# CMBBE 2023 SYMPOSIUM

18th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering

## 3 - 5 May 2023, Paris, France

CHALLENGES IN COMPUTATIONAL BIOMECHANICS FOR TOMORROW'S HEALTHCARE SYSTEMS

# ABSTRACT BOOK POSTER PRESENTATIONS

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CMBBE2023
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# EFFECT OF THE THICKNESS OF PEG HYDROGEL PATCH ON THE DIFFUSION OF WOUND ANTIMICROBIALS

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## 1. Introduction

The occurrence of infections plays a vital role in the transition of wounds from acute to chronic non-healing state [1]. The evolution of drug resistant microbes necessitates the development of novel treatment strategies. Topical application of antimicrobial formulations through hydrogel wound dressings offers beneficial therapeutic outcomes [2]. In this study, a computational model based on the free volume theory (FVT) has been applied to predict the diffusion of the natural and synthetic wound antimicrobials for varied thicknesses of the Polyethylene Glycol (PEG) hydrogel patch.

## 2. Materials and Methods

PEG hydrogel having a molecular weight of 20,000 g/mol is assumed to be in the form of a cylindrical patch of thickness $L$ which is varied from 1 mm to 5 mm. FVT has been utilized to estimate the diffusivity (D) of two plant metabolites with inherent antimicrobial activity namely, Cinnamaldehyde and Curcumin and two synthetic antimicrobial drugs namely, Amphotericin B and Vancomycin as per Eq. 1:

$$\frac{D}{D_o} = \left(1 - \frac{r_s}{\xi}\right) \exp\left(-Y\left(\frac{v_{2,s}}{1 - v_{2,s}}\right)\right) \quad (1)$$

Here, $r_s$ and $D_0$ denote the hydrodynamic radius and diffusivity of the compound in water respectively. $\xi$ and $v_{2,s}$ represent the mesh size and polymer volume fraction of the hydrogel respectively. According to FVT, Y refers to the ratio between the critical volume for diffusion and the available free volume and is usually approximated as 1 [3]. The cumulative drug release fraction can be calculated using Eq. 2:

$$\frac{M_t}{M_\infty} = 1 - \sum_{n=0}^{\infty} \frac{8}{(2n+1)^2 \pi^2} \exp\left(\frac{-D(2n+1)^2 \pi^2 t}{L^2}\right) \quad (2)$$

The diffusion time of the antimicrobial agents is determined when $M_t/M_\infty$ is 1. Furthermore, an empirical exponential relation between the diffusion time and hydrogel patch thickness $L$ has been established.

## 3. Results

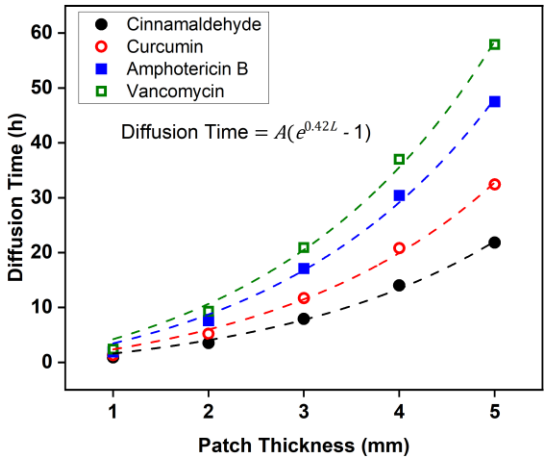


**Figure 1**: Variation of diffusion time of antimicrobial agents with thickness of hydrogel patch (Dashed line: Fitted function)

## 4. Discussion and Conclusions

Fig. 1 shows that an increment in $L$ results in extended diffusion time. The relation is observed to be exponential in nature, with an order of 0.42 $mm^{-1}$ for all the compounds ($R^2$ = 0.99). However, the value of A is observed to be linearly varying with the solute molecular weight, the values being 3.05 and 7.98 for Cinnamaldehyde and Vancomycin respectively. Hence, the present study will be clinically useful for designing the hydrogel wound dressings from simple empirical relations.

## 5. References

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2. Thapa RK et al., Eur J Pharm Sci; 166:105990 (2021).
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## Acknowledgements

Pooja Vardhini Natesan would like to thank the Government of India for providing the Prime Minister's Research Fellowship to carry out this study.