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# Chemicals of Concern in Building Materials: A High-Throughput Screening

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## Abstract

Chemicals used in building materials can be a major passive emission source indoors, associated with the deterioration of indoor environmental quality. This study aims to screen the various chemicals used in building materials for potential near-field human exposures and related health risks, identifying chemicals and products of concern to inform risk reduction efforts. We propose a mass balance-based and high-throughput suited model for predicting chemical emissions from building materials considering indoor sorption. Using this model, we performed a screening-level human exposure assessment for chemicals in building materials, starting from product chemical composition data reported in the Pharos Building Products Database for the USA. Health risks and MAximum chemical Contents from High-Throughput Screening ($MAC_{HTS}$) were determined, combining exposure estimates with toxicity information. Exposures were estimated for >300 unique chemical-product combinations from the Pharos databases, of which 73% (25%) had non-cancer (cancer) toxicity data available. We identified 55 substances as chemicals of high concern, with actual chemical contents exceeding $MAC_{HTS}$ by up to a factor $10^5$, in particular diisocyanates and formaldehyde. This stresses the need for more refined investigations to select safer alternatives. This study serves as a suitable starting point for prioritizing chemicals/products and thus developing safer and more sustainable building materials.

## Keywords

Organic chemicals; Consumer products; Human exposure; Human health risk; MAximum chemical Contents from High-Throughput Screening ($MAC_{HTS}$)

# 1. Introduction

A wide range of chemicals is used in building materials, such as flooring, drywalls and ceiling panels, serving various functions. Examples include plasticizers to increase plasticity, flame retardants to prevent fire, adhesives to bind different components, stabilizers to keep components stable under heat or UV radiation, preservatives/biocides to prevent microbial growth, and many others. Chemicals used in building materials can be a major passive emission source in the indoor environment [1, 2], which has been associated with the deterioration of indoor environmental quality (IEQ) and the emergence of "sick building syndrome" [3]. Various green building rating and certification systems have been developed since the 1990s to maintain high IEQ by limiting the concentrations of hazardous chemicals [4]. However, evaluation studies and regulations have often focused on particular chemicals (e.g. VOCs, formaldehyde, lead) [4-9], while not covering the broad range of chemical substances that are used in building materials.

To assess the potential human exposures and risks for the thousands of chemicals used in building materials, high-throughput screening (HTS) has been identified as a promising approach [10-12]. Recent developments in the assessment of near-field exposures (i.e., exposures occurring near product users, mainly indoors) [11, 13-16] have provided approaches to consistently include product-chemical specific near-field pathways into high-throughput risk and impact assessment contexts. Previous studies have estimated screening-level exposure for hundreds of chemicals used in different consumer product categories to inform chemical prioritization [11, 17, 18]. However, these estimates come with limitations on the exposure side, such as lower-tier conservative or oversimplified assumptions that do not account for the mass-balance nature of competing chemical fate and transport processes. Thus, more refined exposure estimates are needed using more elaborate, mass balance-based, yet high-throughput suited models to cover the various chemical-product combinations.

Accurately predicting the evolution of chemical concentrations in building materials and related emissions forms the basis of estimating human exposures associated with these chemicals. Various models have been developed to simulate chemical emissions encapsulated in building materials [19]. The most widely accepted modeling framework is based on the diffusion of organic chemicals inside the building material, which was first presented by Little et al. [20]. In this framework, the governing equation describing the transient diffusion of chemicals through the building material is given by Fick's 2$^{nd}$ Law, where the emission is assumed to be driven by the concentration gradient between the material-surface boundary-layer and the bulk indoor air [20]. Chemicals released to indoor air can subsequently adsorb to airborne particles and various indoor surfaces, or they can be removed by ventilation [19-26]. Initial models require numerical solution of transcendental equations and calculation of the sum of infinite terms, which is computationally complex and hence not suited for HTS [27]. A recent study developed a parsimonious model for predicting a simplest scenario of chemical emissions from building materials, using simple algorithms and being applicable for a wide range of chemical-product properties [28]. However, this model does not consider sorption to indoor surfaces. Modifying

this model to include indoor sorption for better representing chemical emissions in realistic building materials would make it ideal for high-throughput purposes.

Building on these needs, the present study aims to propose a HTS approach for estimating emissions and related exposures and risks for a wide range of chemicals in building materials with the consideration of indoor sorption, highlighting products and chemicals of concern to inform further research and development. We focus on organic chemicals based on the applicability domain of current indoor emissions, transport and fate modeling approaches [15, 19, 29]. We thereby focus on four specific objectives:

(1) To characterize the product usage and chemical content in commonly used building materials;
(2) To develop a realistic mass balance-based, high-throughput suited modeling method that considers indoor sorption to predict chemical concentration evolutions in building materials and related chemical emissions;
(3) To estimate multi-pathway near-field human exposures for both adult and child building occupants for hundreds of chemical-building product combinations; and
(4) To screen and prioritize human health risks to identify products and chemicals of concern, and to determine maximum chemical contents ($MAC_{HTS}$), combining the high-throughput exposure estimates with toxicity information. Here we focus on the adults, since the exposure and risk estimates for an adult are more accurate and stable over the lifetime of building materials (assumed 15 years in the present study), while the exposure dose and risk for a child would vary over time due to varying developmental stages, behaviors and exposure factors as well as a growing body weight.

Resulting exposure and risk estimates for the many chemical-building product combinations as well as identified products and chemicals of concern may be used to inform decision makers and manufacturers to pinpoint relevant priority products/chemicals and focus future development of safer building materials.



# 2. Methods

## 2.1 Assessment framework

We propose a high throughput quantitative exposure and risk assessment approach for chemicals in building materials that uses the USEtox 3.0beta model [16] to determine Product Intake Fraction (PiF) [13, 15]. We successively determine the amount of chemical used in building product, the corresponding human exposure in mg/kg/d and the associated cancer risks and hazard quotients (Figure 1). This approach has already been applied to identify chemicals of concern in toys, personal care products, cleaning products, and household maintenance products [12, 30].

### *a) Chemical content in building product*

We first quantify the chemical mass of each substance *i* ($m_{i,p}$ , $kg_{chemical\ used}$/household) that is used in a specific building product *p* in a household over the entire building product lifetime:

$$m_{i,p} = M_p \times mf_{i,p} \quad (1)$$

Where $M_p$ ($kg_{product}$/household) is the amount of a building product used in a household, and $mf_{i,p}$ ($kg_{chemical\ used}/kg_{product}$) is the initial content, or mass fraction of chemical *i* in building product *p*. Values of these two parameters were obtained from several sources (see Section 2.2).

### *b) Consumer exposures*

Second, we capture the multi-pathway fate processes transferring chemicals between compartments in the near- and far-field environments, until finally reaching humans. Near-field exposures refer to the exposures occurring within the vicinity of the use of a considered product, which typically include indoor exposures, while far-field exposures refer to the exposures to outdoor environmental media such as ambient air, drinking water and soil [15]. Multimedia chemical mass transfers are structured in a matrix of direct inter-compartmental transfer fractions [15]. By matrix inversion, we obtain cumulative transfer fractions and exposure route-specific (*x*: inhalation, ingestion, dermal) product intake fractions (PiFs). PiF is defined as the chemical mass taken in via multiple exposure pathways *e* (e.g. dust ingestion, dermal contact) by exposed humans *h* ($I_{i,p,h,e}$, $kg_{intake}$/household) per unit mass of chemical in a product [13]: $PiF_{i.p,h,x} = \sum_{e \in x} I_{i,p,h,e}/m_{i,p}$, ($kg_{intake}/kg_{chemical\ used}$) over a given exposure period. The present study focuses on the near-field exposures to chemicals in building materials which include inhalation of indoor air, dermal gaseous uptake of indoor air, dermal contact and dust ingestion. The calculation of direct transfer fractions for these near-field exposures are detailed in Section 2.3.

Combining PiFs with chemical mass in the product, and dividing by the number of exposed humans *h* in the household or in the background population ($N_h$, persons), a human body weight ($BW_h$, $kg_{BW}$/person) and the exposure duration considered when determining the PiF ($\Delta t$, d) yields individual intake doses for exposure route *x* ($D_{i,p,h,x}$, mg/$kg_{BW}$/d) as exposure estimates:

$$D_{i,p,h,x} = \frac{m_{i,p} \times PiF_{i,p,h,x} \times kg\_to\_mg}{N_h \times BW_h \times \Delta t} \quad (2)$$

The exposure duration is determined by the effective lifetime of a product in the building and is assumed 15 years for the present paper.

### *c) Risk characterization*

In the third step, we assess the risks associated with each of the chemical-building product combinations, combining exposure doses with toxicity data. First, carcinogenic risks ($R_{i,h}$, in probability of developing cancer for a lifetime exposure of user *h* via route *x*) are calculated by multiplying the exposure dose by a route-specific cancer slope factor ($CSF_{i,x}$, in incidence/(mg/$kg_{BW}$/d)):

$$R_{i,p,h} = \sum_x D_{i,p,h,x} \times CSF_{i,x} \quad (3)$$

This risk probability can be compared to the defined acceptable incremental lifetime cancer risk of $ILCR_{ref}$ =$10^{-6}$ for the general population or of $10^{-4}$ for occupational exposure settings [31]. Non-carcinogenic effects are characterized by dividing the route-specific exposure dose by a route-specific reference dose ($RfD_{i,x}$, mg/$kg_{BW}$/d) to yield a hazard quotient ($HQ_{i,p,h,x}$) for each route; then a hazard index ($HI_{i,p,h}$) is calculated by summing the HQ from all exposure routes.

$$HQ_{i,p,h,x} = D_{i,p,h,x}/RfD_{i,x} \quad (4a)$$

$$HI_{i,p,h} = \sum_x HQ_{i,p,h,x} \quad (4b)$$

The HQ or HI is not a risk, since HQ is a ratio of two doses, but a HQ (or HI) > 1 (exposure dose higher than reference dose) indicates potentially harmful chemicals that require further scrutiny. The sources for the cancer slope factors and references doses are described in Section 2.4.

