Science of the Total Environment 574 (2017) 1182–1208

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Review

# A review of models for near-field exposure pathways of chemicals in consumer products

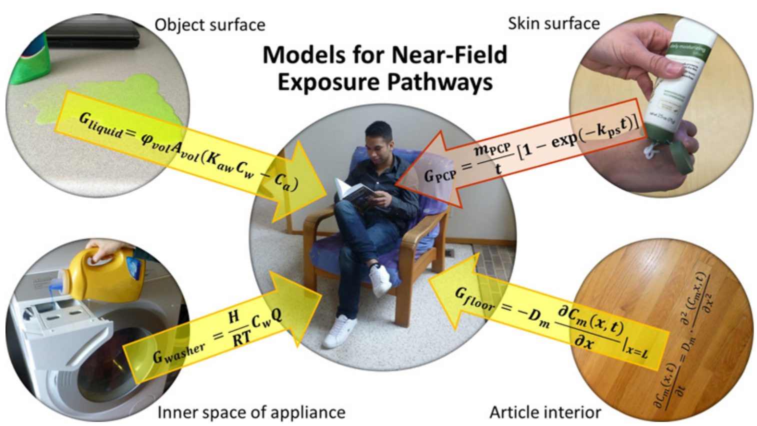
Lei Huang [a,*], Alexi Ernstoff [b], Peter Fantke [b], Susan A. Csiszar [c], Olivier Jolliet [a]

[a] Environmental Health Sciences & Risk Science Center, School of Public Health, University of Michigan, Ann Arbor, MI 48109-2029, United States
[b] Quantitative Sustainability Assessment Division, Department of Management Engineering, Technical University of Denmark, 2808 Kgs. Lyngby, Denmark
[c] Oak Ridge Institute for Science and Education Research Participant, US Environmental Protection Agency, National Risk Management Research Laboratory, Cincinnati, OH 45268, United States

## HIGHLIGHTS

- Near-field compartments for exposure to chemicals in consumer products are defined.
- Models for compartmental transfers and subsequent human exposure are reviewed.
- Key model parameters and impact pathways are identified per compartment of entry.
- Applicability to LCA, alternative assessment & high throughput screening is studied.
- A summary table lists suitable models and research needs for LCA, CAA and HTS.

## GRAPHICAL ABSTRACT




## ARTICLE INFO

*Article history:*
Received 12 April 2016
Received in revised form 15 June 2016
Accepted 15 June 2016
Available online 16 September 2016

Editor: D. Barcelo

*Keywords:*
Human exposure models
High-throughput risk screening
Life cycle impact assessment
Mass transfer fractions
Consumer products
Indoor environment

## ABSTRACT

Exposure to chemicals in consumer products has been gaining increasing attention, with multiple studies showing that near-field exposures from products is high compared to far-field exposures. Regarding the numerous chemical-product combinations, there is a need for an overarching review of models able to quantify the multiple transfers of chemicals from products used near-field to humans. The present review therefore aims at an in-depth overview of modeling approaches for near-field chemical release and human exposure pathways associated with consumer products. It focuses on lower-tier, mechanistic models suitable for life cycle assessments (LCA), chemical alternative assessment (CAA) and high-throughput screening risk assessment (HTS). Chemicals in a product enter the near-field via a defined "compartment of entry", are transformed or transferred to adjacent compartments, and eventually end in a "human receptor compartment". We first focus on models of physical mass transfers from the product to 'near-field' compartments. For transfers of chemicals from article interior, adequate modeling of in-article diffusion and of partitioning between article surface and air/skin/food is key. Modeling volatilization and subsequent transfer to the outdoor is crucial for transfers of chemicals used in the inner space of appliances, on object surfaces or directly emitted to indoor air. For transfers from skin surface, models need to reflect the competition between dermal permeation, volatilization and fraction washed-off. We then focus on transfers from the 'near-field' to 'human' compartments, defined as respiratory tract, gastrointestinal tract and epidermis, for which good estimates of air concentrations, non-dietary ingestion parameters and skin

* Corresponding author.
*E-mail address:* huanglei@umich.edu (L. Huang).

http://dx.doi.org/10.1016/j.scitotenv.2016.06.118

permeation are essential, respectively. We critically characterize for each exposure pathway the ability of models to estimate near-field transfers and to best inform LCA, CAA and HTS, summarizing the main characteristics of the potentially best-suited models. This review identifies large knowledge gaps for several near-field pathways and suggests research needs and future directions.



**Contents**



## 1. Introduction

Collectively, the products we use in our daily lives contain thousands of chemicals (Judson et al., 2009) and new chemical-product combinations are continuously introduced into commerce. Each product has the potential to expose people to chemicals, through using the product and through environmental emissions along a product's life cycle (e.g. from manufacturing). The manner of a product's use and its physical properties (e.g. if solid, liquid, or spray), as well as the properties of the chemicals therein (e.g. vapor pressure) are important factors in determining the fate of and exposures to chemicals within consumer products. For example, some products are intended for use as indoor sprays (e.g. air fresheners) or indoor fixtures (e.g. furniture), or are meant to be directly ingested (e.g. food) or applied to the skin (e.g. skin care products). The multitude of potential uses of products on today's market, and the diversity of chemicals used therein, lead to various chemical exposure magnitudes, durations, pathways, and pose a significant research challenge with respect to quantifying and comparing product-related exposures.

The need for incorporating human exposure information into chemical prioritization has been well identified (Gangwal et al., 2012; Swanson et al., 1997; Wambaugh et al., 2013). Traditionally, physiochemical properties such as vapor pressure, Kow and environmental half-lives of chemicals have been used to rank potentials for human exposures (Gangwal et al., 2012; Swanson et al., 1997; Wambaugh et al., 2013). However, these methods can not reflect well the interaction between various chemical properties that occur for multiple exposure pathways (Wambaugh et al., 2013). Also, the exposure estimates based on these simple properties do not correlate well with monitoring-based estimates of exposures (Gangwal et al., 2012; Wambaugh et al., 2013). Therefore, the use of models, instead of using chemical properties as proxy, is preferred to make estimates of human exposures for chemical prioritization or ranking purposes (Wambaugh et al., 2013).