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Assessing Human Exposure to SVOCs in Materials, Products, and Articles: A Modular Mechanistic Framework

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ASSOCIATED CONTENT
Supporting Information
The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.0c02329.
Nomenclature, list of consensus points, mechanistic modeling framework to predict exposure to SVOCs (Figure S1), emission and transport modeling equations, exposure modeling equations, estimation approaches for model parameters, comparison of K_{oa} values (Figure S2), decision tree for exposure mechanism selection based on the source emission category (Figure S3), and list of signatories who support the proposed framework (PDF)
Complete contact information is available at: https://pubs.acs.org/10.1021/acs.est.0c02329

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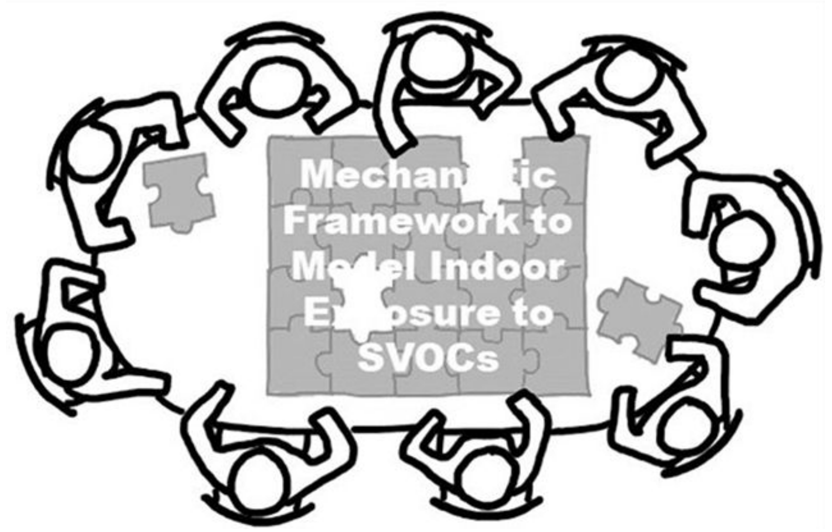
Abstract

A critical review of the current state of knowledge of chemical emissions from indoor sources, partitioning among indoor compartments, and the ensuing indoor exposure leads to a proposal for a modular mechanistic framework for predicting human exposure to semivolatile organic compounds (SVOCs). Mechanistically consistent source emission categories include solid, soft, frequent contact, applied, sprayed, and high temperature sources. Environmental compartments are the gas phase, airborne particles, settled dust, indoor surfaces, and clothing. Identified research needs are the development of dynamic emission models for several of the source emission categories and of estimation strategies for critical model parameters. The modular structure of the framework facilitates subsequent inclusion of new knowledge, other chemical classes of indoor pollutants, and additional mechanistic processes relevant to human exposure indoors. The framework may serve as the foundation for developing an open-source community model to better support collaborative research and improve access for application by stakeholders. Combining exposure estimates derived using this framework with toxicity data for different end points and toxicokinetic mechanisms will accelerate chemical risk prioritization, advance effective chemical management decisions, and protect public health.

Graphical Abstract



INTRODUCTION

Rapid risk-based prioritization of large numbers of chemicals in numerous building materials, consumer products, and consumer articles used indoors (here collectively referred to as sources) has become an increasing focus of chemical management strategies to protect humans from potentially harmful exposures.[1–5] Although these strategies emphasize the need for high-quality, representative exposure data and mechanistic (i.e., process-based) exposure models, approaches for implementation are highly fragmented among countries, authorities, and research institutions.[5,6] We need to implement more efficiently the current understanding of fundamental mechanisms governing indoor exposure to chemicals released from sources. This is especially true for semivolatile organic compounds (SVOCs) due to their multimedia behavior. Unlike volatile organic compounds (VOCs) or most metals, SVOCs partition among multiple indoor compartments, including people, according to their physicochemical properties.[2,7–9] As the number of source/chemical combinations increases steadily, traditional assessment approaches are challenged to keep pace given that key emission and exposure parameters have only been measured for very few combinations that do not necessarily span the full range of exposure conditions.[8,10,11] Potential approaches to facilitate the transition from hazard-driven, single-chemical assessments toward rapid, risk-based, high-throughput (HT) prioritization are already being developed and include procedures to estimate exposure, toxicity, and toxicokinetics.[3,12–16] For example, HT screening methods allow testing of large numbers of samples with highly automated instruments in combination with advanced data processing software.[13,15,17,18] Substantial efforts have been made in generating HT hazard information and HT toxicokinetics, but essential information to predict human exposure to chemicals released from indoor sources is frequently missing.[19,20] To fully realize the potential of new chemical risk assessment approaches, reliable chemical exposure models need to be coupled with quickly accessible toxicity data.[2,21–23]

This paper provides a critical review of mechanistic models for estimating chemical emissions from indoor sources, partitioning among indoor compartments, and exposure to humans indoors. The review develops a generic modular mechanistic framework that provides a roadmap for evaluating exposure scenarios associated with the use phase of materials, products, and articles, within a rapid risk screening and prioritization context. The specific objectives of this paper are thus to (1) define mechanistically consistent source emission categories, (2) review exposure pathways that are congruent with these source emission categories and the subsequent chemical distribution among indoor compartments, and (3) identify relevant knowledge gaps and needs for further research that will facilitate exposure estimates for indoor sources. The focus is on SVOCs, but the modular structure of the framework will make it possible to subsequently include other classes of chemicals released indoors.

Many of the underlying elements forming this framework have been described elsewhere.[24–27] Here, we combine and connect these elements in a consistent and meaningful way to facilitate efficient implementation. To achieve this, we reviewed the existing research in the field, highlighted knowledge gaps, and then assembled a consensus regarding what is known about SVOC emission, transport, and exposure in indoor environments. The result is a framework for rapid exposure estimation that serves as a baseline among researchers and stakeholders regarding SVOC models and conditions of application. Exposure models and concepts underpinning the proposed framework will enable efficient exposure estimates for a wide range of source/chemical combinations, inform scientifically-based chemical management policy and public health decision-making, and provide new insights for manufacturers of building materials, consumer products, and consumer articles.

SEMIVOLATILE ORGANIC COMPOUNDS IN INDOOR ENVIRONMENTS

There are several definitions of SVOCs.[28] The World Health Organization (WHO) defines SVOCs as a group of chemicals with boiling points in the range of (240–260 °C) to (380–400 °C).[29] According to International Standard ISO 16000–6:2011, SVOCs elute after *n*-hexadecane on a nonpolar gas chromatography capillary column.[30] Other definitions refer to a liquid, pure compound vapor pressure range of 10^{-9} Pa to 10 Pa at room temperature[31] or to a saturation mass concentration range of 0.3 μg m^{-3} to 300 μg m^{-3}, corresponding to vapor pressure in the range of about 10^{-6} Pa to 10^{-3} PaPa, assuming an average molecular weight of 400 g mol^{-1} and standard conditions.[32]

SVOCs are present in many different consumer products, building materials, and other indoor articles where they are used as, for example, plasticizers, flame retardants, solvents, and pesticides. Often, they occur as additives that are not chemically bonded to the host polymer. Numerous SVOCs have been associated with adverse health effects, making them of particular concern to scientists, chemical managers, public health professionals, and policy makers.[33–36] Their physicochemical properties make the characterization of SVOCs in indoor environments and exposure estimation challenging because they tend to partition among indoor compartments (e.g., gas phase, airborne particles, settled dust, and surfaces) at different rates.[37]