We then estimate the MAximum chemical Contents based on our High-Throughput Screening results ($MAC_{HTS}$) for the studied chemical-building product combinations. Based on the above-described risk criteria, we define $MAC_{HTS}$ as the content of a chemical in a building product, which results in a reference hazard index $HI_{ref}$ = 1 or $ILCR_{ref}$ = $10^{-6}$. $MAC_{HTS}$s for cancer and non-cancer effects are back-calculated from the exposure and toxicity results, and the minimum $MAC_{HTS}$ between cancer and non-cancer effects is retained as the final $MAC_{HTS}$.

$$MAC_{HTS,\,\text{non-cancer}} = mf_{i,p} \times \frac{HI_{ref}}{HI_{i,p,h}} \quad (5a)$$

$$MAC_{HTS,\,\text{cancer}} = mf_{i,p} \times \frac{ILCR_{ref}}{R_{i,p,h}} \quad (5b)$$

$$MAC_{HTS,\,\text{final}} = \min(MAC_{HTS,\,\text{non-cancer}}, MAC_{HTS,\,\text{cancer}}) \quad (5c)$$

### *d) Identification of chemicals of concern*

We finally define the hazard content ratio (HCR) as the actual mass fraction of chemical in a building product divided by the minimum $MAC_{HTS}$:

$$HCR = \frac{mf_{i,p}}{MAC_{HTS,\,\text{final}}} \quad (6)$$

The chemical-product combinations with HCR > 10 are identified as chemical of higher concern to be further scrutinized in priority, whereas chemicals with HCR between 1 and 10 might also deserve attention. These chemicals of higher concern therefore correspond to hazard index >10 or incremental lifetime cancer risk >$10^{-5}$.

## 2.2 Chemicals composition and usage of building products

Data on the chemical composition of building products are obtained from the Pharos Building Product Library (www.pharosproject.net), which is a database that integrated building products from different manufacturing companies to provide information on the hazard as well as the chemical composition within each product. This database primarily represents building products in the USA. The Pharos database has two versions due to a major reconstruction in 2018: the Common Products Database provides information on 142 common products, characterizing the typical chemical compositions found within a product type, while the individual Products Database contains chemical composition information on 1604 individual branded building products. These two versions are analyzed separately: Each of the 1604 individual products are matched to one of the 142 common products to define the

usage and product properties (see below). Cleanup of both databases are then performed to exclude products used outdoors or underground, or products with unclear usage and properties (resulting in 80 products); Inorganic chemicals, organometallics, mixtures, and substances of unknown or variable composition, complex reaction products and biological materials (UVCBs) are excluded from further analysis. We aggregated the multiple occurrences of a given chemical-product combination that can appear in different components of the same product or serve different functions in the same product combination by summing the chemical contents when assessing exposure and risk. This results in 325 unique chemical-product combinations in the Pharos Common Products Database, and 495 chemical-product combinations in the Pharos Individual Products Database.

For each non-polymer chemical-product combination in the Common Products Database, we use the single average reported chemical content in Pharos to calculate a single chemical content, for example a content of 1.12% for ethylbenzene in Elastic Facade Joint Sealant. For polymers, the polymerized material is considered stable and does not lead to any emissions and exposures. However, we take into account for each polymer a small fraction of residual free monomers that is available for migration and emission. When available in the literature [28-39], polymer-specific ranges of residual monomer in the building product (min and max) are identified; for example, the content of styrene monomer in XPS insulation is between 0.0008% and 0.28%. For the remaining polymers, a residual monomer content ranging from 450 ppm to 2900 ppm is assumed, based on the maximum reported range in the collected references. The content of residual monomer for each polymer material is provided in Appendix A, Section A1.1. In the Individual Products Database, an average possible content is also calculated for chemicals other than residual monomers; for example, dibutyl phthalate in a wood flooring has an average content of 0.03%, while for residual monomers a range (min and max) is also applied to the average content of the corresponding polymer. Detailed explanations of the databases and chemical content calculations are provided in Appendix A, Section A1.1, where maximum possible contents for chemicals in the Individual Products Database are also presented.

For the 80 common building products, we quantify the amounts used in a typical household, by determining the product application area, thickness and density (e.g., vinyl flooring has an area of 96.8 $m^2$, a thickness of 3 mm and a density of 1500 kg/$m^3$), which are detailed in Appendix A, Section A1.2 and Appendix B.

## 2.3 Estimating exposures to chemicals in building products

The first step towards calculating product intake fractions is to determine the relevant direct transfer fractions from building products to indoor air, to human skin via dermal contact, and to the gastrointestinal tract via hand-to-mouth dust ingestion. The direct transfer from building products to indoor air will subsequently lead to inhalation and gaseous dermal exposure. Section 2.3.1 describes the models used to estimate the chemical emissions from building products and chemical concentration at the building product surface. The models for estimating human exposures are presented in Appendix A, Section A3, which include inhalation exposure, dermal exposure by dermal contact, dermal exposure by gaseous uptake, and ingestion exposure by hand-to-mouth activities. The direct transfer fractions for human exposures are calculated using the intake via a specific exposure pathway divided by the

chemical mass in the initial considered compartment (i.e., indoor air for inhalation and dermal gaseous exposures, building product itself for dermal contact and dust ingestion exposures) (Section A3).

### 2.3.1 Models for chemical emissions and surface concentrations

***Existing models***

Models for chemical emissions and surface concentration follow the widely accepted diffusion theory [19]. The simplest model setup [24, 28] assumes that 1) the chemical emission from the building material is driven by its transient diffusion inside the material; 2) the chemical is emitted from the top surface of the material, while the material bottom is impervious; 3) chemicals emitted to indoor air are only lost by ventilation while sorption to indoor surfaces is not considered; 4) chemicals adsorbed on airborne particles are in equilibrium with the gas phase; 5) the indoor air is well mixed; and 6) the air flowing into the house is clean. The two key parameters of this model are the chemical's diffusion coefficient in building material $D_m$ ($m^2/s$) and the chemical's building material-air partition coefficient $K_{ma}$ (dimensionless). The detailed equations and analytical solutions of this model are provided in Appendix A, Section A2.1.

Since the analytical solutions are complex and computationally intensive, we developed in a previous study a simplified, high-throughput suited model that can well approximate the analytical solution for a wide-range of chemical-product properties [28], which is called a "**combined D- and K-limited model**". Briefly, chemical-product combinations are classified as two types: diffusion limited (D-limited) and partition limited (K-limited), based on defined criteria in Eq. 7:

$$\begin{cases} \text{D-limited: } 0.61 \cdot \log D_m + \log K_{ma} < -0.40 \quad or \quad K_{ma} < 0.4 \cdot {D_m}^{-0.61} \\ \text{K-limited: } 0.61 \cdot \log D_m + \log K_{ma} \geq -0.40 \quad or \quad K_{ma} > 0.4 \cdot {D_m}^{-0.61} \end{cases} \tag{7}$$

For both D-limited and K-limited cases, the chemical mass fraction emitted from building material to indoor air from time zero to time $t$ ($TF_{ma}$) can be expressed in the form of two exponentials:

$$TF_{ma} = \frac{m_e(t)}{m_0} = a_1 \cdot e^{b_1 t} + a_2 \cdot e^{b_2 t} + a_0 \tag{8}$$

where $m_e(t)$ is the total chemical mass emitted to air from time zero to time t (μg), $m_0$ is the total chemical mass in building material at time zero (μg), $t$ is time (s), $a_1$, $a_2$, $a_0$, $b_1$, $b_2$ are coefficients that are calculated as functions of convective mass-transfer coefficient $h_m$ (m/s), room ventilation rate $Q$ ($m^3/s$), area of the building material $A_m$ ($m^2$), thickness of building material $L_m$ (m), as well as $D_m$ and $K_{ma}$. Details of the D-limited and K-limited models are described in Appendix A, Section A2.1.2.

***Development of a refined model with sorption to indoor surfaces***

The above-described models only consider one diffusional source of the chemical at a time (i.e., the building product that contains the chemical), and assume that chemicals emitted to indoor air will only be lost by ventilation. However, chemicals in indoor air can also adsorb on various indoor surfaces, which represents a chemical sink [19, 32]. This sorption is especially important for semi-volatile organic compounds (SVOCs) [19, 32]. Thus, we propose a more refined model that considers the sorption to indoor surfaces, adapting the K-limited simplified model to include sorption and verifying it against a numerical model.

***Full model with sorption to indoor surfaces***

This refined model considers the indoor surfaces as a single diffusional sink, which follows the same governing equation and boundary conditions as the diffusional source. For the initial condition, we assume that the chemical concentration in the sorption material is zero. The equations for the refined model system are presented in Appendix A, Section A2.2. The analytical solution for such a model system is very complex [33], so a numerical solution is more practical. We solved it numerically using the Method-of-Lines (MOL) technique and uneven discretization, as described in Huang et al. [28] and details provided in Appendix A, Section A2.2.1. This numerical solution, called "Full numerical model", provides a close-to-exact solution that can be used as a comparison reference for the simplified models described below.

***Simplified model with sorption to indoor surfaces***

For the simplified model, sorption effect is negligible for the D-limited case, so the D-limited model can be directly used. However, for the K-limited cases, sorption is significant and cannot be ignored, so we propose the following modified model. For the K-limited case, we assume that the chemical remains evenly distributed inside the building material and in the sorption material, i.e., no concentration gradient through the materials. The mass balance equations are as follows:

$$\frac{dm_m(t)}{dt} = -\left(\frac{m_m(t)}{A_m L_m}/K_{ma} - \frac{m_a(t)}{V\cdot(1+K_{pa}\cdot TSP)}\right)\cdot h_m A_m \quad (9a)$$

$$\frac{dm_s(t)}{dt} = \left(\frac{m_a}{V\cdot(1+K_{pa}\cdot TSP)} - \frac{m_s}{A_s L_s}/K_s\right)\cdot h_s A_s \quad (9b)$$

where $m_m$ is the chemical mass in building material (μg), $m_s$ is the chemical mass in the sorption material (μg), $A_s$ is the area of sorption surfaces ($m^2$), $L_s$ is the thickness of indoor material (m), $K_s$ is the chemical's sorption material-air partition coefficient (dimensionless), $h_s$ is the convective mass-transfer coefficient on the sorption surfaces (m/s).

