MATHEMATICAL MODEL TO PREDICT THE SKIN DISPOSITION OF DEET AND OTHER VOLATILE COMPOUNDS

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dc.description	Estimation of penetration rates and systemic absorption following the application of a chemical to skin is an important tool used in a variety of fields including personal care, drug delivery and dermal risk assessment for occupational exposures. The objective of this project was to develop a predictive diffusion model for the disposition of volatile compounds on skin. In the first part of this project, the penetration of DEET, a widely used insect repellant, through spilt thickness cadaver skin was measured in non occluded Franz cells. The percent of DEET penetrated after 72 hours increased gradually with dose, up to a dose of about 680 &microg/cm², and declined at higher doses. This lead to the hypothesis that DEET was enhancing its own penetration. The hypothesis was supported by a literature review and by a supplementary study in which DEET pretreatment increased the permeability of skin to benzyl alcohol. Finally a simple diffusion model was developed to predict the absorption of volatile compounds through skin. The model had three parameters – a solubility value for the chemical in the upper stratum corneum M sat ; a mass transfer coefficient for evaporation k evap ; and a characteristic time for diffusion h ² /D . The value of h ² /D decreased with DEET dose in the dose range 30-300 &microg/cm&sup2. In the second part of the project, the model was tested on other volatile and non volatile compounds. Butyl nicotinate and benzyl alcohol displayed skin permeability enhancing properties similar to DEET, and required a diffusivity that varied with dose, while methyl nicotinate, niacinamide and vanillylnonanamide did not. For volatile compounds, the value of k evap was found to be proportional to the logarithm of the saturated vapor pressure, P vp . A qualitative relationship between M sat and lipid and water solubility could be seen, but more compounds must be studied to establish a quantitative relationship. The expected variation of h ² /D with molecular size was weak and not statistically significant. The current model is relatively simple with many approximations, but it has advantages over earlier compartmental models and has the potential to be extended to consider complications such as multi-component diffusion and ingredient interactions.	en_US
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