginate)

		$C_0/(k_BT/v)$	χ	l_p	L	t	$L^{exp}_{g,0.15}$
Chitosan-alginate	4 bilayers	1.7e-2	1.0	15 nm	250 nm	0.8 μm	54.7 μm
	8 bilayers	2.2e-2	1.1	15 nm	250 nm	0.8 μm	50.2 μm

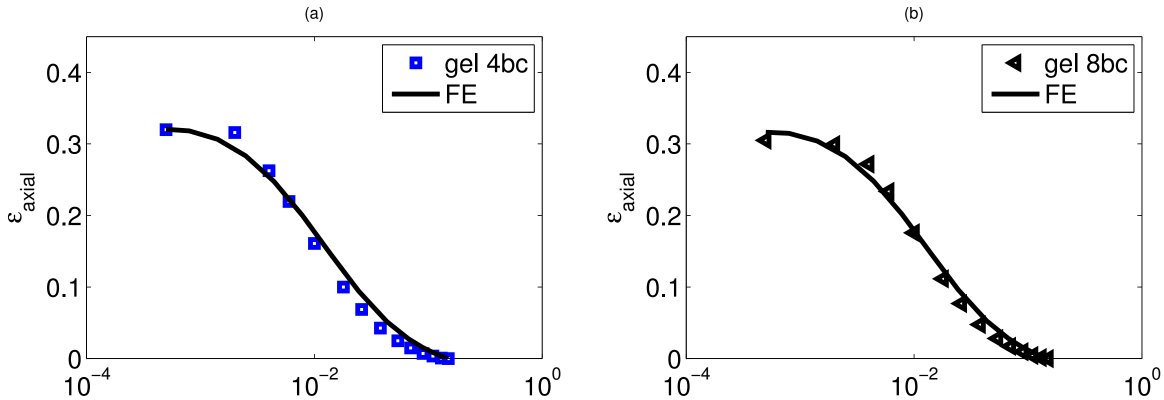

Fig. A.1: Comparison between the axial strain ε_{axial} (eq.(40)) of the hydrogel measured during experiments at different levels of salt concentration and the one computed from finite element analyses with the fitted parameters from Table A.1. Blue squares and black triangles correspond to experimental results for the gel with four and eight bilayer chitosan-alginate coating, respectively. The solid lines correspond to the numerical results. a) ,b) comparison between experimental results and numerical analyses for the gel with four and eight bilayer coating, respectively.

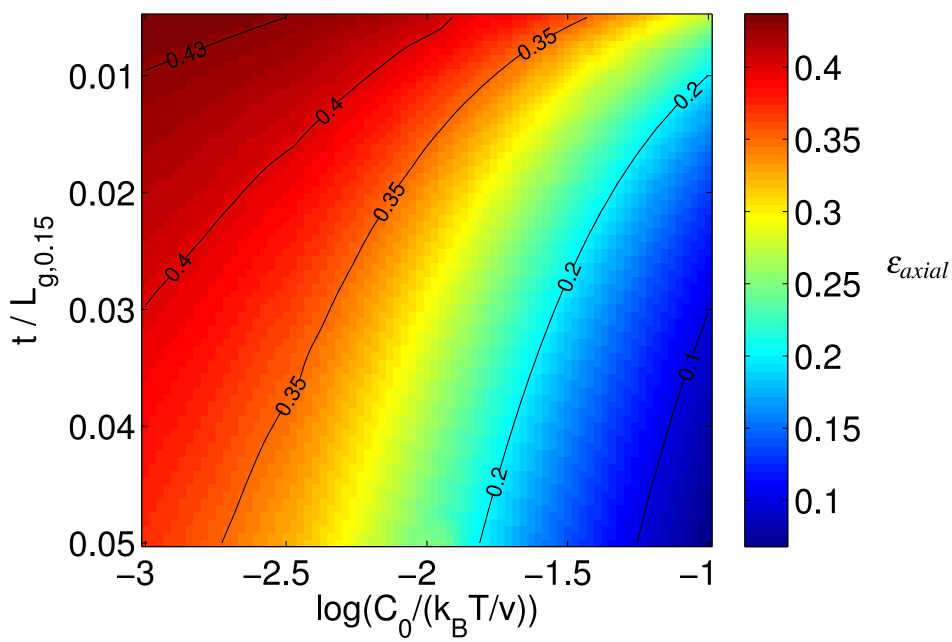

Fig. A.2: Color plot of ε_{axial} (eq.(40)) of the hydrogel with deposited layers at a salt concentration of $5 \cdot 10^{-4}$ M for different values of C_0 (eq.(A.1)) and thickness of the shell and $\chi = 1$.