For the mass balance in the indoor air, since the kinetic of the indoor air is much faster than the kinetic from the emitting and adsorbing surfaces, it equilibrates between these compartments and we thus assume a quasi-steady-state condition for the chemical in the indoor air. Detailed deviation and solution of the K-limited model with sorption are presented in Appendix A, Section 2.2.2.

The D-limited model and the K-limited model with sorption are evaluated by comparing the predicted air concentration to measured values of DEHP in chamber test studies [21], as detailed in Appendix A, Section 2.2.3.

***Criteria for selection of the simplified model and evaluation process***

Criteria are needed to classify chemical-building product combinations as D-limited or K-limited with sorption. We apply the criteria in Eq. 7 which were originally developed for models without sorption, and test their validity by comparison to the numerical solution of the full model with sorption "Full numerical model". The detailed test protocol is described in Appendix A, Section A2.2.4. Briefly, we evaluate the ratio of the mass fraction emitted at the end of simulation between the simplified model with sorption and the numerical solution. Two sets of chemical-product combinations are tested: one is a hypothetical dataset with 10,000 $D_m$-$K_{ma}$ combinations, and the other includes the 325 and 495

resulting chemical-product combinations in the Pharos Common Products Database and Individual Products Database, respectively.

### 2.3.2 Model parameterization

The physiochemical substance properties, building product properties, indoor configurations and exposure factors used to parameterize the models are described in Appendix A, Section A4. Briefly, we model an average residential house in OECD countries, which has 2 adults and 1 child of 2-3 years old as occupants. The house volume is 236 $m^3$ and the air exchange rate is 0.79 $h^{-1}$. 15 years is assumed as the product lifetime for all building products.

## 2.4 Toxicity data for risk characterization

Details of toxicity data are presented in Appendix A, Section A5. Briefly, cancer slope factors (CSFs) for adults are taken from USEtox 2.12 (http://www.usetox.org), and for children we apply an age-dependent adjustment factor (ADAF = 4) to the CSF [30]. The ingestion reference doses (RfD) and inhalation reference concentrations (RfC) are obtained from various databases, and when not available, they are estimated by the *in silico* conditional toxicity value (CTV) predictors if they are within the applicability domain [34]. Dermal CSFs and RfDs are assumed to be the same as the ingestion ones.

# 3. Results and Discussions

## 3.1 Validity of the simplified model with sorption

As detailed in Appendix A, Section A6.1, the simplified model with sorption can accurately predict the air concentration of DEHP from vinyl flooring in two test chambers [21], demonstrating its validity. Figure 2 compares the emitted mass fractions calculated by the simplified model with sorption, with the results of the numerical solution of the model with sorption, using both Pharos datasets for a simulation time of 15 years. The simplified model agrees almost perfectly with the numerical solution for these real chemicals with a material thickness of 100 mm, and its performance is even better with smaller material thicknesses (Appendix A, Section A6.2 Figure A4). For the 325 (495) unique data points of Common Products (Individual Products) combining D- and K-limited cases, the simplified model yields a $Q^2$ of 0.995 (0.991) and a standard error on the log of 0.052 (0.072), indicating that the 95% CI of the predicted mass fraction emitted is within a factor of 1.26 (1.39) from the model prediction. More detailed statistics by chemical function are provided in Appendix A, Section A6. Results predicted by the D-limited and K-limited portions of the simplified model are mostly of similar accuracy, except that the simplified model slightly overestimates the mass fraction emitted by maximum a factor of 2 for certain K-limited cases (Figure 2 B&D). These results demonstrate that the refined simplified model can well approximate the numerical solution for chemical emissions from building materials with indoor sorption. Considering this with the ease of use and parametrization of that model, the refined simplified model is a preferred method for high-throughput purposes, and is thus used to analyze the Pharos data in the

subsequent results. The simplified model with sorption is further compared to the numerical solution for a wider set of condition using 10,000 hypothetical chemicals for two building material thicknesses and two simulation times, again demonstrating its suitability for high-throughput screening (Appendix A, Section A6.2 Figure A3).

## 3.2 Overview of chemicals in building products

Figures 3A-B present an overview of the reported chemical mass fractions in products and the representative product mass per household for the Pharos Common Products Database (abbreviated as CPD). For the residual monomers, only the maximum mass fractions are presented. Chemical mass fractions in building products span several orders of magnitude. For chemicals other than residual monomers, the mass fractions range over 5 orders of magnitude, from $2.7\times10^{-6}$ for Imidacloprid in Exterior door to 0.20 for Butyl benzyl phthalate (BBP) in Elastic façade joint sealant. Higher chemical mass fractions (i.e., >10%) are mostly associated with plasticizers and flame retardants. For residual monomers, the mass fractions range from $1.9\times10^{-10}$ to 0.055. The mass of building product used varies by 6 orders of magnitude, from 0.43 kg of Concrete cork expansion joint to 24,500 kg of Concrete masonry unit per household, indicating large differences in the usage of different building products.

The Individual Products Database (abbreviated as IPD) shows similar patterns (Appendix A, Section A8). Briefly, the average possible mass fractions range from $1.7\times10^{-6}$ to 0.17 for non-residual monomers and from $2.6\times10^{-9}$ to $3.4\times10^{-3}$ for residual monomers, with the highest mass fraction associated with Bis(2-ethylhexyl)terephthalate (DEHT) in Carpet flooring. Chemicals with mass fractions higher than 10% mostly include plasticizers, solvents, blowing agents and flame retardants. The variation in product mass is smaller, ranging from 290 kg to 2,933 kg, since the IPD does not include products used in small quantities such as joint, sealant, adhesive, etc.

## 3.3 Exposure and risk from chemicals in building products

Figures 3C-F present the total mass of chemical used and the resulting adult exposure and health risk for the CPD, ranked according to increasing daily exposure dose summing all exposure routes. The exposure and risk results for a child occupant of 2-3 years old are provided in Appendix B.

Multiplying the chemical mass fraction by the mass of building product (Figure 3A-B) yields the initial chemical mass in each CPD building product in the considered household (Figure 3C). Used chemical mass in CPD ranges widely from $10^{-7}$ to 100 kg per household. Higher chemical mass is generally associated with blowing agents, plasticizers, and flame retardants. The highest chemical mass applied in CPD (113 kg) is for Tris(1-chloro-2-propyl)phosphate (TCPP), a flame retardant, in spray polyurethane foam, due to a relatively high chemical mass fraction (11%) and a large product mass (1,009 kg).

Figure 3D left axis presents for each chemical-product combination the total product intake fractions (PiFs, in $kg_{intake}/ kg_{used}$) summing all exposure routes, which represents the cumulative chemical mass taken in ($kg_{intake}$) by adult occupants per kg chemical initially present in the considered building product. The total PiFs range from $8.9\times10^{-10}$ to 0.12 across the 325 unique chemical-product combinations in CPD.

Combining PiFs with the corresponding initial chemical mass in product and exposure duration yields the average daily exposure doses per adult occupant, as presented in Figure 3D right axis, with the relative contribution of each exposure route presented in Figure 3F. Inhalation is the dominant exposure route for 64% of the cases, while dermal exposure, especially dermal gaseous uptake for high doses, is dominant for most of the remaining cases. Dust ingestion exposure is only important for 2 cases. However, for the child occupant, dust ingestion dominates the exposure for 7 cases, most of which are plasticizers. In CPD, the highest exposure dose of 1.12 mg/kg/d occurs for Benzyl alcohol in Fluid-applied flooring, dominated by dermal gaseous uptake. Our estimated doses are generally comparable to the daily intake back-calculated from biomonitoring studies. For example, the estimated dose for DEHP in vinyl flooring and carpet flooring is 1.85 and 0.98 μg/kg/d, respectively, which are well within the range of the back-calculated dose for USA populations (median of 0.6 – 2.2 μg/kg/d, $95^{th}$ percentile of 3.1 – 16.8 μg/kg/d) [35]. The comparison for other phthalates can be found in Appendix A, Section A10.

Finally, the ratio of the estimated exposure doses divided by reference doses for non-cancer effects, and aggregated across exposure routes yields a single hazard index (HI) per chemical-product combination (Figure 3E, left axis). In CPD, we find the highest HI of 1,950 for 1,6-Hexamethylene diisocyanate (HDI) in Acrylic flooring adhesive, which is mainly contributed by inhalation (43%) and dermal gaseous uptake (56%). Out of 244 chemical-product combinations with toxicity data, 29 (12%) have HI>1. The right axis of Figure 3E displays the estimated incremental lifetime cancer risks (ILCRs), showing that for the chemicals with available cancer toxicity data, about half (43 out of 89 unique chemical-product combinations) have estimated ILCRs>$10^{-6}$, suggesting non-negligible cancer risks, most of which are associated with residual monomers.

A more detailed view of exposure and toxicity results per exposure route and effect type are presented in Appendix A, Figure A4. As a general trend, inhalation exposure is the main contributor to both non-cancer and cancer effects, while dust ingestion is negligible for most cases. Note that dust ingestion becomes more important for several plasticizers when a child occupant is considered, which is more obvious in the results for Pharos IPD (Appendix A Section A8 and Appendix B). For non-cancer effects, an inhalation HQ > 1 was estimated for 20 chemical-product combinations out of 244 in CPD, and of which only 1 with inhalation HQ > 100 (HQ = 839). A dermal HQ > 1 was estimated for 16 chemical-product combinations and only one has dermal HQ > 100 (HQ = 1110). For cancer effects, 13 and 1 chemical-product combinations have estimated ILCR > $10^{-4}$ for inhalation and dermal exposures, respectively, potentially indicating very high concern on cancer effects.

Results for the IPD show similar patterns and are presented in Appendix A, Section A8, with 32% of chemical-product combination with HI>1 and 75% with ILCRs>$10^{-6}$. Detailed exposure and risk results for adult and child occupants for CPD and IPD are provided in Appendix B.

