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Linking dermal modeling and loading data to predict long-term doses from intermittent dermal contact

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In this paper we assess dermal exposure and dose resulting from intermittent contact with residue-contaminated surfaces. These estimates require an understanding of (1) the quantitative relationship between exposure and absorbed dose; (2) the impact of intermittent exposure on absorbed dose; and (3) the temporal resolution required of exposure data to model absorbed dose. We apply a numerical model of dermal absorption to evaluate integrated dermal uptake from a series of contacts with residue-contaminated surfaces. A range of exposure scenarios and contaminant properties are considered. We use results from dermal transfer studies in which dermal loading, resulting from a series of controlled contacts with surface residues, was measured using fluorescent imaging techniques. These experimental results allow us to define archetypal temporal boundary conditions with varying skin loading and removal (via rinsing and pressing). We apply these boundary conditions in a numerical model of contaminant transport through the stratum corneum (SC) and viable epidermis (VE). This model uses a Crank-Nicholson approach to solve the transient Fickian diffusion problem with an explicit approach to connect the SC and VE. We successfully tested the model against analytical solutions of single-contact exposure scenarios for a range of compound properties. The model allows us to investigate accumulated doses from short-term and intermittent contacts, thereby avoiding important limitations of analytical solutions. Our results indicate that increasing the partition coefficient between the SC and VE (k_{sv}) decreases the time-integrated mass transferred through the VE as total contact time increases. This effect is caused by residual contaminant in the SC that reduces the concentration gradient (that drives transport from the skin surface into the SC) for subsequent contacts. Because of this "residual effect," multiple single-contact estimates cannot accurately capture integrated dose. The extent to which the single-contact estimate differed from the true dose varies with contaminant and skin properties. Below a k_{sv} of about 0.1 the time-integrated mass transferred through the VE is relatively unaffected by changes in k_{sv}, because the skin clears quickly with low k_{sv}. We also describe the sensitivity of the time-integrated uptake (i.e., through the VE) to (1) the thickness and diffusivity of both the SC and the VE and (2) the contaminant-to-SC partition coefficient. Our results indicate that estimates of integrated dose resulting from a series of intermittent exposures can be practically obtained from the numerical model and related to compound properties. Results of this study can be used to guide dermal exposure model refinements and exposure measurement study design.

Disclaimer
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