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Prediction of relevant exposure sources to aggregate chemical exposures from general and occupational environments: exploration of a decision tree approach

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Abstract

Objectives: To understand the total exposure of a human population to a chemical, it is necessary to aggregate exposures from different exposure routes (ingestion, inhalation, dermal uptake) and exposure sources (eg food, air, consumer products) from different environments (ie general, occupational, consumer use). Preventive actions or regulatory decisions require decisions to be taken on priority exposure routes and sources. This study explores the development of a quantitative decision tree to identify relevant exposure sources in the context of aggregate exposure. As a case study for spray applications, it focuses on joint exposure to a specific chemical in a consumer product through domestic use of hairspray, and exposure at the workplace involving surface spraying, such as spray application of paints.

Methods: Determinant of the exposure models ART (for workers) and ConsExpo (for the general population) were used to generate a wide range of realistic exposure scenarios. The dominance of one source over another was analyzed through pairwise random comparisons. Exposure estimates from one source containing a specific determinant are compared with those from the other source, scaled by a dominance ratio that defines how much higher one source's exposure must be to be considered dominant. For each comparison, the number of times one source exceeds the other by at least a dominance ratio is counted, resulting in the occurrence. The occurrence is compared with a predefined threshold (eg 80%). If the threshold is met or exceeded, the higher-contributing source is considered dominant and no exposure aggregation is needed; otherwise, aggregation of both sources is recommended.

Results: The findings indicated that the use of high- or medium-specification glove boxes, as forms of permanent encapsulation or encasing of the emission source, results in occupational exposure that is negligible compared with the exposure from consumer product use. When these glove boxes were used, hair spray exposure was the dominant source in 89% and 82% of cases, for high and medium specifications, respectively. A spraying activity with surface liquids performed outdoors (close to buildings) showed a significant trend toward occupational exposure dominance in 81% of cases. Using these three determinants, a three-layer quantitative decision tree was built to help users quickly decide whether aggregation was relevant before performing calculations. Aggregation was suggested in 91% of cases and avoided it in 9%.

Keywords: aggregate exposure; chemicals; consumer exposure; decision tree; exposure models; occupational exposure.

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What's Important About This Paper?

Assessing aggregate exposure is a major challenge in the prevention and regulation of chemical risks. Existing approaches for decision-making about exposure aggregation are scarce and remain mostly qualitative or based on expert judgment. This study demonstrated the feasibility of a decision-making tool for aggregating and prioritizing exposure sources.

Introduction

Humans are exposed to chemicals from the general environment, such as drinking water, food, and consumer products, as well as in their occupational environment, via 1 or more routes of exposure. Aggregate exposure is defined as the exposure to a single substance through all relevant sources (ie: water, air, dust, diet, etc.) and routes (ingestion, inhalation, dermal contact) (WHO/IPCS, 2009; U.S. EPA, 2011; ECHA, 2016c; OECD, 2018).

To understand the total exposure of a human population to a chemical, it is necessary to aggregate exposures from all relevant sources and routes. Therefore, decision-making on aggregation necessitates the examination of all available data related to the substance and its exposure scenarios, which can be resource-intensive and complex for substances with limited data.

REACH regulation (Registration, Evaluation, Authorization and Restriction of Chemicals) requires exposure assessment and subsequent risk characterization to be carried out for substances subject to registration. Exposure estimates can be derived from measured data sets or modeled predictions (ECHA, 2016a). The in silico approach involves assessing exposure to chemicals using exposure determinants that describe exposure conditions, whether in the occupational or in the general environment. These models are either mechanistic, ie based on the understanding of the fundamental processes behind the observed phenomena, or empirical, ie relying on observed data to identify patterns and make predictions. Several tools are available, such as ART (Advanced Reach Tool 1.5, www.advancedreachtool.com) and ConsExpo (https://consexpoweb.nl/), which are higher-tier chemical exposure assessment tools in the workplace, and for consumer exposure, such as the use of personal care products, respectively (ECHA, 2016b, 2016c).

The gap in current legislation regarding aggregate exposure assessment is increasingly recognized, highlighting the necessity of an integrated approach (Schlüter et al. 2022). Determining which routes and sources are to be considered is a key decision in aggregate exposure assessment. This is currently based on assessing the exposure corresponding to each route and source of exposure independently (ie each pathway of exposure), using specific models. The relative contributions of each route and source are then compared with determine which are relevant to keep in the assessment of overall exposure (U.S. EPA, 2001).

The preliminary decision regarding the necessity to aggregate exposures constitutes a critical element in exposure assessment. Addressing this, (ECETOC, 2023) identified limitations in cross-sectoral methodologies and data for evaluating aggregate consumer exposure, highlighting the need for integrated data platforms. Quantitatively, the probabilistic PACEM model (Delmaar et al. 2024) simulates aggregate exposure distributions from consumer products by leveraging usage survey data and accounting for co-occurrence. Also, the CEFIC LRI-funded TAGS project (Sarigiannis et al. 2012) introduced a tiered framework based on specific criteria to determine the need for comprehensive aggregate assessment. Institutional reports have qualitatively addressed the need to narrow the scope of exposure assessments as the many potential exposure scenarios could make it difficult to perform an aggregate assessment. Overall, existing approaches for decision-making about exposure aggregation are scarce and remain mostly qualitative or at the methodological level (U.S. EPA, 2001; WHO/IPCS, 2021). Quantitative tools like PACEM effectively model the aggregation of exposure from specific consumer product usage scenarios. However, they do not inherently address the challenge of a prior identification of relevant exposure sources and routes that should be considered in the aggregation process before quantitative assessments are conducted. Developing a quantitative and generic decision-making tool is therefore necessary to enable an a priori decision to be taken on the need to carry out an overall exposure assessment.

