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Published in:
Proceedings of Indoor Air 2016

Publication date:
2016

Document Version
Peer reviewed version

[Link back to DTU Orbit](#)

Citation (APA):
Morrison, G., Weschler, C. J., & Bekö, G. (2016). Further advances in modeling transdermal uptake of SVOCs. In *Proceedings of Indoor Air 2016* [268]

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Further advances in modeling transdermal uptake of SVOCs

Glenn Morrison^{1,*}, Charles J. Weschler^{2,3}, Gabriel Bekö³

¹ Missouri University of Science & Technology, Rolla, MO, USA

² EOHSI, Rutgers University, Piscataway, NJ, USA

³ Technical University of Denmark, Lyngby, Denmark

* *Corresponding email: gcm@mst.edu*

SUMMARY

To better simulate dermal uptake of SVOCs from air, we develop an enhanced transport model that includes skin surface lipids (SSL). As modeled, clothing can remove SSL by contact transfer and it can act as a source or sink for gas-phase transfer to and from SSL. Addition of SSL increases the overall resistance to uptake of SVOCs from air but also allows for more rapid release of SVOCs to sinks like clothing or clean air. We compare the model results to reported experimental uptake of di-ethyl phthalate (DEP) and di-n-butyl phthalate (DnBP), normalized by exposed skin area and the phthalate air concentration during exposure (Weschler et al., 2015). Overall, the model predicts total uptake values that are consistent with those observed in the experiments. The model predicts a normalized mass uptake of DEP of $3.1 (\mu\text{g}/\text{m}^2)/(\mu\text{g}/\text{m}^3)$ whereas the experimental results range from 1.0 to 4.3 $(\mu\text{g}/\text{m}^2)/(\mu\text{g}/\text{m}^3)$. The model somewhat over-predicts uptake of DnBP: $4.6 (\mu\text{g}/\text{m}^2)/(\mu\text{g}/\text{m}^3)$ vs the experimental range of 0.49 to 3.2 $(\mu\text{g}/\text{m}^2)/(\mu\text{g}/\text{m}^3)$.

PRACTICAL IMPLICATIONS

This improved model of dermal uptake under transient conditions can be used to enhance exposure models and improve estimates of population uptake of SVOCs.

KEYWORDS

dermal uptake, exposure model, phthalates, clothing, skin lipids

1 INTRODUCTION

Dermal uptake is emerging as an important component of the overall body burden of SVOCs from indoor air. In controlled chamber exposure studies, Weschler et al. (2015) observed substantial dermal uptake of DEP and DnBP for six bare-skinned participants. The inhalation and dermal pathways were equally important for the 6h exposure. Gong et al. (2014) developed a dynamic, mechanistic model of transdermal uptake that accounted for external resistance to uptake through the convective boundary layer over human skin. While a significant improvement over a steady-state model, the Gong et al. model over-predicted uptake observed in the Weschler et al (2015) study. To improve estimates of uptake, we enhance the Gong et al. model by including skin surface lipids and consider the impact of clothing.

2 MATERIALS/METHODS

The Gong et al. (2014) model was comprised of three layers separating the SVOC in air from the dermal capillaries: air boundary-layer adjacent to skin (ABL), stratum corneum (SC), viable epidermis (VE). Transport was assumed to be Fickian, and input parameters, such as partition coefficients and diffusion coefficients, were drawn from a variety of independent sources (see Gong et al. (2015)). Our model adds a layer of skin-surface lipids (SSL) that is assumed to be in equilibrium with both the adjacent outer surface of the SC and the inner

layer of the ABL. By including SSL as a separate layer, we can model loss of SSL by contact transfer to clothing. In this model, clothing can also act as a sink for diffusive transport of an SVOC through the air gap between SSL and clothing. The SSL-cloth air gap is assumed to be equivalent to the thickness of several human hairs (0.2 mm), simulating tightly fitting clothing. The SSL-air partition coefficient is assumed to be equal to the octanol-air partition coefficient at 32°C.

We test the model by simulating exposures of six human participants reported by Weschler et al. (2015). In that experiment, six subjects were exposed to elevated concentrations of di-ethyl phthalate (DEP) and di-n-butyl phthalate (DnBP) for six hours. After leaving the chamber, all subjects don clothing. All urine was collected from just prior to exposure until 48 hours after exposure for subsequent analysis of phthalate metabolites.

3 RESULTS

Modelled results, normalized by chamber concentration and estimated exposed skin area, for DEP and DnBP are 3.1 and 4.6 ($\mu\text{g}/\text{m}^2$)/($\mu\text{g}/\text{m}^3$) respectively. The experimental results for DEP (from Weschler et al., 2015) range from 1.0 to 4.3 ($\mu\text{g}/\text{m}^2$)/($\mu\text{g}/\text{m}^3$) for six participants. The model somewhat over-predicts uptake of DnBP: the experimental range for participants was 0.49 to 3.2 ($\mu\text{g}/\text{m}^2$)/($\mu\text{g}/\text{m}^3$). Simulations including transfer of SSL to clothing result in lower uptake for DnBP and better match the experimental results. SSL transfer has little impact on DEP uptake.

4 DISCUSSION

Adding SSL and clothing to the Gong et al. model results in dermal uptake that is a good match for the experimental results. The model tends to over-predict uptake somewhat for DnBP. Uncertainty in model inputs, including partition and diffusion coefficients, could account for over-predictions associated with DnBP simulations. Including a mechanistic model of transport through clothing may further improve predictions.

5 CONCLUSIONS

The model suggests that SSL and clothing are important modifiers of phthalate uptake from air. Therefore, population exposure estimates will be improved through a better understanding of the fate of SSL by transfer to clothing and other surfaces. Further, the type of clothing, fit, dimensions, storage and washing history and many other factors likely also influence dose.

ACKNOWLEDGEMENT

This research was supported by the Otto Mønsted Guest Professor Fellowship and the International Centre for Indoor Environment and Energy at the Technical University of Denmark.

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