## 3.4 Identified chemicals of higher concern (CoCs) and maximum chemical contents ($MAC_{HTS}$)

The chemical-product combinations with a calculated HCR>10, identified to be of higher concern (or CoCs), are presented in Table 1. Again, this prioritization focuses on the exposure and risk results for

adult occupants, as explained in the Introduction. A total of 55 chemicals of concern were identified, each associated with one or more types of building products (Table 1). The chemicals are ranked by decreasing maximum HCR across all building products, indicating decreasing concern. Figure 4 details the actual chemical mass fractions in products, cancer and non-cancer $MAC_{HTS}$ and HCRs of the 55 identified CoCs. In addition, Appendix B provides the full list of chemicals considered, including chemicals with HCR between 1 and 10 that might also deserve attention.

Note that these $MAC_{HTS}$ and HCRs are calculated using an air exchange rate of 0.79 $h^{-1}$ which represents an average residential house in OECD countries. However, as ventilation is one of the primary loss mechanisms for chemicals indoors, especially for volatile chemicals, variation in the air exchange rate can significantly affect the $MAC_{HTS}$ and HCR. As the air exchange rate increases, the $MAC_{HTS}$ would increase and the corresponding HCR would decrease, which is more prominent for VOCs since inhalation is the dominant exposure pathway for these chemicals. The relationship between air exchange rate and $MAC_{HTS}$ as well as HCR is presented in Appendix A, Section A11. Thus, in practical applications the maximum chemical contents need to be adjusted according to the actual house configurations and may differ from the values in Table 1.

It should also be noted that the $MAC_{HTS}$ values reported here are based on the results of a high-throughput screening of exposure and risk. This high-throughput screening aims to represent a realistic but also pragmatic chemical/product usage and exposure scenarios, which does not necessarily represent conservative or worst-case assumptions. Thus, the $MAC_{HTS}$ values are intended to be used for comparative assessments between chemicals and providing tentative reference values for future product design. The $MAC_{HTS}$ should not be taken as substitutes for regulatory limits of chemical contents in products.

*Diisocyanates*

The results for the two diisocyanates HDI (1,6-Hexamethylene diisocyanate) and MDI (Methylene bisphenyl diisocyanate) indicate great concern as they rank 1$^{st}$ and 4$^{th}$ in Table 1, with hazard content ratios (HCRs) ranging from 30 to 244,000 for HDI and 60 to 4,000 for MDI, the variation between application being primarily linked to variation in actual chemical mass fraction in the different products (Figure 4A). These two chemicals have no carcinogenic data, MDI being classified as Group 3 (Not classifiable as to its carcinogenicity to humans) by the International Agency for Research on Cancer (IARC). However, very low non-cancer inhalation RfCs ($10^{-5}$ mg/m$^3$ for HDI and $6\times10^{-4}$ mg/m$^3$ for MDI) are reported by IRIS. This means that even when only considering inhalation, HDI and MDI still greatly exceed the risk criteria of the current analysis . Since no ingestion and dermal RfDs are reported, these are assumed equal to the inhalation RfC-derived RfDs. This may represent high-end toxicity estimates, considering that dermal exposure (especially dermal gaseous uptake) is as high as or even higher than inhalation exposure for HDI and MDI.

MDI is generally used to react with polyols (organic compounds containing multiple hydroxyl groups) to form polyurethanes [36]. Spray polyurethane foam systems with unreacted MDIs have been identified by the California EPA as a priority product [36], and the U.S. EPA has issued an action plan for MDI and related compounds [37]. However, after the reaction with polyols is completed, MDIs as a residual monomer in cured polyurethane foams are at ppm levels [38], which do not pose a significant health risk

to building occupants based on our calculations. The cases we identified as of concern are MDI in various flooring and composite wooden boards with mean mass fractions ranging from 0.09% to 10%, for which no clear function was indicated in Pharos IPD. If these MDIs are in fact polymer precursors and would be polymerized when being applied in the house, the health risks for building occupants would be greatly reduced. Nonetheless, the determination of $MAC_{HTS}$ enables to back-calculate independent targets to compare with actual chemical contents, indicating that the free MDI mass fraction should not exceed 10 ppm in flooring products and 20 ppm in wooden furniture to remain below the risk criteria of the current analysis (Table 1).

For HDI, its exposure and risk have been studied for decades, but mainly in occupational settings [39-42]. The HDI reported in Pharos CPD occurs in Acrylic flooring adhesive as a crosslinker and has relatively high mass fraction (1.4%), while the HDI in Pharos IPD was reported in various flooring products with unknown function and mass fractions ranging from 10 ppm to 5%. The highest HCR is for HDI in carpet flooring with relatively high mass fraction (5%) and product mass (774 kg). Similar to MDI, if the HDI would polymerize when the building products are applied, the calculated health risks would be greatly reduced. To meet the calculated $MAC_{HTS}$ , the HDI mass fraction should not exceed 0.2 ppm in carpet flooring, 7 ppm in acrylic flooring adhesive, and 0.1 ppm in wood, cork, and vinyl flooring (Table 1).

*Formaldehyde*

Formaldehyde is identified as a CoC in many different building products with HCRs up to 52,000 (Table 1, Figure 4B), all based on cancer effects, indicating extremely high cancer risk potential from exposure to formaldehyde in building products. Formaldehyde is a well-known carcinogen, and its emission from building materials has been extensively studied [5, 7, 43, 44]. It can be used as a preservative/biocide in wood products, drywall, and water-based paints. Formaldehyde can also occur as a residual monomer in various polymers, such as urea formaldehyde (UF), phenol formaldehyde (PF) and melamine-urea-formaldehyde (MUF) resins, which are important binders used in composite wood products. The estimated cancer risks for formaldehyde used as a preservative in IPD products are very high, especially for several wood and drywall products with ILCR > $10^{-2}$, due to relatively high mass fractions (0.08% to 0.35%), product mass (881 to 2933 kg), and the high cancer slope factor. Formaldehyde as a residual monomer poses lower cancer risk due to the lower mass fractions, but still exceeds the calculated $MAC_{HTS}$ by several hundred times.

Our estimates of formaldehyde contents in and emission from building materials are consistent with previous studies, with details presented in Appendix A, Section A9.1. However, there is an uncertainty in the carcinogenicity of formaldehyde, for which we used the inhalation CSF of 2.17 $(mg/kg/d)^{-1}$ from USEtox that is 38 times higher than the CSF from U.S.EPA's IRIS (Appendix A, Section A9.1). As a result, the carcinogenicity of formaldehyde may be a high-end estimate in the present study, but cancer risk from formaldehyde in building products would remain high and well above the $10^{-6}$ limit even if the IRIS toxicity data are used. In addition, there could be non-linearity in the carcinogenic effect of formaldehyde as suggested by the WHO [45], which may also lead to lower estimates of the lifetime cancer risk.

As indicated in Table 1, the free formaldehyde content should not exceed 30 to 80 ppb in building products applied in large quantities, such as furniture, base cabinetry, flooring, gypsum wallboard and

ceiling, and foam insulation when using the USEtox CSF to remain below the risk criteria of the current analysis (or 1 to 3 ppm using IRIS data). The free formaldehyde contents in hollow core wood doors and carpet can be slightly higher, at 100 ppb (or 4 ppm using IRIS data), while the contents in countertops and sealants can go up to 5 ppm (or 190 ppm using IRIS data). However, since formaldehyde generally occurs in more than one building products, which would result in aggregate exposure, the presented results suggest that it is better to keep formaldehyde below 30 ppb (or 1 ppm using IRIS data) in all building products. The actual formaldehyde residual monomer contents reported by Pharos are far larger than this limit, around 10 to 100 ppm in various building products. This indicates that manufacturers would need to lower the free formaldehyde content by 1000 to 10,000 times (or 30 to 300 times using IRIS data) in formaldehyde-related resins to remain below the calculated $MAC_{HTS}$, which is difficult to achieve with current technologies. This suggests that usage of formaldehyde containing resins may need to be completely avoided in building materials. In addition, the results of the analysis suggest that manufacturers should avoid using formaldehyde as a preservative and consider less toxic alternatives in building products. Our analysis, for example, indicates that several preservatives/biocides reported in Pharos, such as thiabendazole, methylchloroisothiazolinone (CIT, CMIT), carbendazim, and chlorothalonil used in flooring, paint and sealant products result in HCRs from 0.0036 to 0.16 and thus much lower human health risks than formaldehyde, which could be potential alternatives.

*Other residual monomers*

Based on the screening results, 10 other residual monomers are identified as CoCs, all based on cancer effects (Table 1). Note that the residual monomers have wide ranges of HCRs because the calculations consider the ranges of residual monomer contents in polymer materials. The highest HCRs of 200 to 3,200 are calculated for ethyleneimine (Aziridine). The other residual monomers include 2-chloro-1,3-butadiene, oxirane, 1,3-butadiene, melamine, vinyl chloride, n-methylol acrylamide, acrylonitrile, 2-methyloxirane (Figure 4C), and styrene (Figure 4B). Except for the first 3 monomers in the list, these monomer chemicals result in limited risk levels according to our calculations (HCR < 10 in Table 1) if minimum monomer contents are used, but would exceed the $MAC_{HTS}$ by up to a factor 400 if maximum contents are used. Since we did not find any information on reported monomer contents for the first 3 monomers in the list, we assumed a minimum of 0.045% and a maximum of 0.29%. More accurate risk estimates are needed, but our results suggest that a residual monomer content of 0.045% of these three compounds would still be of concern. Based on calculated $MAC_{HTS}$ ,these monomer chemicals should not exceed for example 10 ppm for styrene in insulation and 0.6 ppm for vinyl chloride in flooring (Table 1), which could serve as a tentative reference for manufacturers of building products..

