In silico Study of Transdermal Drug Delivery Through the Stratum Corneum: Testing the Impact of Lateral Diffusion

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Transdermal drug delivery (TDD) has emerged as a reliable alternative to invasive drug administration techniques. However, current methods used to test the process of TDD are inefficient and costly. While TDD offers a steady absorption rate of drugs bypassing first-pass metabolism, the successful permeation of medications through the stratum corneum (SC) remains a critical challenge. This study utilized a spatially resolved Tetrakaidecahedra (TKD) model to examine drug penetration and lateral diffusion within the SC. The model incorporated distinct diffusion coefficients for corneocytes represented by TKD within an intercellular lipid matrix, with both subdomains resolved using triangulation. The diffusion coefficient for corneocytes was set at 5.1x10^-7 cm^2/h, while the coefficient for lipids was set at 1.1x10^-4 cm^2/h. A vertex-centered finite volume method was employed to discretize the diffusion equation and was subsequently solved numerically via a supercomputer. The partial differential equation was solved using the toolbox UG4 which led to about 6,000,000 computed Degrees of Freedom (DoFs). Furthermore, the iterations were computed to achieve the reduction of the norm of the defect by factor 10^-8. These results have shown that the saturation time did not significantly depend on the boundary conditions. Examining such complex phenomena will help the pharmaceutical industry in optimizing TDD methods to their full potential while also gaining a deeper insight into the biological complexity present. This holds promise for advancing drug delivery approaches in a targeted manner that accelerates industry innovation and facilitates healthier patient outcomes.

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