SVOC emissions can occur directly during use (e.g., spraying of indoor pesticides or application of varnish) or from the application itself, because the additive migrates over time, resulting in delayed exposure (e.g., migration from plastic products such as PVC shower curtains). Exposure to SVOCs is possible via inhalation, dermal uptake (i.e., transfer from a source to the skin surface) and ingestion (including hand-to-mouth transfer and mouthing).[38] In 2004, Bennett and Furtaw[39] introduced a fugacity-based model to describe exposure to SVOCs in indoor environments, while in 2006, Xu and Little[40] extended a model originally developed for VOCs to predict emission rates of SVOCs from polymeric materials. As with SVOCs outdoors, Xu and Little showed that SVOC emission and transport are subject to external control, that is, partitioning, convective mass transfer and sorption to surfaces and airborne particles.[40] In 2008, Weschler et al.[41] investigated the distribution of phthalates among the gas phase, airborne particles, and settled dust, and provided a model for the gas/particle partition coefficient K_p, which allows an estimation of the SVOC concentration in airborne particles if the gas-phase concentration is known. Weschler and Nazaroff[31] presented the first framework for characterizing equilibrium partitioning among indoor compartments for SVOCs. One key finding was that SVOCs might persist in indoor environments for years, depending on their vapor pressure, even after the original source has been removed.[31,42] Several studies followed, presenting both measurements and models describing SVOC emission, transport, and subsequent exposure, often with a focus on phthalates such as di-2-ethylhexyl phthalate (DEHP).[43–48]

In 2012, Little et al.[37] proposed a framework for rapid exposure estimates based on the source type in which the respective SVOC is present. Accounting for source composition and use (i.e., additive vs reactive use in the host polymer) as well as for emission characteristics, a simple method to estimate exposure to additives in sources used indoors and for sources sprayed or applied to interior surfaces was developed.[37] The key parameters needed for these models have since been investigated, and reliable measurement methods of various levels of complexity are now available.[49–57] Other aspects, such as the influence of clothing on dermal SVOC exposure,[58,59] the dermal uptake of SVOCs from air,[24,60,61] the impact of organic films on indoor surfaces on SVOC dynamics,[48,62,63] and the influence of occupants on indoor exposure to SVOCs[64,65] are being studied in increasing detail.

Li et al.[66–68] developed a framework for describing the fate of chemicals at different product life-stages (Production-to-Exposure or PROTEX model). PROTEX is comprised of four modules, including a technosphere module, which is based on a flow analysis approach, a nested indoor-urban-rural fate module, a food-web bioaccumulation module, and a human toxicokinetic module, all based on the fugacity approach.[68] PROTEX yields exposure estimates based on near- and far-field exposure pathways.[68] Its modular structure and the consideration of different product life-stages make the PROTEX model a good example of how different aspects of chemical fate can be combined. However, the estimation of indoor emission rates in the technosphere module is based on empirical relationships to estimate emission factors[68,69] or on mechanistic models that the framework presented here aims to expand and update.[40,67] The modular structure of PROTEX allows the integration of consistent mechanistic models to describe the fate of SVOCs in indoor environments during the product use stage, thus making PROTEX highly complementary to the proposed framework.

Dietary exposure to SVOC residues present in food and beverages is an important component of overall exposure to certain SVOCs, for example to DEHP, diethyl phthalate (DEP), and triphenyl phosphate (TPHP).[70–73] This exposure route can occur due to "far field" effects of bioaccumulation through the food web or due to migration from food contact materials and appliances.[74,75] To assess the far-field dietary exposure pathway, it would be necessary to expand the framework discussed here; however, a detailed review of the relevant mechanisms is beyond the scope of this critical review. One example of how to connect indoor exposure and dietary exposure as well as far-field exposures can be found in the PROTEX framework, which includes a food-web bioaccumulation module.[66,76]

A FRAMEWORK FOR PREDICTING EXPOSURE TO INDOOR SVOCS

Figure 1 illustrates a mechanistic modeling framework for estimating exposure to SVOCs emitted from sources present or used in the indoor environment. The central elements of the framework are (1) the modeling of emissions based on mechanistically consistent source emission categories (SECs), (2) the modeling of transport, chemical transformations, and resulting concentrations in the respective indoor environ- mental compartments, and (3) the estimation of exposure via different pathways based on the concentrations in the compartments for different exposure scenarios. Based on this framework and with the SECs as starting points, we review the scientific background and underlying assumptions of the mechanistic models for emission, transport, chemistry, and exposure, as well as their main input parameters, assumptions, uncertainties, limitations, and conditions of model application.

In the framework, the focus is on mechanistic modeling as the underlying principles are robust, and the model can be applied to multiple chemicals when predicting exposure.[21,25,77,78] Mechanistic models, also referred to as process-based models,[19] rely on well-established physicochemical processes such as diffusion or sorption. They are generalizable and can vary in complexity based on the needs of a given assessment context, in contrast to empirical models.[27] However, if suitable mechanistic models are not available, other approaches such as machine-learning, expert opinions, statistical, or empirical models may serve in a preliminary role.[78]

Assumptions.

The following general assumptions are often made for SVOC emission, transport, and exposure models. They are valid in many cases, but there are exceptions that increase the uncertainty of the derived exposure estimates.

The indoor compartments considered in this framework are the gas phase, airborne particles, dust, and surfaces. We included clothing as an additional compartment because its role in exposure scenarios is particularly important.[58,79] People are in constant, intimate contact with clothing. Clean clothing has been shown to protect against dermal uptake of SVOCs from air, while clothing that had been exposed to contaminated air can serve as an additional exposure source leading to potentially increased dermal uptake and inhalation exposure.[58,80,81] These characteristics, together with other properties discussed below, distinguish clothing from other environmental compartments.

The relationship between the indoor compartments is fundamentally dynamic. In some cases, equilibrium conditions between gas phase, particle phase, dust, and surfaces can be assumed to simplify the models.[52,82] However, the greater the capacity of an environmental compartment, the longer it will take for that compartment to reach equilibrium with other compartments, and the less applicable the equilibrium assumption will be. A detailed discussion of this issue can be found in Mackay et al.,[83] including recommendations for identifying and quantifying kinetic delays.

SVOC emissions from source materials are mostly externally controlled, meaning that internal mass transfer (e.g., diffusion) is faster than external mass transfer.[31,40,84] Furthermore, the material-phase SVOC concentration C_0 can be considered constant as depletion usually happens at a very slow rate, as shown by Xu and Little,[40] Xu et al.[85] and Pei et al.[86] However, these assumptions are only valid for sufficiently small external mass transfer coefficients and SVOCs with relatively low vapor pressures.[87] Internal diffusion may become important when considering transfer in, for example, clothing.[57,88]

It is generally assumed for modeling purposes that the air in the indoor environment is well-mixed, but this may not be the case for many indoor environments, especially not for indoor air in poorly ventilated spaces, for example within cabinets and closets.[89,90]

In some cases, it may be reasonable to assume that background outdoor concentrations of SVOCs are negligible for exposure assessments of chemicals released from indoor sources. This assumption depends on the type of SVOC considered, as some are present both indoors and outdoors, for example, pesticides and polycyclic aromatic hydrocarbons (PAHs).[91–93] If an SVOC has an outdoor source, its concentration in the infiltrating air and the possibility of transport into the indoor environment with outdoor dust should be taken into account.[94]

Emission.

