Read across for the derivation of Indoor Air Guidance Values supported by PBTK modelling

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Abstract

Polyurethane Flexible Foams (PUF) are versatile materials used in upholstered furniture and bed mattresses. Due to the production procedure, fresh foams emit volatile organic compounds (VOC) which may contribute to indoor air exposure. To evaluate the risk for consumers, the VOC concentration measured in chamber tests can be matched against existing benchmarks for indoor air like "Richtwerte" (RW) of the German UBA (Umweltbundesamt), "Lowest Concentration of Interest" (LCI) for construction products or derived no effect levels (DNEL) for consumer inhalation exposure. In a previous paper a method for the derivation of Indoor Air Guidance Values (IAGV) for VOC without RW, LCI or DNEL was developed. The method described made use of a sufficient toxicological database. For substances with an insufficient database, read across to structural analogues is a way forward to estimate Indoor Air Guidance Values (IAGV). In this work a read across exercise, supported by an open source physiology based toxicokinetic (PBTK) modelling program is demonstrated. The use of enzyme kinetic data for phase I and phase II metabolism is discussed and areas for further work were identified. For two substances with very limited toxicological data, allyloxypropanol (isomer mixture of 1-allyloxy-2-propanol and 2-allyloxy-1-propanol) and 2,3-di-ethyl-2,3-dimethylsuccinodintrile, Tentative Indoor Air Guidance Values of 750 µg/m³ and 65 µg/m³ were derived.

Issue

Vol 17 (2018)

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