*Solvents*

Our calculations also indicate that another important group of CoCs is solvents (Figure 4D), which includes 13 chemicals such as Ethyl carbamate, N-Methyl-2-pyrrolidone, Diethylene glycol, Ethylene glycol monobutyl ether (EGBE), 2-(2-butoxyethoxy)ethanol, and Ethylbenzene in various flooring, insulation and ceiling products, of which the screening results for Ethyl carbamate in flooring indicate an extremely high HCR of 58,000 to 140,000 based on cancer effects and ranks 2$^{nd}$ in Table 1. Ethyl carbamate is a by-product in food fermentation process and its presence in various food products including alcoholic beverages, soy sauce and other fermented foods has been widely studied [46-48]. It

is reported to be used as a solvent in flooring with mass fraction ranging from 1.4% to 10%, leading to very high cancer risks in the screening results. Due to its high toxicity and the large product mass of flooring, ethyl carbamate in flooring should not exceed 0.2 ppm to remain below the risk criteria of the current analysis. However, since ethyl carbamate is found in various food products, food ingestion is likely the predominant exposure pathway for this chemical compared to exposure to ethyl carbamate embedded in a flooring. The other solvent chemicals are discussed in Appendix A, Section A9.2.

*Plasticizers*

Based on our calculations, only one phthalate plasticizer BBP is identified as CoC in Table 1 and Figure 4E, mostly in vinyl and carpet flooring, and all based on cancer effects. However, results for two other plasticizers Diisononyl phthalate (DINP) and Di-(2-ethylhexyl) phthalate (DEHP) indicate moderate concern with HCRs around 9 (Appendix B). The $MAC_{HTS}$s for BBP, DINP and DEHP in flooring are 60 ppm, 0.4% and 0.4%, respectively. These suggested maximum contents are too low for the plasticizers to fulfill their function in flooring products, since the contents of plasticizers generally need to be higher than 1% to make the plastics flexible. Therefore, our results indicate that these three plasticizers in vinyl and carpet flooring should be replaced by less toxic alternative plasticizers. Several other plasticizers, such as bis(2-ethylhexyl)terephthalate (DEHT), dipropylene glycol dibenzoate, diisoheptyl phthalate (DIHP), are not identified as of concern due to lack of toxicity data, which do not implicate that they are safe but instead call for more toxicity data to better evaluate these chemicals.

As mentioned in Section 3.3, dust ingestion exposure becomes important for plasticizers for the child occupant. Thus, when considering the child occupant, several plasticizers become of concern due to increased exposure via dust ingestion. For example, DINP and DEHP would be of concern with HCRs > 20; Dibutyl phthalate (DBP) in wood flooring would be marginally of concern with HCR slightly higher than 1. In addition, for DEHT and DIHP in various flooring products, dust ingestion dominates the exposure for the child occupant, which needs further investigation once toxicity data for these chemicals are available.

*Others*

Other important CoCs include Tris(1-chloro-2-propyl)phosphate (TCPP) (flame retardant), Triethanolamine (TEA) (water reducer), Urea (formaldehyde scavenger), Vinyl acetate (performance enhancer), and synthetic antioxidants such as Butylated hydroxyanisole (BHA) and Butylated hydroxytoluene (BHT). They are further discussed in Appendix A, Sections A9.3-A9.5.

## 3.5 Study limitations

The present study has several limitations, and there are uncertainties associated with the results. First, in terms of chemical content, for certain chemicals in the IPD, Pharos report a wide range of chemical contents in specific products, leading to uncertainty in their chemical contents. In addition, we assumed a residual monomer content of 0.045% to 0.29% for all polymer materials except those with available literature data, based on the measured content of monomers in acrylic polymers by Davy et al. [49], which needs better estimates. Moreover, the Pharos database represents the building product composition in the USA. Although building product composition is not expected to vary significantly by

geographic location, there may be other chemicals used in other countries/regions, so the identified list of CoCs is not an exhaustive list worldwide.

Second, in terms of exposure, limitation and uncertainty come from two aspects: the estimated chemical emission from building materials and the estimated human exposure. The emission estimates for certain VOCs with good physiochemical data (e.g., formaldehyde, ethylbenzene) in building materials directly in contact with indoor air (e.g., wall, ceiling, flooring, etc.) are relatively accurate as they would be 100% emitted after 15 years. However, for SVOCs whose emission is much slower, the emission estimate could have a larger uncertainty. Also, emissions could be overestimated in certain cases, since we assume for example that all building products are in direct contact with the indoor air, which is not true for insulation products that are usually installed behind the drywall, or that the entire flooring area is installed with vinyl flooring or carpet, which would overestimate the product mass and the chemical mass. In addition, many building products may have non-considered surface coating that acts as a diffusion barrier, which can greatly reduce emissions. For the estimated human exposure, the uncertainty associated with inhalation exposure is relatively small, since the indoor inhalation intake fraction is well quantified. However, the dermal exposure, especially the dermal gaseous exposure, has a larger uncertainty due to the estimated skin permeation coefficient. The estimated dermal gaseous exposures for certain chemicals are relatively high, up to 10 times higher than inhalation exposures, which needs to be further investigated. The dust ingestion exposure also has relatively large uncertainty due to the large variations in the exposure factors such as dermal contact area, dermal contact frequency and dust ingestion rate. In addition, the SVOC levels in dust may be under/over-estimated since we assumed that dust comes solely from the abrasion of the building material, so the SVOC levels in dust are the same as those in the source building material. However, there are many sources of dust and dust may have high content of organic carbon that attracts SVOCs, leading to lower or higher levels of SVOCs in dust than in the source material. Thus, the dust could be treated as a separate compartment in the future, and the removal of dust via vacuum cleaning and surface cleaning needs to be considered.

Third, in terms of toxicity, many chemicals (93 out of 252 in the present study) lack toxicity data (either experimental or QSAR-predicted) so that the hazard index or cancer risk cannot be calculated. With that, the risk evaluation for the studied chemicals in building products is not comprehensive. Furthermore, for certain chemicals, toxicity data are only available for one exposure route, requiring route-to-route extrapolations. This suggests an urgent need for more experimental toxicity data for more exposure routes and prediction methods with wider applicability to support HTS of health risks to chemicals in building materials and other product applications. On the other hand, for chemicals with toxicity data available, the toxicity estimates may have large uncertainties. For example, the CSF for formaldehyde can vary by one to two orders of magnitude, and the RfD for urea can vary by a factor 1000 according to different sources. Thus, uncertainties in the chemical toxicity need to be quantified when in-depth assessments are conducted for specific CoCs.

Fourth, the present study only assesses the health risk at the level of individual chemical-product combinations. We do not consider the cumulative exposures from a chemical present in multiple building products, or from multiple chemicals with similar health effects. Thus, while a chemical can be identified as not of concern in one product, its simultaneous presence in multiple building products or

the presence of other chemicals with the same health effects may still pose a significant health risk to the occupants, which may be overlooked in the present study. As a result, cumulative exposures should be a focus for future studies that are higher-tier and are more in-depth.

Finally, the estimated risks combining exposure and toxicity in the present study are relatively high. For example, certain chemical-product combinations have estimated HIs > 1000, or estimated ILCR > $10^{-3}$. Formaldehyde in several wooden products in Pharos IPD is even estimated to have potential ILCRs higher than 0.01, which is unlikely. This suggests that estimated risks could be either on the high-end or conservative estimates of the potential risks. Although the absolute risks in the present study might be high-end estimates in certain cases, they nevertheless can provide useful insights on the relative ranking across chemicals and chemical prioritization. Thus, the chemical-product combinations identified as CoCs deserve more refined studies to better quantify their exposures and risks for building occupants.

## 3.6 Linking to national and international efforts for addressing chemicals of concern in building products.

The building and construction sector is one of the largest end markets for chemicals downstream of the chemical industry and the sector is expected to grow following increased urbanization, especially in the Asian and African regions [50]. Construction furthermore has been identified as priority sector for action on the emerging policy issue of Chemicals in Products (CiP) under the Strategic Approach for International Chemicals Management (SAICM) [51]. Considering the potential for (indoor) exposure during use of building products and the potential barriers that chemicals of concern can pose for material circularity, addressing chemicals of concern in building products can offer significant opportunities for advancing sustainable consumption and production and protecting human health and the environment from harmful impacts of chemical pollution in line with the UN Sustainable Development Goals.

A recent report by the UN Environment Programme has identified almost 30 chemicals of concern relevant for building and construction products that have already been addressed by national and international regulatory risk management action [52]. The analysis however excluded chemicals for which scientific knowledge concerning risk to human health and the environment is emerging. Given that scientific knowledge on chemical uses and hazards is constantly evolving, addressing chemicals of concern in building products requires a holistic approach, including continued regulatory action but also targeted action by industry stakeholders at upstream stages of the product value chain. Designers and manufacturers of building products, for example, should actively track and manage chemical composition of their materials and assess potential impacts of chemicals of concern along their life cycle. High-throughput-screening can offer accessible and fast instruments for such assessments at the design stage and can provide important support for upstream action on chemicals of concern and for avoiding regrettable substitution in products of the construction sector.

# 4. Conclusions

Based on a high-throughput exposure and risk assessment for chemicals in building materials, the present study suggests that inhalation is the dominant exposure route, followed by dermal intake, while dust ingestion is a negligible pathway for the various considered chemicals across a wide range of building materials. Using criteria of hazard index > 10 or lifetime cancer risk > $10^{-5}$, 55 chemicals in various building products were identified as chemicals of concern. These results indicate that a significant number of chemical-product combinations used in building materials may pose a non-negligible potential risk to human occupants. Although overestimates can occur in such screening assessment, more refined investigations are warranted for the chemicals identified with very high risks. Maximum chemical contents calculated in this study provide tentative chemical-product specific reference values that are easy-to-use in the design of sustainable building products. Such tentative reference values can provide useful and easily actionable information for practitioners and can serve as a good starting point for prioritizing chemicals/products of greatest concern thus informing the development of more sustainable building products.




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# Conflict of Interest

The authors declare no conflict of interest, whereas Dr. Jolliet discloses his role as a member of the USEtox Center scientific advisory board and chair of the project on Global guidance for Life Cycle Impact Assessment a project supported by the Life Cycle Initiative, hosted at UN-environment.