The framework is structured to distinguish between contact and mediated exposure (Figure 1). Contact exposure can occur immediately via direct dermal uptake or (inadvertent) ingestion of chemicals in the source, which includes mouthing or licking of a source. Mediated exposure occurs when emission from the source to environmental compartments happens first, followed by partitioning and chemical transformations, resulting in accumulation in one or more compartments where exposure may take place. Frequently, exposure pathways are categorized as “direct” and “indirect”, but these categories are used inconsistently in the literature, thus we chose different terms.

Chemical emission from a source depends largely on chemical characteristics, on the source characteristics, and on the properties of the environmental compartment into which the chemical is emitted.[37] However, all indoor environmental compartments can serve as both sources and sinks, even simultaneously, depending on the chemical and the direction of the chemical fugacity (or chemical activity) gradient. The general direction for chemical mass transfer in this framework is the transport from sources with high fugacity to sinks (including humans) with lower fugacity, thus the arrows in Figure 1 point from the left (sources) to the right (human exposure). It should be noted that the direction of the chemical fugacity gradient may reverse.

Traditionally characterized sources of emission are furniture, building materials including flooring and carpet, electrical and electronic products, personal care products, as well as combustion processes (e.g., burning a scented candle) and cooking (e.g., heating oil in a pan). For our modeling framework, we derived SECs from a continuum of possible sources (Figure 2). We recognize that there is some overlap between the categories and that some sources may not fit perfectly into one category. In such cases, multiple scenarios may have to be considered.

For SVOCs, Little et al.[37] differentiated between two main categories of sources: One included solid sources in which SVOCs are present as additives or surface coating components and the other category included sources containing SVOCs that are either sprayed or applied. Mechanistic emission models were presented for both categories.[37] Here, we modify and extend the list of categories to include the following SECs: solid sources, soft sources, sources that humans frequently contact, liquid applied sources, liquid sprayed sources, and high temperature sources, resulting in a total of six mechanistically consistent SECs (Figure 2), which cover most sources of SVOCs.[10,95]

These SECs can be mapped to those defined by organizations such as the Organisation for Economic Co-operation and Development (OECD) and the U.S. EPA. The sources in the categories “solid”, “soft”, and “frequent contact” are usually “articles” as defined by the OECD, that is, solids, polymers, foams, metals or woods that are continuously present in the indoor environment during their useful life.[96] “Applied”, “sprayed”, and “high temperature” sources correspond to “products” as defined by the OECD, which are consumable liquids, aerosols, or semisolids that are used a certain number of times until they are exhausted.[96] Furthermore, the Level 1 and Level 2 product use categories (PUCs) listed in Isaacs et al.[97] overlap to a large extent with the SECs “frequent contact”, “applied”, and “sprayed” and to some extent with the categories “solid” and “soft”. The PUCs were derived from the products listed in the U.S. EPA’s Chemicals and Product Database (CPDat).[97] Although they do not align completely, it would be possible to map each PUC to an SEC and potentially to incorporate PUCs in this framework. Descriptors and schemes used in other instances for tracking and managing products and source/chemical combinations could potentially be adapted as well, given that the categories proposed here are intended to be relatively flexible, while still remaining mechanistically consistent.[98]

The SEC-based emission rates and chemical concentrations for each indoor compartment can be used in combination with the exposure estimation models presented as part of the framework or independently in different types of specific exposure and intake models to derive exposure estimates in the required format.

Solid Sources.—Solid sources containing SVOCs include, for example, PVC flooring, electronic devices such as TVs, plywood furniture, and previously painted walls. They have relatively large emitting surface areas relative to the volume of most indoor environments or to the area that may come in contact with an exposed person. Exposure to SVOCs present in these solid sources is predominantly mediated. Contact exposure contributes much less to overall exposure.[76,99]

As discussed above, depletion of the SVOC in the source can often be assumed to be negligible.[40,85,86,100] Including the variability of source strength over time in the model increases its complexity, but the mechanisms governing emission from solid sources remain the same. A prerequisite for calculating the depletion rate is that C_0 is known.

From a solid source, emission may occur either into the gas phase or by migration into dust in direct contact with the solid source material.[37,101] Governing parameters for emission into the gas phase are the SVOC gas-phase concentration immediately adjacent to the source material y_0 and the mass transfer coefficient h_m (Section 1a in the Supporting Information (SI)).[25,37,102] y_0 is itself a function of C_0 (SI Section III)[53,56] and can also be measured[49] or derived using the material/air partition coefficient, K_{ma}.[103,104] Addington et al.[105] developed a quantitative structure−activity relationship (QSAR)-based method for estimating activity coefficients and y_0 for plasticizers based on chemical structure, polymer characteristics, and physicochemical properties. An expansion of this approach to other types of SVOCs and chemicals in general would greatly facilitate our ability to estimate indoor emissions.

If it is assumed that a linear equilibrium relationship exists between the settled dust and the gas layer directly adjacent to the source material (SI Section 3), the critical parameters for modeling emission into dust are y_0, h_m (SI Section IV), the dust/air partition coefficient K_{dust} (SI Section VI), the particle deposition velocity v_d, and the concentration of airborne particles, which is usually given as total suspended particles, TSP.[25,43,106,107] Instead of TSP, other particle concentration ranges such as $PM_{2.5}$ can be used, depending on the research question.[9,41]

Soft Sources.—Exposure to soft sources can occur both via contact exposure due to frequent close contact of a person with these sources and via mediated exposure due to their often large emitting surface areas.[108–110] Soft sources include cushions, mattresses, foams, carpets, upholstery, draperies, and clothing. Note that this SEC includes clothing as a source, while clothing as environmental compartment is discussed in the Transport section below. New clothing may contain SVOCs introduced during manufacture, transport, storage, or from contact with packaging materials, or because they have been added deliberately for product enhancement, for example water-resistant/repellent coatings.[79] These SVOCs may be emitted into the indoor environment after the clothing has been brought into a building and even after laundering.[79] Stored clothing may accumulate SVOCs from the air and reactions of oxidants with soiled clothing can be a source of SVOCs; thus they serve as an additional environmental compartment.[58,111] Emission from soft sources into the gas phase or into settled dust can be modeled using the equations in SI Sections 1a and 3, respectively.

Frequent Contact Sources.—Exposure to certain SVOCs in solid sources that are frequently handled (e.g., smartphones, smartwatches, toys) or mouthed by children (e.g., teethers and pacifiers) is more likely to occur via contact exposure.[112] These sources are not stationary, usually irregularly shaped and their emitting surface area is comparatively small and thus contributes less to the SVOC concentrations in the environmental compartments; however, their frequent handling can increase their importance as an exposure source. Emission may be modeled as for solid sources.[79]

Applied Sources.—A liquid source that is directly applied to the body (e.g., lotion, shampoo, sunscreen) is mainly linked to contact exposure. With a liquid source applied to the body, aside from the direct dermal exposure, emission into the gas phase and further partitioning occurs, which may contribute to total exposure to a lesser extent, depending on the SVOC and individual occupant behavior.[113,114]

If the liquid source is applied to a surface or remains open to the indoor air, mediated exposure via inhalation of the gas phase and aerosols dominates for more volatile SVOCs.[9,115,116] Examples are floor care products, other cleaning products, detergents, or wet paint. Emission from an applied source is usually confined to a relatively short period of time during and shortly after application. For certain cases, for example the application of paint (and depending on which constituents in paint are being considered, for example, solvents or PCB-11 as a degradation product of pigments[117]), it might be necessary to consider the application exposure scenario first, and then exposure from the essentially solid source after the paint has dried.[118,119]

After initial release, SVOCs partition onto indoor surfaces (including exposed skin, hair, and clothing), airborne particles and dust, from where long-term exposure may occur even if the initial short-term source has evaporated or been depleted. In the case of dried paint or other dried sources, emission into the gas phase can be modeled using the same approach as for emission into the gas phase from a solid source (SI Section 1a).[40]

Sprayed Sources.—A liquid source that is sprayed toward the body can result in both contact and mediated exposure. Dermal uptake by direct contact with the source occurs together with exposure by dermal uptake from air and inhalation of both gas and particle phases. Examples are deodorants, perfumes, or sprayed sunscreens. If the source is sprayed away from a person, for example, air freshener or window cleaner, mediated exposure may contribute more.