In this study, we conducted a proof of concept of a decision tree using a case study focused on spray applications. The example exposure scenario involves a non-volatile chemical present both in hairspray, as a source of consumer exposure, and surface spraying with liquids, as a source of occupational exposure.

The aim is to enable an a priori decision to be taken on the need to carry out an overall exposure assessment for the combination of 2 sources of exposure in different human environments. This is the first step to develop a more comprehensive decision-making tool involving multiple exposure routes and sources.

Aggregate exposure is one of the priorities of the European Partnership for the Assessment of Risks from Chemicals (PARC) project, aiming at the development of the next-generation of chemical risk assessment to protect human health and the environment (Marx-Stoelting et al. 2023). This work was conducted as part of Work Package 6, "Innovation in regulatory risk assessment," and more specifically within Project 6.2.1.b, "Strategy for aggregate exposure."

Materials and methods

An inventory and scoring of existing exposure models carried out by the PARC P.6.2.1b Aggregate exposure project has classified exposure models according to their methodology, scope, efficiency, and usability (Blassiau et al. in preparation). ConsExpo Web and ART were the models among the highest scores for modeling exposure to consumer products and in the workplace, respectively. Thus, we used the ConsExpo Web (version 1.1.1, https://consexpoweb.nl/) and ART (Advanced Reach Tool 1.5, www.advancedreachtool.com) models to identify the determinants that describe the different possible exposure scenarios when using a hair spray (consumer exposure) or when spraying a surface with a liquid (occupational exposure), respectively. An exposure scenario is defined under REACH regulation as the conditions of manufacture and use which are needed for controlling the risks to human health and the environment. This includes operational conditions and risk management measures (ECHA, 2011). Both models were also used to estimate chemical concentrations in the air, hence external exposure. In this paper, "consumer exposure (external)" refers to the chemical concentration in the air to which individuals may be exposed in their general environment through the domestic use of consumer products, while "occupational exposure (external)" refers to the chemical concentration in the air to which the same individuals may be exposed in their occupational environment.

ConsExpo is a modeling tool that can be used to estimate consumer exposure to a wide variety of products and of circumstances (Delmaar and Schuur 2017). The ConsExpo Spray Model "toward person" estimates the indoor inhalation exposure to slightly evaporating or nonvolatile compounds in droplets that are released from a spray can or trigger spray (Delmaar and Bremmer 2009). Exposure determinants needed for this model, including spray and room characteristics, ventilation, and substance properties are described in Table S1.

ART is a higher-tier exposure assessment tool incorporating a mechanistic model of inhalation exposure at the workplace and a database of empirical exposure information (Schinkel et al. 2011). The "surface spraying of liquids" model belonging to the "spray application of liquids" activity class was used. This activity class is used to estimate exposure when a liquid is atomized into droplets for dispersal on surfaces (surface spraying) or into the air (air spraying), such as spray application of paints on, eg ships or spraying cleaning agents on surfaces. For low-volatile substances, the model estimates the exposure to mists (Fransman et al. 2013). Exposure determinants needed for this model, such as chemical properties (vapor pressure, weight fraction, viscosity), application method (rate, direction, technique), environmental conditions (dispersion, surface contamination), exposure duration, and control measures are described in Supplementary Tables 2 and 3.

Generation of exposure scenarios

Thirteen determinants were used for hairspray use exposure scenarios, and 13 for the occupational exposure through surface spraying. These determinants and their variation ranges are detailed in Table 1 for the exposure to hairspray and in Table 2 for the exposure at the workplace. In the context of this paper, "determinant value" refers to the categories or the values a categorical or numerical determinant can take.

Each determinant (numerical or categorical) can take more than 1 value. For each scenario, 1 value is randomly selected for each determinant, ensuring a wide range of combinations. If the resulting combination of determinants is unique, it is added to the overall dataset of scenarios, ensuring that all scenarios are distinct. For example, for the spray technique, for each scenario, 1 of the 2 spray categories: propellant spray (high compressed air use) or pump spray (low or no compressed air use), was selected using random sampling from a discrete uniform distribution.

Using MATLAB software (The MathWorks Inc., MATLAB Version: 23.2.0.2409890 [R2023b] Update 3), we created 2 distinct datasets, each containing 5.10^4 exposure scenarios, ie sets of combinations of values for exposure determinants. One dataset represents exposure scenarios related to hair spray, while the other represents scenarios related to surface spraying of liquids at the workplace. A dataset size of 5.10^4 was chosen to generate the maximum number of potential exposure scenarios while maintaining a reasonable computation time.

Some occupational scenarios are technically not possible and therefore do not constitute realistic situations. These scenarios were avoided, such as the use of vapor recovery systems as localized control. