

EFFECT OF THE SCALE FACTOR OF FREE VOLUME THEORY ON THE DIFFUSION PROPERTIES OF POLYETHYLENE GLYCOL HYDROGEL

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Doi:https://doi.org/10.34107/YFMV730915

ABSTRACT

Free volume theory (FVT) based approach has been frequently utilized by the researchers to characterize the diffusion-mediated hydrogel drug delivery systems. The scale factor is a crucial parameter in the FVT premise which governs the diffusion dynamics of the solute by means of the available free volume. In this study, the influence of the scale factor (Y) of FVT on the diffusion characteristics of polyethylene glycol (PEG) hydrogel has been explored for wound healing applications. A computational model has been implemented to simulate the diffusion of two antimicrobial plant metabolites namely, Cinnamaldehyde and Curcumin and two synthetic antimicrobial drugs namely, Amphotericin B and Vancomycin through PEG 20000 hydrogel matrix. A reduction in the diffusion coefficient and diffusivity ratio of about 36% has been observed with an increase in the scale factor from 0.5 to 2, while the diffusion time is found to be extended by more than 50%. This shows that the theoretical assumption of a constant Y value of 1 may not be suitable for practical cases as the scale factor significantly influences the diffusion kinetics. The outcomes of the present study will contribute to the physical understanding of the FVT scale factor and its impact on the diffusion characteristics of hydrogels which in turn will aid in the appropriate selection of the model parameters during the in silico validation of tuned drug delivery systems.

Keywords: Hydrogel, Diffusion, Free Volume Theory, Scale Factor, Antimicrobial Agents, Wound Healing

INTRODUCTION

A wound can be defined as the loss in the cohesiveness of the epithelium, with or without the loss of the underlying elemental connective tissues which ultimately disintegrates the normal anatomic structure and defensive function of the skin [1]. Infection is one of the most common complications occurring in the chronic wounds due to the presence of biofilms which protect the pathogenic microbes from the antibodies and antimicrobial therapies [2-4]. Topical antimicrobial treatments have been used empirically in an attempt to prevent the wound infections as they exhibit fewer systemic side effects [5-6]. The presence of biofilms, altered local pH, emergence of drug resistant microbes, inflammation of the tissues and heterogeneity of the wound environment are the crucial challenges which need to be tackled during the delivery of the antimicrobial formulations [7-8]. This necessitates the urgent development of non-conventional therapeutic strategies that are capable of enhancing the efficacy of the drug delivery process.

Hydrogels are three-dimensional, physically or chemically crosslinked swollen polymer networks which exhibit an exceptional ability to imbibe large quantities of water or biological fluids without dissolution [9]. The pore space of the hydrogels accommodates the solute molecules and can be tuned to facilitate the sustained delivery of natural and synthetic therapeutic agents [10]. PEG hydrogels are one of the potential candidates for wound healing applications as they mimic the native skin micro-environment, maintain an optimum level of moisture in the wound bed, absorb the excess exudates and provide a suitable platform for the loading of biomacromolecules [11]. The fundamental release