Sprayed sources are pulse emission sources with constant or variable time patterns. The emission mechanism of sprayed sources differs from that of applied liquid sources because of the force with which the product is released within a relatively small volume of air, resulting in high concentrations for a short period of time. The formation of aerosol droplets that interact with airborne particles, dust, and indoor surfaces enhances the potential for exposure that may occur long after the initial release. Additionally, powdery sources may fall into this category, as their application can also result in high concentrations in a short period of time and the release of particles into indoor air. Further research is needed to develop mechanistically consistent models describing the mechanism for this SEC.

High Temperature Sources.—High-temperature events like candle burning, cooking, or using a fireplace are pulse emission sources that can release both gas-phase and particle-phase SVOCs over a longer period of time compared to sprayed sources.[9,120] Appropriate mechanistic modeling approaches are also needed for this SEC. In addition, transformations and reactions (including oxidation) possibly happening during and shortly after emission must be taken into account. Exposure to these types of sources is primarily mediated via inhalation. Although all sources may undergo temperature variations that influence their chemical activity and thus emission behavior, this category targets sources that participate in intentional events and experience high temperatures for a certain period of time.

Transport.

SVOC transport and partitioning occur among the compartments as shown in Figure 1. The lower their saturation vapor pressure p_s (SI Section I) and the higher their octanol/air partition coefficient K_{oa} (SI Section II), the more SVOCs tend to partition to particles, dust or surfaces.[37,41]

Airborne Particles.—Particles enter either from outdoors (via unintentional infiltration or intentional ventilation) or are emitted by occupants, for example, as exhaled aerosols, and from other occupant activities.[84,120–122] Gas/particle partitioning is described in SI Section 4. The equation in SI Section 7a shows the mass balance for particle transport, taking into account particle infiltration, dust resuspension, particle generation, and removal via ventilation and deposition. Particle residence time and air change rate are directly correlated.[82] For less volatile SVOCs, instantaneous equilibrium between the gas and particle phases cannot be assumed, and dynamic models exist that account for particle residence times.[82,123,124] Particle composition also plays an important role for both the dominant partitioning mechanism (ad- or absorption) and the amount of an SVOC that a particle can accumulate.[52,125,126] The gas/particle partition coefficient K_p is a lumped parameter reflecting these considerations. Estimation strategies for K_p are described in SI Section V.

Dust.—Airborne particles contribute to settled dust when they are deposited on surfaces, while settled dust can be resuspended and become airborne.[127] Occupants can also contribute to settled dust, e.g. by shedding of skin flakes.[25,121] SVOC partitioning may occur between the gas phase and dust settled on source surfaces (SI Section 5a) and on indoor surfaces (SI Section 5b). A mass balance for dust settled on indoor surfaces can be found in SI Section 8.

SI Section VI shows strategies for the estimation of the dust/gas partition coefficient K_{dust}. Clausen et al.,[128] Schripp et al.[129] and Liu et al.[101] focus on the kinetic process of SVOC uptake by dust particles and explore the relationship between the source surface and layers of settled dust. Dust may also contribute to SVOC losses due to a combination of abiotic and microbial degradation, if the relative humidity is elevated.[130] Cleaning can have a short-term removal effect on the SVOC mass balance, but the long-term effect depends on the specific scenario and on the volatility of the SVOC.[65,127] However, the possibility of enhanced SVOC removal should be considered when exploring unusual exposure scenarios.

Indoor Surfaces.—From the gas phase, SVOCs partition to indoor surfaces, which form substantial reservoirs that act as both sinks and sources.[37,131] Here, surfaces are defined as the readily accessible interfacial region (air–substrate interface and bulk substrate near the interface) of materials such as wood, painted walls, furnishings, glass, nonclothing fabrics, and upholstery. The sink surface/gas partition coefficient K_s depends on SVOC and surface material characteristics, and has been measured for some SVOC/surface material combinations (SI Section VII).[51,56,132–135] SI Section 6a describes surface/gas partitioning for solid indoor surfaces, while SI Section 6b describes surface/gas partitioning for soft indoor surfaces with dust settled on those surfaces.

Modeling the uptake of SVOCs by indoor surfaces is strongly influenced by thin organic films that are likely present on most indoor surfaces (SI Section 6c).[39,62,133,136] Their presence affects the SVOC dynamics and is thus also relevant for modeling of partitioning onto surfaces, because the presence of organic materials on surfaces and their properties (i.e., chemical composition, phase state) change partitioning parameters, especially K_s, and potentially simplify the model.[51] Weschler and Nazaroff[62] developed a model of the growth of organic films on impermeable surfaces and its effect on partitioning of SVOCs with different octanol/air partition coefficients K_{oa} and predicted that SVOCs with a $\log K_{oa}$ between 10 and 13 would be predominantly present in the film. Furthermore, the growth rate of the film was predicted to be initially high and to decrease over time. Low molecular weight SVOCs reach their equilibrium surface concentration relatively quickly, compared to higher molecular weight SVOCs.[24,62] Eichler et al.[63] added a mass-transfer model that describes the initial formation of an organic film on clean impermeable surfaces, identifying a two-stage process that requires the film to reach a critical thickness before the growth model becomes applicable. This approach is supported by Liang et al.[137] Coarse particle deposition via gravitational settling on upward-oriented surfaces is also likely to influence the growth of organic surface films, depending on the gas-phase concentration of SVOCs with higher $\log K_{oa}$ values, the concentration of airborne particles and their organic matter fraction.[62]

Finally, the equation in SI Section 9 shows the general mass balance for indoor SVOCs, combining the previously listed elements. The mass balance includes entry of gas- and particle-phase SVOCs into the indoor environment from outdoors, removal of gas- and particle-phase SVOCs by ventilation, SVOC emission from source surfaces, mass transfer to surfaces, deposition of particles on surfaces, and resuspension of dust from surfaces. It does not include clothing-mediated sink or source effects or chemical elimination by humans, but these processes may be relevant in some scenarios. For lower volatility SVOCs, it has been shown in models that humans may affect the indoor mass balance significantly, if no degradation in the particle phase occurs and if large reservoirs are present.[37,64,138] Potential removal pathways by humans include hand washing, bathing, skin peeling and skin renewal, and chemical elimination in the body (exhalation, biotransformation, and excretion).[138] To better quantify the effect of humans on the SVOC mass balance, further research on human activity patterns as well as on chemical and biological removal rates is warranted.