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# Tables

Table 1. Identified chemicals of concern (CoCs) and the associated building products from the Pharos databases. $MAC_{HTS}$: MAximum chemical Content based on High-Throughput Screening in ppm corresponding to HI=1, ILCD=$10^{-6}$. HCR: hazard content ratio = actual chemical content/$MAC_{HTS}$. Note that the residual monomers have wide ranges of HCRs because they consider the ranges of residual monomer contents in polymer materials.

| CAS | Chemical | Product categories* | Chemical function | $MAC_{HTS}$ (ppm) | $MAC_{HTS}$ endpoint | Actual content (ppm) | HCR | Database |
|---|---|---|---|---|---|---|---|---|
| 822-06-0 | 1,6-Hexamethylene diisocyanate (HDI) | Carpet flooring | Crosslinker | 0.2 | Non-cancer | 48800 | | CPD+IPD |
| | | Acrylic flooring adhesive | Crosslinker | 7 | Non-cancer | 13650 | 1950 | |
| | | Flooring (wood, cork, vinyl) | Crosslinker, Residual monomer | 0.1 | Non-cancer | 2.8 - 236 | 28 - 2360 | |
| 51-79-6 | Ethyl carbamate | Flooring (rubber, cork, wood) | Solvent | 0.2 | Cancer | 11560 - 28800 | | IPD |
| 50-00-0 | Formaldehyde | Wooden furniture, Base cabinetry | Preservative, Residual monomer | 0.1 | Cancer | 6.6 - 3102 | | CPD+IPD |
| | | Flooring (wood, cork, bamboo, fluid-applied) | Preservative, Residual monomer | 0.1 | Cancer | 6.58 - 1890 | | |
| | | Gypsum wallboard | Preservative | 0.03 | Cancer | 1032 | | |
| | | Foam insulation (polyurethane, spray), Gypsum ceiling | Preservative, Residual monomer | 0.1 | Cancer | 2.8 - 236.8 | 35 - 2960 | |
| | | Hollow core wood veneer door, Carpet flooring | Preservative, Residual | 0.1 | Cancer | 1.5 - 27.6 | 15 - 276 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | monomer | | | | | |
| | | Cellulose countertops, High pressure laminate, Drywall acoustical sealant | Preservative, Residual monomer | 5 | Cancer | 30 - 3215 | 6 - 643 | |
| | | (Glass or mineral fiber) insulation and ceiling | Preservative | 90 | Cancer | 540 - 1170 | 6 - 13 | |
| 101-68-8 | Methylene bisphenyl diisocyanate (MDI) | Flooring (rubber, carpet, fluid-applied, wood) | Unknown | 10 | Non-cancer | 610 - 40500 | 61 - 4050 | IPD |
| | | Wooden furniture | Unknown | 20 | Non-cancer | 78400 | 3920 | |
| 151-56-4 | Ethyleneimine (Aziridine) | Flooring (wood, cork), Wooden furniture | Residual monomer | 0.02 | Cancer | 3.94 - 63.2 | 197 - 3160 | IPD |
| 102-71-6 | Triethanolamine (TEA) | Concrete mansory unit | Water reducer | 0.02 | Cancer | 25 | 1250 | CPD |
| 25013-16-5 | Butylated hydroxyanisole (BHA) | Carpet flooring | Antioxidant | 6 | Cancer | 5202 | 867 | IPD |
| 111-76-2 | Ethylene glycol monobutyl ether (EGBE) | Cork flooring | Solvent | 50 | Cancer | 39600 | 792 | IPD |
| | | Polyurethane foam insulation | Solvent | 200 | Cancer | 11600 | 58 | |
| 872-50-4 | N-Methyl-2-pyrrolidone (NMP) | Flooring (wood, cork) | Solvent | 10 | Cancer | 3050 - 6920 | 305 - 692 | IPD |
| 85-68-7 | Butyl benzyl phthalate (BBP) | Flooring (vinyl, carpet) | Plasticizer | 60 | Cancer | 12480 - 41400 | 208 - 690 | CPD+IPD |
| | | Elastic facade joint sealant | Plasticizer | 10000 | Cancer | 150000 | 15 | |
| 75-01-4 | Vinyl chloride | Flooring (carpet, vinyl, VCT) | Residual monomer | 1 | Cancer | 0.36 - 241.2 | 0.6 - 402 | CPD+IPD |
| | | Polyurethane Foam Insulation | Residual monomer | 1 | Cancer | 1.2 - 11.4 | 2 - 19 | |
| 124-09-4 | 1,6-Hexanediamine | Carpet flooring | Unknown | 300 | Non-cancer | 114000 | 380 | IPD |
| 111-46-6 | Diethylene glycol (DEG) | Polyurethane Foam Insulation | Solvent | 50 | Cancer | 15200 | 304 | IPD |
| | | Gypsum Ceiling | Solvent | 20 | Cancer | 4720 | 236 | |
| 100-42-5 | Styrene | Insulation (XPS, EPS, PS foam) | Residual monomer | 10 | Cancer | 3.7 - 2990 | 0.37 - 299 | CPD+IPD |
| | | Flooring (rubber, cork, carpet) | Residual monomer | 2 | Cancer | 0.052 - 334 | 0.026 - 167 | |
| 108-05-4 | Vinyl acetate | Flooring (carpet, cork, wood) | performance enhancer | 70 | Cancer | 1470 - 16660 | 21 - 238 | IPD |
| | | Gypsum wallboard | performance enhancer | 30 | Cancer | 1020 | 34 | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 108-31-6 | Maleic anhydride | Flooring (wood, cork), Wooden furniture | Intermediate | 30 | Non-cancer | 2640 - 6750 | 88 - 225 | IPD |
| 126-99-8 | 2-Chloro-1,3-butadiene | Base cabinetry | Residual monomer | 0 | Cancer | 13.6 - 89.2 | 34 - 223 | CPD |
| 100-41-4 | Ethylbenzene | Flooring (wood, fluid-applied) | Solvent | 3 | Cancer | 108 - 666 | 36 - 222 | IPD |
| 75-07-0 | Acetaldehyde | Gypsum Wallboard | Solvent | 5 | Cancer | 1065 | 213 | IPD |
| 112-34-5 | 2-(2-butoxyethoxy)ethanol | Flooring (wood, cork) | Pigment solvent | 3 | Non-cancer | 267 - 609 | 89 - 203 | CPD+IPD |
| | | Low VOC flat acrylic ceiling paint | Rheology modifier | 100 | Non-cancer | 1200 | 12 | |
| 128-37-0 | Butylated hydroxytoluene (BHT) | Carpet flooring | Antioxidant | 30 | Cancer | 5940 | 198 | IPD |
| 106-99-0 | 1,3-Butadiene | Flooring (rubber, cork, carpet) | Residual monomer | 2 | Cancer | 0.06 - 384 | 0.03 - 192 | CPD+IPD |
| 108-78-1 | Melamine | Flooring (wood, cork) | Residual monomer | 3 | Cancer | 15.6 - 552 | 5.2 - 184 | CPD+IPD |
| | | Wooden furniture, Base cabinetry | Residual monomer | 4 | Cancer | 4.8 - 600 | 1.2 - 150 | |
| 57-13-6 | Urea | Flooring (wood, cork), Wooden furniture | Formaldehyde scavenger | 300 | Non-cancer | 18000 - 54900 | 60 - 183 | IPD |
| 75-21-8 | Oxirane | Spray foam insulation | Residual monomer | 3 | Cancer | 51 - 396 | 17 - 132 | CPD |
| 140-31-8 | Aminoethylpiperazine | Fluid-Applied Flooring | Epoxy curing agent | 200 | Non-cancer | 21800 | 109 | IPD |
| 141-43-5 | Ethanolamine | Cork Flooring | Surface active agent | 200 | Non-cancer | 18400 | 92 | IPD |
| 77-99-6 | 1,1,1-Tri(hydroxymethyl)propane | Carpet Flooring | Unknown | 300 | Non-cancer | 26700 | 89 | IPD |
| 1717-00-6 | Dichlorofluoroethane (HCFC-141B) | Polyurethane Foam Insulation | Foam blowing agent | 1170 | Cancer | 62010 | 53 | IPD |
| 96-29-7 | Methyl ethyl ketoxime (MEKO) | Wood Flooring | Blocking agent in coatings | 5 | Cancer | 278.46 | 51 | IPD |
| 191-24-2 | Benzo[g,h,i]perylene | Carpet Flooring | Unknown | 2 | Cancer | 116.62 | 49 | IPD |
| 111-90-0 | Eiethylene glycol monoethyl ether | Waterborne flooring finish | Coalescent | 700 | Non-cancer | 34300 | 49 | CPD |
| 25265-77-4 | Texanol | Wood flooring, Gypsum ceiling | Coalescing solvent | 300 | Non-cancer | 6000 - 12300 | 20 - 41 | IPD |
| 2855-13-2 | Isophorone diamine | Flooring (fluid-applied, wood) | Crosslinker | 200 | Non-cancer | 3600 - 6400 | 18 - 32 | CPD+IPD |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 24800-44-0 | Tripropylene glycol | Carpet Flooring | Unknown | 400 | Non-cancer | 12000 | 30 | IPD |
| 13674-84-5 | Tris(1-chloro-2-propyl)phosphate (TCPP) | Spray foam insulation | Flame retardant | 4000 | Non-cancer | 52000 - 112000 | 13 - 28 | CPD+IPD |
| 74-98-6 | Propane | Spray Polyurethane Foam | Blowing agent | 2000 | Non-cancer | 16000 - 56000 | 8 - 28 | CPD |
| 6711-48-4 | Tetramethyldipropylenetriamine | Polyurethane Foam Insulation | Unknown | 2000 | Non-cancer | 56000 | 28 | IPD |
| 85-44-9 | Phthalic anhydride | Carpet Flooring | Intermediate for phthalates | 1000 | Non-cancer | 27000 | 27 | IPD |
| 52-51-7 | Bronopol | Cork Flooring | Biocide | 100 | Non-cancer | 2600 | 26 | IPD |
| 79-10-7 | Acrylic acid | Wood flooring | Unknown | 30 | Non-cancer | 720 | 24 | IPD |
| 115-10-6 | Methyl ether | Spray Polyurethane Foam | Blowing agent | 3000 | Non-cancer | 22800 - 69000 | 7.6 - 23 | CPD |
| 924-42-5 | n-Methylol acrylamide | Firestop Joint Spray | Residual monomer | 50 | Cancer | 150 - 1000 | 3 - 20 | CPD |
| 107-13-1 | Acrylonitrile | Polystyrene foam board insulation | Residual monomer | 2 | Cancer | 0.008 - 40 | 0.004 - 20 | IPD |
| 75-56-9 | 2-Methyloxirane | Spray foam insulation | Residual monomer | 10 | Cancer | 20 - 170 | 2 - 17 | CPD |
| 74-85-1 | Ethylene | Carpet flooring | Unknown | 2000 | Non-cancer | 32000 | 16 | IPD |
| 811-97-2 | 1,1,1,2-Tetrafluoroethane (HFC-134A) | Polyurethane foam insulation | Blowing agent | 6000 | Cancer | 84000 | 14 | IPD |
| 111-40-0 | Diethylenetriamine | Wood flooring | Crosslinker | 100 | Non-cancer | 1400 | 14 | IPD |
| 1330-20-7 | Xylenes | Fluid-applied flooring | Solvent | 500 | Cancer | 7000 | 14 | IPD |
| 123-91-1 | 1,4-Dioxane | Polyurethane Foam Insulation | Solvent | 20 | Cancer | 280 | 14 | IPD |
| 78-40-0 | Triethyl phosphate (TEP) | Polyurethane Foam Insulation | Solvent | 900 | Non-cancer | 11700 | 13 | IPD |
| 95-63-6 | 1,2,4-Trimethylbenzene (1,2,4-TMB) | Flooring (cork, wood) | Solvent | 300 | Cancer | 2100 - 3600 | 7 - 12 | IPD |
| 35691-65-7 | Bromothalonil | Cork Flooring | Preservative | 200 | Non-cancer | 2400 | 12 | IPD |
| 100-51-6 | Benzyl alcohol | Flooring (fluid-applied) | Solvent | 4000 | Non-cancer | 44000 | 11 | CPD |
| 345 | Dipropylene | Flooring (cork, wood) | Surfactant | 80 | Non- | 8000 | 10 | IPD |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 90-94-8 | glycol monomethyl ether | | | 0 | cancer | | | |

