Chemical Potential

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September 30, 2020

1 Crosslink Fraction

In ref [1], the crosslink fraction, α, is given by:

$$\alpha = \frac{2x}{m_T}$$

$$\begin{aligned} \text{x} &= \text{Concentration of doubly bound Calcium} = B_{C2} \\ m_T &= \text{Total monomer concentration} \\ &= m + 2x + w + v + y \end{aligned}$$

The concentrations per solvent volume (units: mol/L) of the polymer species are denoted by:

$$x = [M_2Ca],\ m = [M^-],\ v = [NaM],\ w = [MCa^+],\ y = [HM]$$

However, in the gel notes, the crosslink fraction, α, is given by:

$$\alpha = \frac{2B_{C2}}{\tilde{z}\theta_n}$$

$$\begin{aligned} \tilde{z} &= \text{Total density of monomer binding sites} \\ \theta_n &= \text{Network volume fraction} \end{aligned}$$

Therefore, we need to determine why the denominators are different in the two formulations above (or why they seem different) and then implement the more appropriate equation in the code.

2 References

[1] S. Sircar, J. P. Keener, and A. L. Fogelson. The effect of divalent vs. monovalent ions on the swelling of Mucin-like polyelectrolyte gels: Governing equations and equilibrium analysis. *J. Chem. Phys* **2013**, 138, 5-6. [Link]