Clothing.—Clothing has been identified in recent years as an important mediator of human exposure to chemicals and particles because of its close proximity to people at almost all times, potentially acting as a barrier to exposure or having a prolonging effect.[59,79] Newly purchased clothing as a source of emission has been discussed above. Postpurchase, clothing contains a mix of SVOCs (among other chemicals) present at the time of purchase and those sorbed while stored or in use.[79,111,139] Laundering clothing can remove SVOCs to some extent.[140] Several studies have shown that SVOCs present in indoor air can accumulate in clothing.[58,59,88,141,142] Partitioning between clothing and air can be modeled using the equation in SI Section 10a. For very thin clothing, diffusion inside the material can be ignored, and a simplified model can be applied (SI Section 10b).[57,88] The simplified model includes the clothing/air partition coefficient K_{ca}, which can be approximated for cotton based on K_{oa}.[111,142] Partitioning between multiple layers of clothing can be derived from the respective K_{ca} values of each layer. Morrison et al.,[141,142] Cao et al.,[57] and Saini et al.[111] reported values for K_{ca} for polychlorinated biphenyls (PCBs) and phthalates in different types of clothing material (SI Section VIII). Additionally, clothing may take up SVOCs from personal care products applied to skin, from laundering detergents and dry-cleaning additives, and also from cross-contamination with other fabrics during laundering and storage.[79,111,140] Partitioning between clothing and particles has only been studied to a limited extent, but clothing can serve as a source of biotic and abiotic particles that may contribute to the particle mass balance indoors and thus to human exposure. Potential strategies to determine emission rates of particles from clothing can be found in Licina et al.[79]

Indoor Chemistry.

Indoor chemistry involves thousands of species that undergo transformations, resulting in changes in the composition of the gas and particle phases, and countless different indoor materials serve as sinks, sources, and reaction sites with at times very different properties.[24,143–148] In the context of exposure assessments, the focus is usually on one specific chemical; however, the effect of chemical mixtures on partitioning behavior, reactivity, and subsequent exposure, and the potential relevance of additive exposures may affect the outcome of the assessment. Occupants influence indoor chemistry as well, serving as sinks and sources and providing surfaces for chemical transformations.[138,149,150] The formation of secondary organic aerosols (SOA), that is, the generation of particles as a result of the oxidation of some reactive organic species in the gas phase by indoor oxidants, including ozone and the OH radical, is also important when evaluating gas/particle partitioning of SVOCs.[144,150–152] Because of their reactivity and composition, SOA emission rates and their partitioning can only be assessed using detailed chemical models.[153] Efforts have been made to develop thermodynamic models that consider oxidative aging of SVOCs[154] and nonideal thermodynamic mixing on SOA partitioning.[155] Although still at a rudimentary stage, the possibility of the formation of SVOCs should be addressed at least qualitatively as part of any exposure assessment.

Finally, ozone and other oxidants react with organic species sorbed to surfaces, including human skin.[144,149,151,156–158] For example, a recent study by Zhou et al.[159] found that the chemical fate of PAHs embedded in organic oil is affected by the phase state and morphology of the film. The reactivity of SVOCs with oxidizing agents varies greatly and thus indoor chemistry may not be relevant for all applications.[160] For chemical reactions in the gas phase to affect indoor environments, their reaction rate has to be shorter than or close to the air change rate.[121] This time constraint does not apply to reactions on indoor surfaces, making those reactions particularly important.[121] Indoor chemistry modeling approaches are available, but still limited regarding their parametrization, especially for SVOCs, and are a focus of ongoing research.[121,151,152]

Exposure.

Based on the equations discussed in the previous sections, SVOC concentrations in specific indoor compartments can be predicted and then used to estimate exposure on an individual level. The following general exposure routes are considered: dermal exposure, inhalation exposure, and nondietary ingestion. Dermal exposure can be regarded as a two-step process: Skin-surface lipid uptake refers to the transfer of a chemical to the skin surface, whereas transdermal uptake describes transfer through the skin into body tissues and blood. For transdermal uptake, the permeability of the skin becomes important.[150,161] The equations in the SI yield exposure rates (μg h^{-1}) for each exposure route. The details of the equations are discussed below. The exposure rates can be used to express exposure (or intake) in the metrics necessary for a specific research question or risk assessment approach, for example as intake fractions (unitless) or steady-state whole-body concentrations (ng kg^{-1} BW).

As shown in Figure 1, contact exposure can occur via dermal uptake by direct contact with the source and by ingestion of a source and mouthing of the source (source-to-mouth behavior). Mediated exposure pathways are (1) inhalation of air (gas phase and airborne particles), (2) dermal uptake from the gas phase, from airborne particles, and from contact with dust, surfaces or clothing, and (3) nondietary ingestion, that is, ingestion of dust and mouthing of nonsource objects such as clothing and hands.

Dermal Uptake by Direct Contact with the Source.—When the skin is in direct contact with a source (products and articles), partitioning of SVOCs between the source and the skin-surface lipids takes place (SI Section 12a). A simple approach to describe the flux from a solid source surface to the skin surface has been used by the U.S. Consumer Product Safety Commission (U.S. CPSC). It incorporates a migration rate and the skin surface area in contact with the source.[162] Other approaches assume that the transferred amount of SVOC depends on the SVOC concentration in the source and relate this property to either a thin layer of SVOC present on the source surface or to the diffusive flux of SVOC from within the source to its exterior.[163,164] A summary of these equations can be found in Huang et al.[26] However, further research to develop a full mechanistic model is needed. For describing the transfer from liquid sources applied to the skin, a simplified form based on the approaches used by Wormuth et al.[71] and Giovanoulis et al.[165] can be used.

Following the transfer from the source to the skin-surface lipids, the subsequent transdermal uptake from the skin-surface lipids to the dermal capillaries can be described by multiplying the concentration of SVOCs on the skin surface C_{ssl} with the dermal permeability coefficient k_{p_ssl}.[24,150] Huang and Jolliet[166] proposed calculating the dermal uptake by direct contact with a given material by dividing the dermal permeability coefficient k_{p_ssl} by the material −water coefficient K_{mw} (see SI Sections 12 and IX).

Dermal Uptake from the Gas Phase and Airborne Particles.—The transdermal exposure rate Ex_{trans} from SVOCs present in the gas phase to dermal capillaries depends on the SVOC gas phase concentration C_g, the overall transdermal permeability coefficient k_{p_g} and the exposed body surface area A_{exp} (SI Section 13a).[161] k_{p_g} can be calculated based on a resistor-in-series model that takes into account the mass transfer coefficient from the bulk gas phase through the boundary layer of the skin as well as the compound-specific permeability coefficient through the stratum corneum/viable epidermis composite.[24,150,161] The model has been extended for dynamic conditions by Gong et al.[167] and further by Morrison et al.[60] Kinetic models are also available that include the impact of clothing and chemical reactions of skin lipids and ozone.[81,168] These dynamic models demonstrate that transdermal uptake of SVOCs can be a slow process and that steady-state models might not be appropriate for modeling short-term exposures.

