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Ion-binding-mediated swelling of a mucus-like polyelectrolyte gel model

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Swelling and deswelling of polyeletrolyte gels play important roles in many biophysical processes. The swelling behavior of such charged polymer gels depend strongly on their ionic environment. Found in many physiological systems, mucus is a network of polymeric proteins that is often regarded as a polyelectrolyte gel. Maintenance of a consistent mucus layer lining the gastric wall is critical to healthy stomach function and is thought to be dependent on the swelling of fresh mucus secreted from epithelial cells lining the stomach wall [1]. In this work, we present an extension to our previous two-fluid model for ion-binding-mediated mucus swelling that eliminates certain assumptions about the relative size of network monomers and solvent molecules [2]. In particular, the model accounts for the various electrochemical potentials that may drive dynamic rearrangement of the polymer network/solvent aggregate. We present a series of numerical experiments meant to represent samples of dense mucus allowed to swell in baths of differing ionic compositions. We show that the various forces driving swelling behavior are influenced by the chemical affinity between dissolved cations and the polymer network, as well as the resulting distribution of charges within the mixture. The dependence of the swelling rate on ionic bath composition is quantified, and this analysis highlights the importance of the electromigration of ions and the induced electric field in regulating the rate/degree of gel swelling.

REFERENCES

[1] R. A. Cone, Barrier properties of mucus. *Adv Drug Deliv Rev.*, Vol. **61(2)**, pp. 75–85, 2009.

[2] S. Sircar, J. P. Keener and A. L. Fogelson, The effect of divalent vs. monovalent ions on the swelling of mucin-like polyelectrolytle gels: governing equations and equilibrium analysis. *J Chem Phys.*, Vol. **138(1)**, pp. 014901, 2013