Modeling the Combined Effect of Convection and Diffusion in Cross-linked Alginate Capsules

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Introduction: Alginate is a biopolymer and hydrogel comprised of (1,4)-linked β-D-mannuronic (M) and (1,3)-α-L-guluronic (G) acid residues. In this effort, the experiments were designed to meet a single research objective of modeling and predicting the effect of convection in addition to passive diffusion on the upper limit of size exclusion of the cross-linked hydrogel membrane reported to be 66 kDa [1].

Materials and Methods: Microcapsules (MCs) made of 2% (w/v) alginate formed by polyelectrolyte complexation were extruded into a 1% (w/v) calcium chloride solution and cross-linked for 60 min. The MCs were subjected to a single compression/stress relaxation cycle. The effect of convection was simulated by equating the maximum compressive stress obtained for the first cycle (σ_max=12kPa) to the flowrate of the marker diffusing into the capsule during recovery. Theoretical diffusivities, reflection coefficients and membrane pore size data were obtained from previously-established efforts [1,2]. The convection-diffusion equation [Equation 1] was used to model the distance diffused through the membrane using the Comsol software (version 5.1). The ratio of the marker concentration (R_M) at the (R=0, C_R0) and (R=10μm, C_R) has been used to compare the radial diffusion profiles.

Results and Discussion: Assuming that the elastic modulus of the membrane has not changed during the compression and there is no significant change in cross-link density, there is a marked difference in the simulated radial profiles of the markers shown in Figures 1a & 1b at 10 s: Numerical values of the ratio R_M are 0.5 and 0 for the 4kDa and 66 kDa, respectively. The profile at 10s is representative of a steady state solution for this simulation during which convection has not been shown to be effective for pushing the 66 kDa marker through the membrane. Shown in Figure 1c, is a characteristic 100 μm long, 10 μm thick cross-section used for modeling the combined convective and diffusive fluxes.

Conclusions: Addition of convection to passive diffusion is not an effective method for increasing the upper limit of size exclusion for alginate. Future studies will model the simultaneous effect of a decreased elastic modulus and convection/diffusion forces on marker diffusivity.

References