Dermal absorption of SVOCs associated with airborne particles is expected to be much smaller than dermal absorption from the gas phase because particles diffuse much more slowly than gases.[161] A model for dermal uptake of SVOCs associated with airborne particles or dust is given in SI Section 13b. From the skin-surface lipids, transdermal uptake could be modeled as for direct dermal contact with a source. SI Section 13c shows a model for the dermal uptake of SVOCs from contaminated indoor surfaces. The equation employs a contact rate and an availability factor, because it can be assumed that not all of the SVOC deposited on the indoor surface is transferred when touched.[169] Both parameters, however, are not well-established for SVOCs and further research is necessary.[26] Dermal uptake from contact with clothing materials can be modeled using the equation in SI Section 13d. Critical parameters are the SVOC concentration in skin-surface lipids, which depends on the partitioning between clothing and skin-surface lipids and the SVOC concentration in the clothing material, the transdermal permeability coefficient from the skin-surface lipids into dermal capillaries and the exposed skin surface area. The model can be varied in complexity as described by Morrison et al.[59] and Cao et al.[88] However, because the equation in SI Section 13d assumes equilibrium between the skin-surface lipids and the clothing, it describes a worst-case scenario. In many cases, the duration of contact between clothing and skin is shorter than the time needed to reach equilibrium.[31]

Inhalation.—For inhalation exposure, the inhalation rate IR_{inh} and the total SVOC concentration in the air (gas plus particle phase SVOCs) are critical parameters (SI Section 14).[24] IR_{inh} is well documented in the U.S. EPA Exposure Factors Handbook for different age ranges, activity levels and sexes.[170] However, larger particles may be deposited in the respiratory tract and some fraction may be exhaled again or swallowed.[24,26,171] Thus, intake, bioaccessibility, and bioavailability fractions should be taken into account for exposure calculations in general.[172] The intake fraction is the amount of a compound that enters the human body compared to the amount that has been released from a source.[173] Following Wei et al.,[171] we define the bioaccessible fraction as the amount of a compound that is released into body fluids and available for absorption, while bioavailability describes the fraction that is able to cross a biological membrane and enter systemic circulation. Assuming intake, bioaccessibility, and bioavailability fractions of one, respectively, will lead to an overestimation of the actual amount being taken up by, and distributed in, the human body. The concept of intake fraction (iF) as described by Shin et al.[174] and Fantke et al.[175] can be used to provide further insight for including these concepts in exposure estimates for screening purposes, and equally when evaluating exposure to particulate matter indoors.[176]

Ingestion and Mouthing of a Source.—Nondietary inadvertent ingestion of a source (e.g., shampoo, lotion) and mouthing or licking of a source is particularly relevant for young children. In both cases, the SVOC mass fraction in the source w_0, derived from C_0, needs to be known. For ingestion, the source intake rate $\mathrm{IR}_{\mathrm{source}}$ is the most critical parameter (SI Section 12b). To estimate exposure by mouthing of a source, the mouthed area of the source A_{mouthing}, the migration rate during mouthing MR, the exposure frequency EF, the accessible fraction f_{A} and the exposure duration d are important (SI Section 12c). Studies have been conducted to explore the solubility and leachability of chemicals in saliva from various children's products, which may affect f_{A}.[162,177]

Ingestion of Dust, Hand-to-Mouth and Object-to-Mouth Exposure.—Ingestion of dust can occur via hand-to-mouth and object-to-mouth contact, especially for young children.[178] Exposure via dust ingestion can be estimated using the dust intake rate $\mathrm{IR}_{\mathrm{dust}}$ and the weight fraction of SVOCs associated with the dust (SI Section 15a).[24,26] As with $\mathrm{IR}_{\mathrm{inh}}$, the U.S. EPA Exposure Factors Handbook provides values for $\mathrm{IR}_{\mathrm{dust}}$, although these values contain considerable uncertainty.[24,179] SVOC bioaccessibility in dust must also be taken into account, as discussed by Raffy et al.[180] For calculation of exposure to SVOCs via mouthing of the source, mouthing of hands (hand-to-mouth) or contaminated objects like clothing (object-to-mouth), the frequency of contact events per unit time (EF) and the amount transferred to the mouth during each contact have to be included.[24,26] Also, the amount present on the hand or object must be specified along with the fraction of the surface area in contact with the mouth.[24,26,181] Huang et al.[26] propose a removal efficiency relationship that has been used in a similar form by Isaacs et al.,[169] who obtained their relationship by using the Stochastic Human Exposure and Dose Simulation Model for Multimedia, Multipathway Chemicals (SHEDS-MM) to fit available data.

Uncertainty Considerations.

Uncertainty is introduced in the equations at any point where a parameter is being estimated or measured. Generally, measured parameters are preferred to estimated ones, except where generalized estimated parameters might be more representative than parameters measured for one specific situation but applied to another. However, measured parameters have uncertainty associated with the experimental procedures and should only be used in models within the bounds of the experimental data (i.e., temperature and relative humidity). Uncertainty is usually included within the modeling framework as probability distributions of the modeled parameters. The material-phase concentration C_0, the octanol/air partition coefficient K_{oa}, and the saturation vapor pressure p_{s} are critical parameters for modeling SVOC emission, transport, and subsequent exposure, because they are commonly used to estimate partition coefficients.[31,41,53,182] Dust and particle properties such as the settled dust density ρ_{dust}, the particle density ρ_{part}, and the organic content of dust $f_{\mathrm{om\_dust}}$ and of particles $f_{\mathrm{om\_part}}$ are also necessary to describe SVOC distribution between different phases indoors.[182,183] Dust and particle properties vary greatly among different indoor environments (e.g., due to smoking, pets, occupant habits) and modeling cannot always account for the broad range of individual settings, but has to rely on averages based on measurements or target specific scenarios. Salthammer and Schripp[183] reviewed the results of several dust sampling campaigns and concluded that an organic content of 35% and a density of 1 g cm^{-3} appear to be reasonable parameters. Other frequently used values can be found in Weschler and Nazaroff.[43] The uncertainty associated with any of the parameters used in the models (e.g., C_0, K_{oa}, p_s, ρ_{dust}, ρ_{part}, f_{om_dust}, f_{om_part}) propagates further when using them to obtain other modeling parameters.

C_0 can be measured with chemical extraction methods and GC-MS analysis.[184,185] Suspect-screening analysis and non-targeted analysis of chemicals in products can further expand our knowledge of product composition.[186] Databases such as the U.S. EPA's CPDat, which is part of the CompTox Chemistry Dashboard, provide additional information on product composition and reference values that can be used for modeling.[187,188]

In contrast to C_0, p_s and K_{oa} are often poorly known for SVOCs, particularly at room temperature and for less volatile compounds, which makes calculating partition coefficients challenging.[183] Salthammer and Schripp reviewed the available literature and reported that values of p_s for one SVOC can span several orders of magnitude for different measurement techniques.[183,189] They estimated that uncertainty can be expressed as $p_s \pm 0.95 \cdot p_s$, following a normal distribution.[183] O'Meara et al.[190] provide a quantitative assessment of state-of-the-art p_s estimation methods for VOCs, SVOCs, and low volatility organic compounds (LVOCs). Aside from a statistical evaluation, they discuss restrictions in the coverage of different elements and functional groups for the representation of organic structures, as well as the treatments of the temperature dependence. O'Meara et al. further provide insight into the impact of combinations of different normal boiling point and vapor pressure estimation methods on predicted SOA mass concentrations based on a large number of compounds in their test set, indicating that the best vapor pressure estimation methods do not necessarily result in the best predictions of SOA mass concentrations. In the absence of reliable measurements and when the set of functional groups of the system components allow its application, the EVAPORATION model by Compernolle et al.[191] is the recommended p_s estimation method.

