Multi-objective Optimisation Modelling of Biodegradable Chitosan/pEGDA Hydrogels for Contact Lens Applications

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Over 140 million people worldwide rely on daily silicone contact lenses, generating ~15,000 tonnes of plastic waste annually and contributing to microplastic contamination through improper disposal. Developing biodegradable alternatives is hindered by costly, time-intensive trial-and-error material design, whereas computational modelling offers a more efficient pathway to optimise formulations. This project aimed to synthesise an alternative biodegradable hydrogel that meets contact lens biocompatibility and optical standards. A chitosan–PEGDA hydrogel was selected, with poly(ethylene glycol) diacrylate (PEGDA) acting as a photopolymerisable crosslinker to enhance porosity, equilibrium water content (EWC), and O2 permeability. An optimised formulation was identified using multi-objective optimisation modelling based on literature-derived correlations between synthesis parameters and material properties. Monte Carlo sampling and differential evolution were applied to target five key properties: EWC (55–75%), O2 permeability (=30Dk), Young's modulus (300–900kPa), refractive index (1.37–1.41), and light transmittance (=90%). The model predicted an optimal formulation of 1.77 w/v% chitosan, 12.41 w/v% PEGDA, and 1.5 w/v% photoinitiator under 12.5 minutes of UV irradiation. Experimental synthesis yielded EWC 69.8±0.2%, O2 permeability 39.65±2.50 Dk, Young's modulus 793.7±24.2 kPa, refractive index 1.3810±0.0015, and transmittance 90.7±0.8%. A paired t-test showed no significant difference between predicted and experimental values (t=1.10, a=0.05, df=4). The hydrogel degraded by 88% after 8 hours in 10 mM lysozyme and is estimated to be 2–3× cheaper than conventional lenses, demonstrating strong potential as a cost-efficient, biodegradable alternative.

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