* Wooden furniture includes HDF, MDF, OSB, plywood, particleboard and other composite wood products.

# Figures

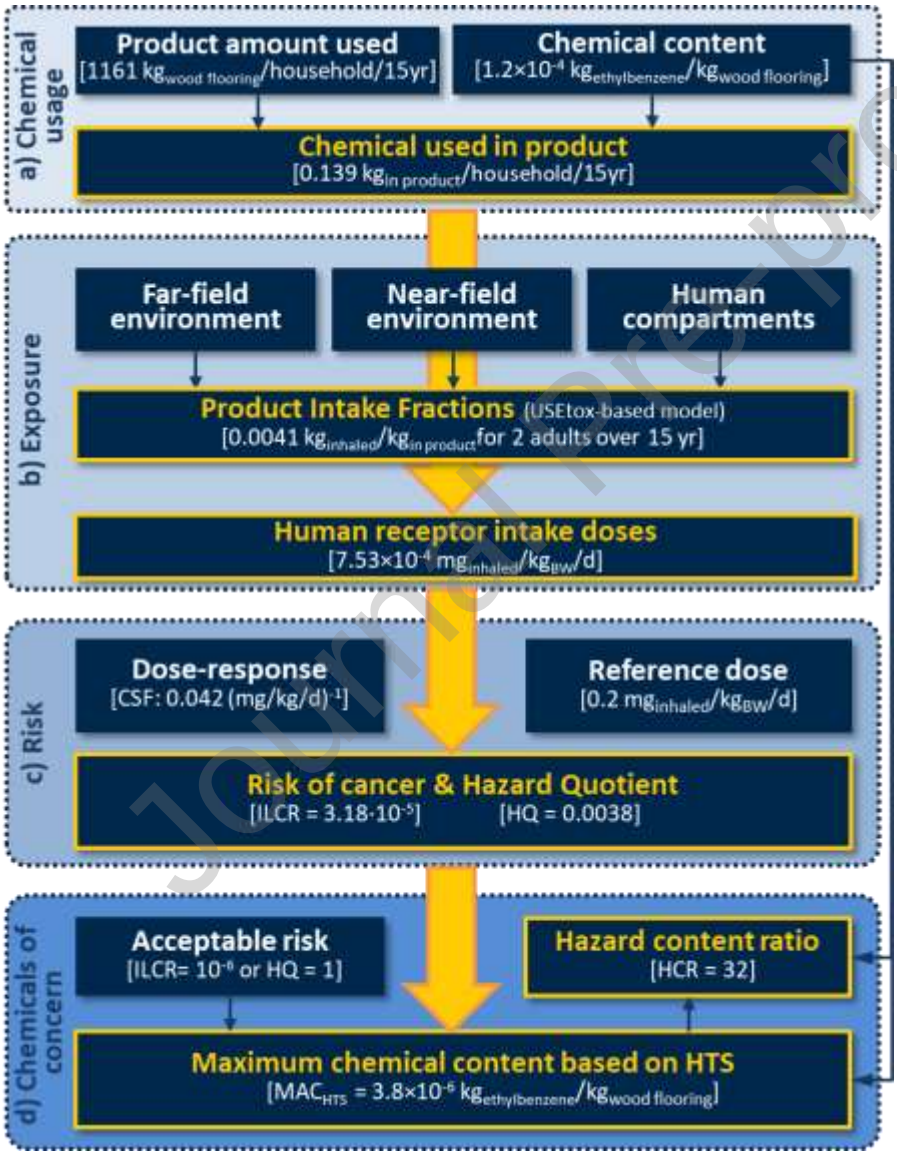


Figure 1. Diagram of the assessment framework, from mass in product to health risks, illustrated with the example of ethylbenzene in wood flooring. Adapted from Huang et al. 2019 [4].

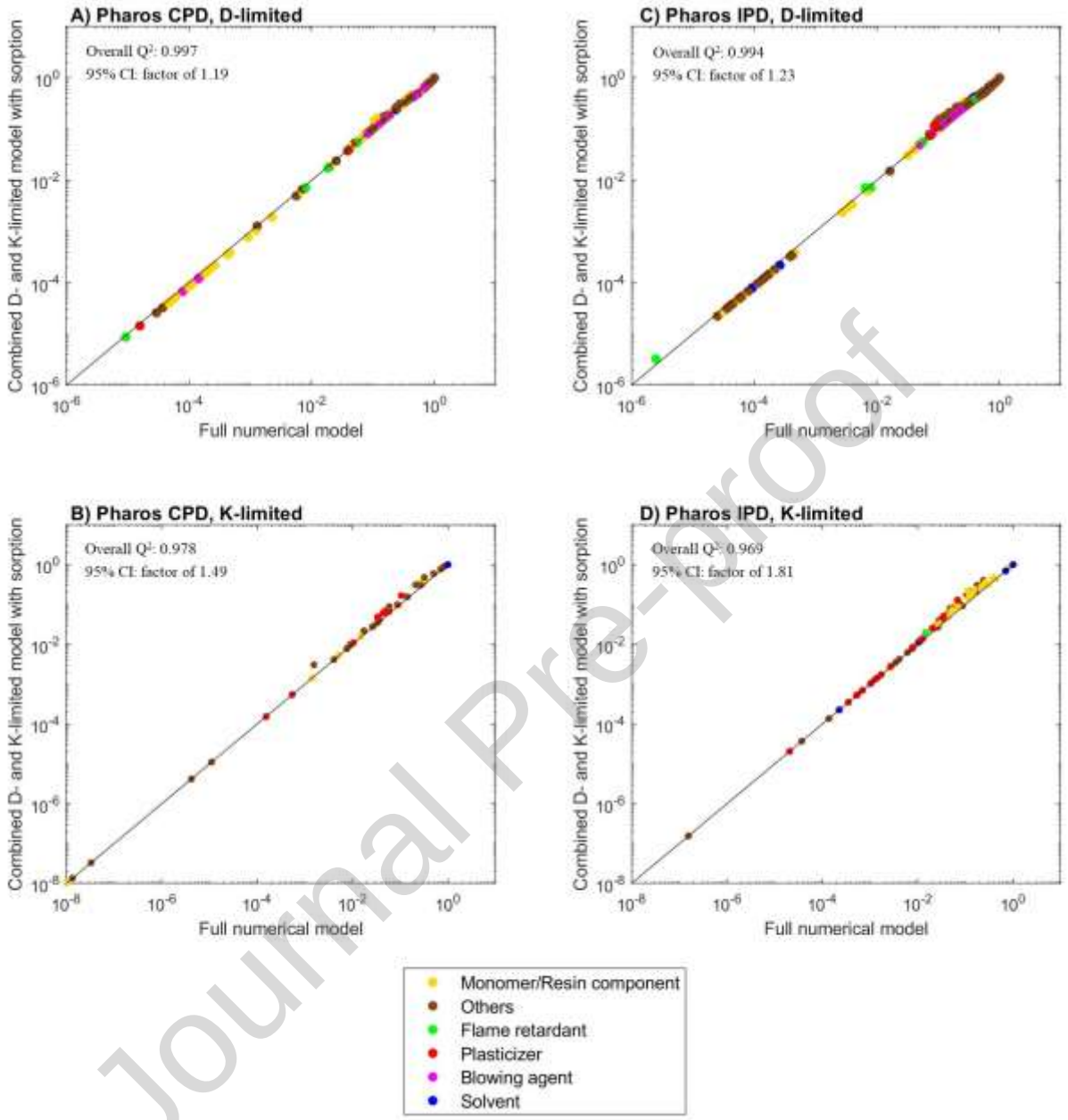




Figure 2. Mass fraction emitted at the end of a 15-yr simulation period predicted by the simplified model (combined D- and K-limited model with sorption) compared to the numerical solution of the full model. Values for the 325 and 495 unique chemical-product combinations are presented in (A)(B) Pharos Common Products and (C)(D) Individual Databases, respectively, with a building material thickness of 100 mm and a thickness of sorption material of 1.27 cm.