K_{oa} can be determined experimentally,[192] but many K_{oa} values found in the literature have been derived from the air/water partition coefficient K_{aw}, the octanol/water partition coefficient K_{ow} and/or Henry's law constant H, which introduces additional uncertainty.[183,193,194] When K_{oa} is obtained from K_{aw} and K_{ow}, the uncertainty of K_{oa} can be calculated as the combined uncertainty of the parameters used to obtain K_{oa}. For example, if $K_{oa} = K_{ow}RT/H$ is used, the uncertainty of K_{oa} is the combined uncertainty of K_{ow} and H.[183] Numerous algorithms and quantitative structure−property relationship (QSPR) approaches have been developed for the prediction of chemical properties.[195] These are available via tools like SPARC, EPI Suite, LSER, and COSMOTHERM to estimate K_{oa} and p_s, as well as online tools such as UManSysProp.[107,183,196,197] However, the results differ depending on the selected algorithm and, in case of QSPR approaches, on the quality of the input data and data training sets. Moreover, associated uncertainties are difficult to quantify.[193] Alternatively, K_{oa} can be determined from linear free energy relationships as described by Schwarzenbach et al. [198]

K_p calculated using K_{oa} can be quite different from K_p calculated using p_s.[193] Additional uncertainty might arise from the sigmoidal shape of the equation predicting the fraction of a component partitioned to the particle phase, especially for compounds of intermediate volatility (10^{-6} Pa < p_s < 10^{-2} Pa). Small changes in p_s, K_{ow}, and H (and thus K_{oa}), and in the particle concentration result in large differences in the concentration ratio between gas and particle phase.[183,193] In those cases, it is not possible to predict reliably if an SVOC is predominantly in the gas or in the particle phase. Additional difficulty arises from the humidity-dependent potential of liquid−liquid phase separation in multicomponent aerosol particles or films, affecting the equilibrium partitioning of SVOCs.[155] Generally, the range of error of both experimentally derived and calculated values for K_p is within 1 order of magnitude, but can be much greater, particularly for polar compounds.[107,199]

y_0 is a critical parameter to describe emission and can be measured directly.[49,54] Furthermore, y_0 can also be derived from correlations with C_0 for certain SVOCs.[53,56,105] Similarly, regressions for different classes of SVOCs partitioning to certain types of sink materials have been established to estimate K_s.[40,137,200] However, these correlations also depend on p_s and have similar challenges to those discussed above.

When operating with parameter distributions, Monte Carlo simulations are helpful to quantify how uncertainties propagate to derived parameters. Wei et al.[182] reviewed published data for K_p and K_{dust} and described the distributions of $\log_{10}K_p$ and $\log_{10}K_{dust}$ for 72 SVOCs that can be used as references for Monte Carlo simulations. They also developed an empirical linear relationship between $\log_{10}K_p$ and $\log_{10}K_{dust}$, which may serve to estimate K_{dust} based on K_p or vice versa, if no other sources are available.[182] Additionally, modeling parameters, especially partition coefficients, are influenced by indoor environmental factors, for example, temperature, humidity, ventilation, size fractions of airborne particles, and potential biodegradation of SVOCs.[25,52,106,130,132] These relationships require further research, but utilizing parameter distributions as model inputs provide some sense of the uncertainty associated with their estimation.

Limitations and Conditions of Model Application.

As discussed above, the current limitation of this framework is model parametrization. Availability and quality of data for input parameters impact significantly the confidence in modeling outcomes and thus constitute a priority for further research, for exmple, through integration of existing data sets, QSAR and QSPR approaches, and expert opinions to decrease uncertainties and improve the predictive power of models. It is often not possible or feasible to measure parameters directly, thus they have to be estimated or obtained from databases. The implementation of the proposed framework has to include ways to access databases like the U.S. EPA CompTox Chemistry Dashboard, including CPDat for information on C_0, and other platforms that contain data derived from HT screening approaches or QSARs/QSPRs that can serve as input for mechanistic models.[103,166,188,201,202] Parameter estimation approaches vary greatly in their accuracy, and thus different forms of uncertainty are introduced, which have to be addressed appropriately.[199] The SI provides information on approaches to estimate important parameters together with ranges of applicability and uncertainty, if available. However, the comparison of estimated parameters used in exposure models with empirical data is an important component of model evaluation.

The modular structure of the framework allows aspects of exposure modeling to chemicals released indoors to be included or excluded. The framework could, for example, be extended to include VOCs or other groups of chemicals, such as per- and polyfluoroalkyl substances (PFAS), by including additional processes and parameters. It has to be noted that the models provided with this framework have been derived for neutral SVOCs and are not directly applicable to ionic and ionizable species, which includes many PFAS.[203] Some modules are better understood than others, making it tempting to ignore those that might introduce complexity. However, even if some parts of the framework are not addressed quantitatively, they should be part of the broader discussion of the resulting exposure estimates so that they can be placed in the right context.

In addition to chemical-related model parameters, those parameters describing specific exposure scenarios may also be unknown or highly uncertain. Whenever possible, variability has to be taken into account with respect to exposed populations and occupant characteristics,[204,205] occupant behaviors,[9,64,146,206] and indoor environmental settings.[207,208] Applying Monte Carlo-based approaches to include parameter distributions and addressing certain activities to identify high exposure situations should be part of the application of the framework. It has been shown that cooking and cleaning activities greatly enhance the levels of SVOCs in indoor environments compared to background levels.[9,65,206] The possibility of aggregate exposures due to certain occupant behaviors and potential consequences for exposed individuals should thus be incorporated in the exposure assessment.[209] When assigning parameter distributions, one needs to be mindful that much of the indoor literature is based on data representative of midsocio-economic status (SES) households. However, low SES individuals can be particularly vulnerable to higher exposures resulting from poor quality housing and higher SVOC emissions.[35,205] Although the models are fundamentally “neutral”, their parametrization may be biased toward mid-SES situations that do not capture indoor exposures of vulnerable populations in low SES communities.[210,211]

Concepts of bioaccessibility and bioavailability, as discussed for example by Wei et al.[171] for inhalation exposure and by Raffy et al.[180] for dust ingestion, should be considered in the calculations when estimating intake rates based on the models presented in the SI. SVOC bioaccessibility and bioavailability can span a wide range, depending on the pathway, the specific substance, and many other influencing factors.[171,180] If bioaccessibility and bioavailability factors are not taken into account, the resulting intake rates might overestimate exposure. For higher-complexity modeling purposes, exposure estimates derived with this framework should be combined with a mechanistic model describing, for example, the fate of gas and particle phase species in the human respiratory tract, possibly followed by the application of physiologically based pharmacokinetic (PBPK) models and similar strategies to quantitatively predict concentrations in plasma or target tissues, as has been done, for example, in the PROTEX model.[2,66,68,171,212,213]

Additional uncertainty may be introduced when evaluating SVOC sources that are not in direct contact with the indoor environment, such as those present in the building envelope (e.g., rim joists, vapor barriers, and building insulation). Strongly varying temperatures and infiltration paths into the indoor environment may significantly affect the infiltration rate of SVOCs from the building envelope into the indoor environment.

THE IMPORTANCE OF MECHANISTIC MODELING FOR SOLVING KEY CHALLENGES

Mechanistic models have been identified as a critical element for addressing key challenges in exposure modeling.[21,25,77,78] Mechanistically consistent SECs are the basis of the proposed framework and allow modelers and users to identify relevant exposure pathways quantitatively, including assessments of uncertainty and parameter sensitivity. For modeling these pathways, mechanistic models with different levels of complexity are available and can be applied to derive exposure estimates, but gaps remain. Specific mechanistic model development needs for each SECs are listed in Table 1.

Factors influencing the complexity of modeling SVOC emission, transport and exposure in indoor environments include the following:

1. Assumption of quasi-instantaneous equilibrium or of dynamic, kinetically limited conditions;
2. Consideration of the influence of indoor environmental factors on model parameters, especially on partition coefficients (e.g., temperature, humidity, ventilation, size fractions of airborne particles, and source loading factor), and respective uncertainties;
3. Consideration of indoor chemistry, its effect on partitioning behavior, reactivity and subsequent exposure, and SVOC transformation products resulting from oxidation, hydrolysis, and other reactions; and
4. Influence of occupancy (e.g., in terms of surface soiling, dust resuspension, cleaning habits, and other occupant behavior) and occupant characteristics (e.g., age, sex, socio-economic status, variability of exposure factors) on exposure estimates.

