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Modelling Behaviour of anionic hydrogels

Thesis in **Transport phenomena**

Supervisor: Candidate:

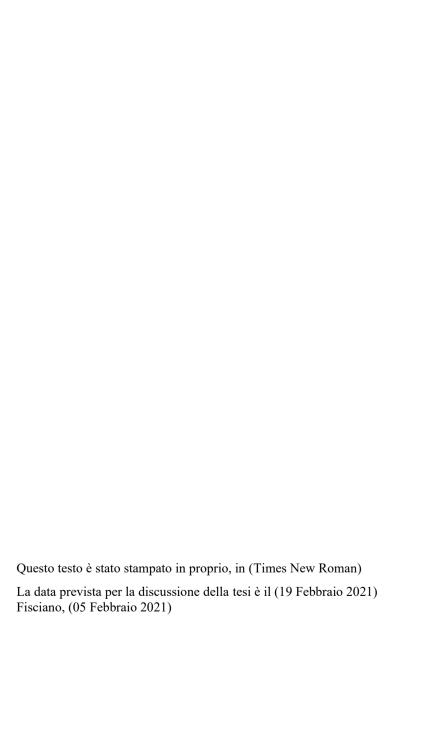
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To my Family



Summary

Summary	I
Figures Index	III
Tables index	V
Abstract	VIII
Introduction	1
1.1 The importance of hydrogels in food systems	2
1.2 Natural anionic hydrogels in food	2
1.2.1 Sodium Alginate	3
1.2.2 Xanthan Gum	
1.2.3 Olive	5
1.3 Polyelectrolyte hydrogel	5
1.3.1 Introduction	5
1.3.2 Chemical characterization	6
1.3.3 Poroviscoelastic behaviour	_ 10
1.4 Modelling approach	11
1.5 Project objectives	12

Mathematical Modelling	13
2.1 introduction to continuum mechanics	14
2.1.1 The displacement field and the deformation gradient	15
2.2 Model Assumptions	16
2.3. Dissipation Inequality	17
2.3.1 Elastic contribution:	18
2.3.2 Free Energy of mixing	23
2.3.3 Free Energy of Ionization	24
2.3.4 Free energy of dissociation	25
2.3.5 Electroneutrality conditions and charges balance	25
2.3.6 Helmholtz free energy for a "large" electroneutral anionic hydrogel	27
2.3.7 Volumetric constraint	
2.4 Derivation of Constitutive Equation	29
2.5 Steady-State Analysis	31
2.5.1 External concentration calculation	31
2.5.2 External chemical potential	
2.5.3 Internal chemical potential	32
2.5.4 Implementation in Matlab	35
Results and discussion	37
3.1 Swelling analysis	38
3.2 Analyze the effects of the number of ionizable on the hydrogel	_
Conclusion	47
Bibliography	50

Figures Index

Figure 1. Hydrogel application in food
Figure 2. Soduim alginate [17]
Figure 3. Xanthan Gum [17]4
Figure 4. Stimuli-responsive swelling of the hydrogel6
Figure 5. Structure of anionic hydrogel [23]6
Figure 6. pH-dependent ionization of Anionic Hydrogels [24]7
Figure 7. Structure of cationic hydrogel [23]
Figure 8. pH-dependent ionization of cationic hydrogels [24]7
Figure 9. The pH-responsive swelling of (a) anionic and (b) cationic hydrogels.8
Figure 10. Debye length region [27]9
Figure 11. hydrogel Structure [28]10
Figure 12. Type of gel deformation [28]10
Figure 13. A system defined as a continuum
Figure 14. The deformation function χ _Dand the displacement vector uD15
Figure 15. Internal gel and external solution with the system species [27]17
Figure 16. A dry network is taken to be the state of reference. In the current state, the network is immersed in an aqueous solution subject to a set of mechanical forces [7]
Figure 17. SLS model [16]22
Figure 18. External Concentration
Figure 19. Reference concentration
Figure 20. General parameters
Figure 21. Initial concentrations

Figure 22. Qualitative analysis of the trend of polyelectrolyte hydrogels that increase swelling with increasing pH	. 38
Figure 23. Swelling analysis	. 39
Figure 24. The influence of pH values of buffer solution on the equilibrium o PAA [43].	
Figure 25. Swelling behavior for GA1.	. 43
Figure 26. Swelling behavior of GA2	. 44
Figure 27. Swelling behavior of GA3	. 44
Figure 28. Swelling behavior of GA4	. 45
Figure 29. Swelling behavior of GA5	. 45
Figure 30. swelling behavior for the five gels using the model data	. 46

Tables index

Table 1. First Simulation parameters	39
Table 2. Compositions and characters of the GA hydrogels	41
Table 3 General Model parameters.	42



Abstract

Anionic polysaccharides polymers are class of polyelectrolyte hydrogels. They have a wide range of application in the food industry, such as shelf-life extension, flavour release, nutraceutical preservation, and food packaging. Polyelectrolyte hydrogels are linear, slightly crosslinked polymers containing ionizable groups on their backbone. Additionally, they are sensitive to pH changes.

In this work, the monophasic model is used to describe the steady-state behaviour of polyelectrolyte hydrogels. As a result of ionizable groups' existence, there are four contributions in the Helmholtz free energy: the elastic ones, the term of mixing of the solvent with the network, the term of mixing of the ions with the solvent, and the term of dissociation of acidic groups. Electroneutrality assumption also has been considered in this work.

In the comparative study, the model has been used to simulate hydrogels' behaviour reported in the literature. From the results, it can be established that the model's swelling ratios can be calibrated to fit the actual behaviour of the literature findings. This conclusion is evident from the simulation results, as the initial concentration of the ionizable groups present in the polymer chain increased with an increase in the PAA concentration of each gel reported. Comparing the model's results and literature showed a proportional dependence of the swelling behaviour on the number of dissociation groups, indicating the model's realistic results.

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