EXPERIMENTAL AND NUMERICAL INVESTIGATION OF 5-FLUOROURACIL RELEASE KINETICS FROM HETEROGENEOUS MATRICES

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The development of controlled drug delivery systems requires a comprehensive understanding of the mass transport mechanisms. This study focuses on characterizing the release of 5-fluorouracul, the anti-cancer drug, from hydrogels located on polycaprolactone foams into a surrounding liquid environment. The research methodology integrates laboratory-scale experimental data with Computational Fluid Dynamics (CFD) simulations. During the experimental phase, drug concentration levels were monitored at specific time intervals to establish release profiles.

The experiments involved multiple batches characterized by varying initial drug loadings into hydrogels and into hydrogels and foams simultaneously. To replicate these processes numerically, the hydrogel and foam were modelled as a porous zone with stable structural properties. Mass transport within the system was simulated using the Species Transport model to track the diffusion of the drug through the fluid phase. The numerical framework accounts for the resistance of the porous matrix and the subsequent mass transfer across the carrier-liquid interface. Initial drug concentrations within the domain were precisely defined to match the experimental starting conditions for each individual case.

The simulation aims to capture the concentration distribution of the drug as it migrates from the carrier into the solution. A significant aspect of this research is the investigation of how the physical dimensions and shape of the carrier may influence the resulting release kinetics. By comparing numerical results with experimental concentration curves, the model's ability to predict diffusion-driven transport is evaluated. In the CFD environment, the effective diffusion coefficient was adjusted to represent the internal tortuosity of the porous network. The interface between the hydrogel and the external fluid was treated as a continuous boundary to ensure the conservation of mass flux. Furthermore, User-Defined Scalars (UDS) can be optionally implemented to account for complex sorption and desorption phenomena within the gel structure. The research examines whether subtle variations in carrier thickness and surface area lead to measurable changes in the transport rate. This comparative analysis is essential for identifying the primary factors that dictate the system's kinetic behaviour.

The findings from this study contribute to a more detailed characterization of porous carriers in biomedical engineering.