Modeling of complex scenarios within indoor environments is a challenging task. There will always be a need to make assumptions, accept uncertainty, and adapt to new knowledge. However, modeling affords the opportunity to incorporate state-of-the art mechanistic understanding, evaluate the sensitivity to assumptions and data gaps, and to quantify uncertainty. As such, advancing exposure modeling approaches to appropriately reflect real-world conditions will increase transparency and confidence in exposure analyses and the resulting risk management decisions.

IMPLICATIONS AND RECOMMENDATIONS

The proposed framework integrates the current state of knowledge of SVOC exposure in indoor environments to advance chemical exposure assessment. Exposure science plays a crucial role in a fully integrated system of chemical risk assessment to inform and prioritize higher tier toxicity testing, describe and rank risks, and develop and evaluate models.[214–221]

The driving context for development of this framework was to facilitate efficient integration of exposure estimates derived using this framework with toxicity data for different end points and toxicokinetic mechanisms to accelerate chemical risk prioritization.[21,222,223] As an example of such an approach, Shin et al.[224] proposed a strategy to combine exposure estimates based on intake rates with toxicity data derived from ToxCast in vitro bioactivity assays, deriving bioactivity quotients (BQ) for HT risk ranking and prioritization. Another example can be found in Li et al.,[225] who used a dimensionless risk assessment factor (RAF), that is, the ratio of actual emission or application rate to a critical emission or application rate, to rank chemicals. The choice of metric depends on the respective research question and on the requirements of the risk assessment strategy.

More broadly, the proposed framework can be employed to inform chemical management decision contexts beyond rapid risk prioritization.[6,226] We envision this mechanistic exposure modeling framework to be developed and used as a community model available to better leverage ongoing research and inform chemical management decisions. Such a platform would enable further evaluation of the proposed framework through a continuous improvement process. This includes consideration of additional SVOC modeling and parameter estimation approaches, and of new empirical data as they become available. A common platform would also allow rapid and simple optimization of different components, depending on the user’s needs and the knowledge available. As work progresses, the source categories can be adjusted, VOC and aerosol emissions can be added, and indoor chemistry can be included. The Community Multiscale Air Quality (CMAQ) model[227–229] could serve as an example of how the framework can be developed, with open-source contributions from researchers worldwide and participation of relevant stakeholders.

Finally, understanding the health effects of exposures to chemicals has important implications for public health and also for more sustainable design and production of building materials and other indoor articles and products, which is especially relevant in a circular economy context.[230] Currently, chemical management authorities, regulators, and policy makers focus on evaluating risks from exposures to individual or groups of chemicals based on the properties of those chemicals. This approach rarely enables policy makers to link increased risk of public health outcomes to chemical management actions. As a result, chemical managers are challenged to anticipate impacts of chemical use and focus resources on addressing the most pressing concerns. A public health perspective, as described by Gwinn et al.,[231] starts with the health outcome of concern and incorporates multiple data streams to inform preventative policy decisions. The goal is to extend the scope of the considerations that support chemical management decisions and advance the tools for integrating this more complex information. Our framework can support this approach by informing design of exposure studies, facilitating interpretation of exposure data (i.e., chemical occurrence, biomonitoring and other exposomic measurements), and enabling risk assessments for environmental epidemiology studies. The proposed framework may therefore serve as the foundation for developing an open-source community model to better support collaborative research with improved access for application by stakeholders to advance effective chemical management decisions and protect public health.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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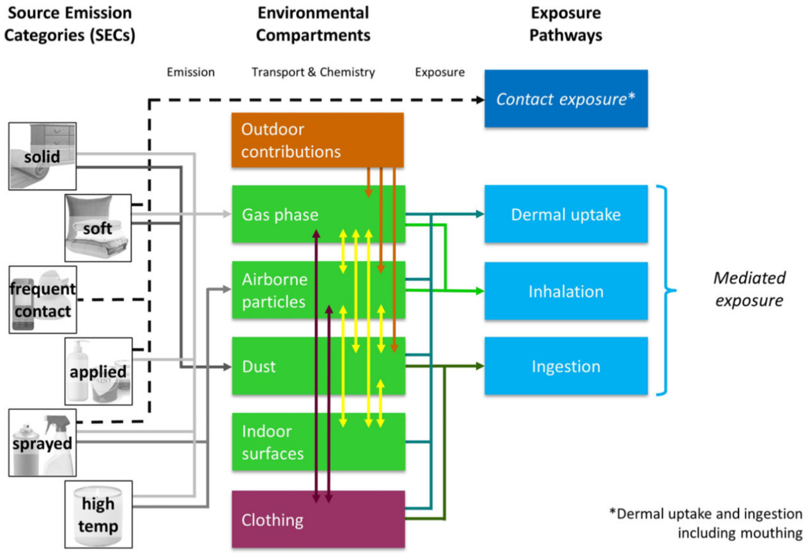

Figure 1.

A modular framework for modeling indoor SVOC emission, transport, chemistry and exposure.

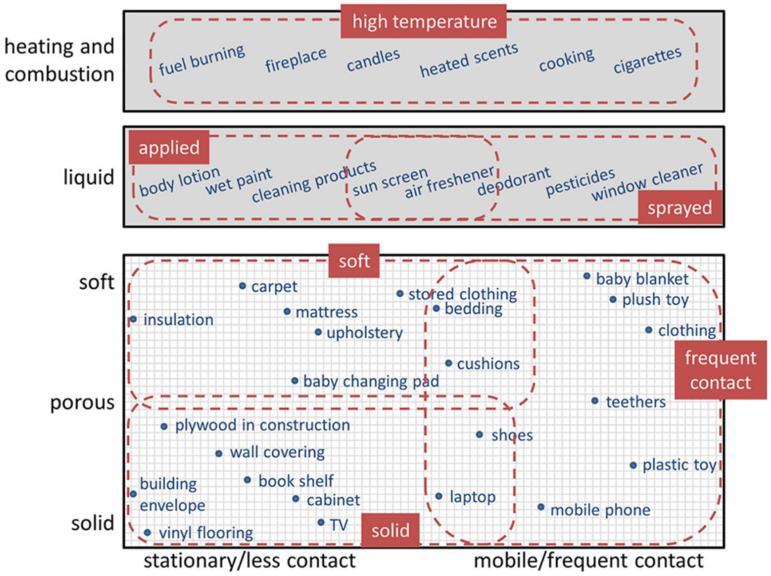

Figure 2.

Classification of source emission categories (SECs) from a continuum of possible sources, which range from solid to soft, from stationary to frequent contact, and including certain specific uses such as applied, sprayed, and heated/combusted.

Table 1.

Mechanistic Model Development Needs for Each Source Emission Category (SEC)

source emission category (SEC)	model development needs
solid, soft and frequent contact	• estimation of y_0 based on chemical structure, polymer characteristics and physicochemical properties for a broad range of SVOCs
applied liquid	• dynamic pulse emission model, slow release to the gas phase
sprayed liquid	• dynamic pulse emission model, pressure release to the gas phase
	• dynamic pulse emission model for release of airborne particles
high temperature	• dynamic pulse emission model for emission into the gas phase
	• dynamic pulse emission model for release of airborne particles
	• inclusion of chemical reactions and reaction products