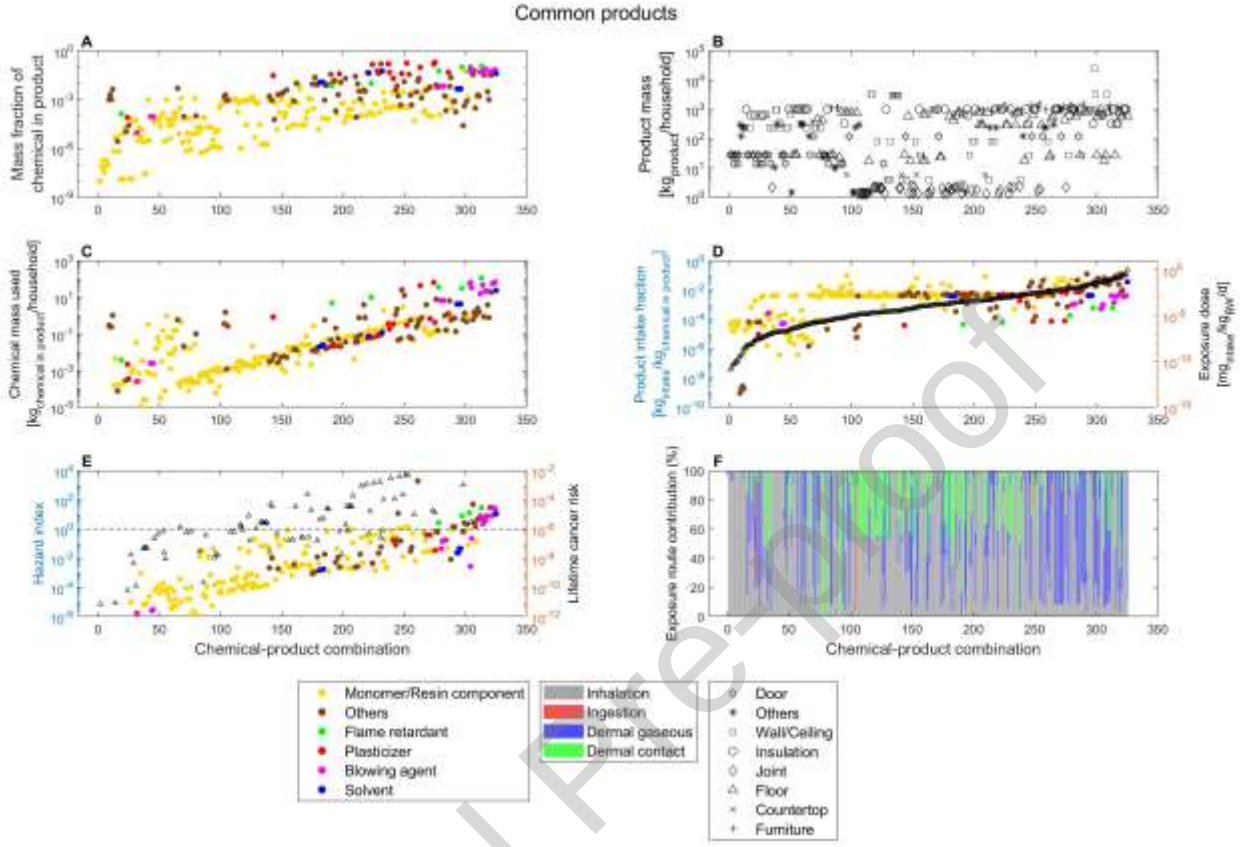


Figure 3. Summary screening results for the 325 unique chemical-product combinations in the Pharos Common Products. (A) Chemical mass fraction in product [- or $kg_{chemical}$/ $kg_{product}$]; (B) product mass [$kg_{product}$/household]; (C) amount of chemical used [$kg_{chemical\ in\ product}$/household]; (D) product intake fractions [$kg_{intake}$/ $kg_{chemical\ in\ product}$] (left axis, colored points) and daily exposure doses summing all routes [mg/kg/d] (right axis, black triangles); (E) resulting Hazard Index [-] (left axis, colored points) and Incremental lifetime cancer risk [-] (right axis, black triangles); and (F) exposure route contributions. The dotted line in (E) represents the threshold of applied risk criteria as HI = 1 and cancer risk = $10^{-6}$. All plots are ranked according to increasing total daily exposure dose summing all exposure routes. Only the results for adult occupants are presented. For residual monomers, the maximum monomer mass fractions in polymers are presented (see Section 2.2 for explanation).

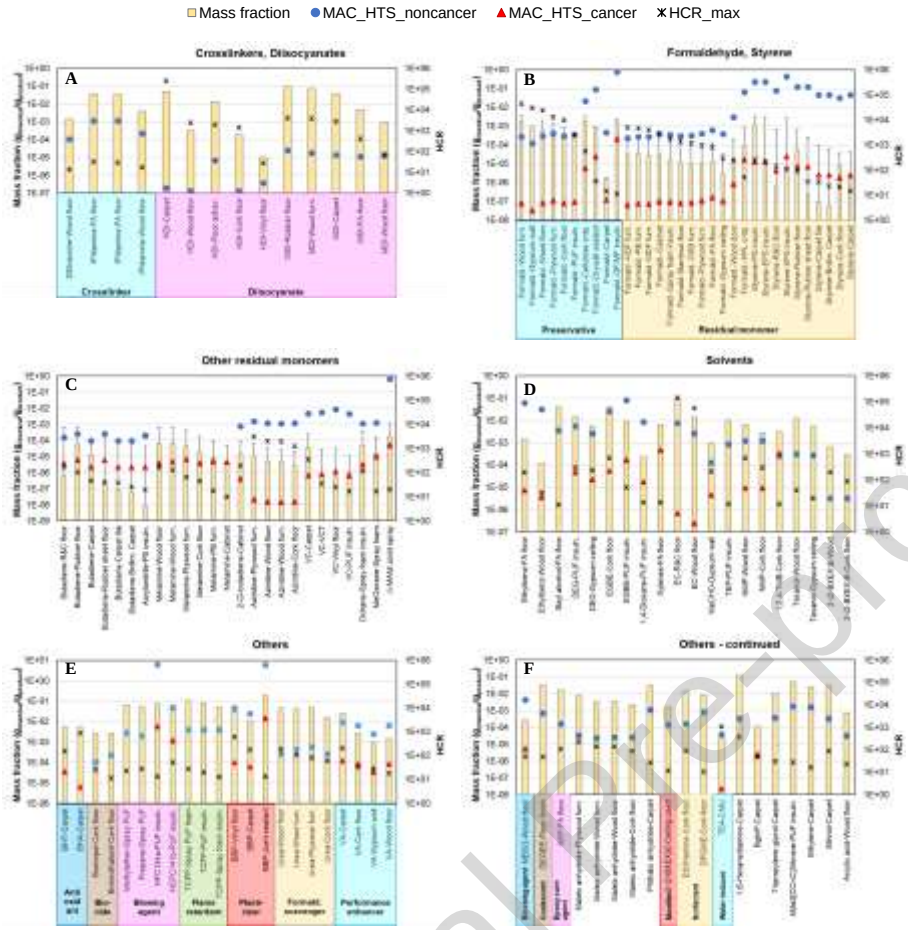


Figure 4. Actual chemical mass fraction (bars) compared to calculated maximum chemical content ($MAC_{HTS}$) for cancer (blue points) and non-cancer (red triangles) for the identified chemicals of concern (left axis), and resulting Hazard Content Ratios (HCR) (black crosses - right axis), for A) crosslinkers and diisocyanates, B) formaldehyde and styrene, C) Other residual monomers, D) Solvents, E) Antioxidants, biocides, blowing agents, flame retardants, plasticizers, formaldehyde scavengers and performance enhancers, and F) Other remaining functions.

FA floor: fluid-applied flooring. Adhsv: adhesive. Furn: furniture. Insuln: insulation. Cntp: countertop. PUF: polyurethane foam. GF/MF insuln: glass or mineral fiber insulation. HDF: high density fiberboard. PB: particleboard. MDF: medium density fiberboard. OSB: oriented strand board. HPL: high pressure laminate. PS: polystyrene. EPS: expanded polystyrene. XPS: extruded polystyrene. R&C floor: rubber & cork flooring. Brdlm carpet: broadloom carpet. VCT: vinyl composition tile. CMU: concrete masonry unit.

DEtriamine: diethylenetriamine. IPdiamine: isophorone diamine. HDI: 1,6-hexamethylene diisocyanate. MDI: 4,4'-methylene bisphenyl diisocyanate. Formald: formaldehyde. Butadiene: 1,3-butadiene. 2-Cl-butadiene: 2-chloro-1,3-butadiene. VC: vinyl chloride. MeOxirane: 2-methyloxirane. n-MAM: n-methylol acrylamide. Ethylbenz: ethylbenzene. Bzyl alcohol: benzyl alcohol. DEG: diethylene glycol. EGBE: Ethylene glycol monobutyl ether. EC: ethyl carbamate. MeCHO: acetaldehyde. TEP: triethyl phosphate. NMP: N-Methylpyrrolidone. 1,2,4-TMB: 1,2,4-trimethylbenzene. 2-(2-BXEX)E: 2-(2-butoxyethoxy)ethanol. BHT: Butylated hydroxytoluene. BHA: butylated hydroxyanisole. TCPP: Tris(1-chloro-2-propyl)phosphate. BBP: Butyl benzyl phthalate. VA: vinyl acetate. MEKO: methyl ethyl ketoxime. DEGEE: diethylene glycol monoethyl ether. AEP: Aminoethylpiperazine. 2-(2-BXEX)E: 2-(2-butoxyethoxy)ethanol. EtOHamine: ethanolamine. DPGME: dipropylene glycol monomethyl ether. TEA: triethanolamine. BghiP: benzo[g,h,i]perylene. 4Me2[CC=C]3Amine: tetramethyldipropylenetriamine. Ethriol: 1,1,1-tri(hydroxymethyl)propane.

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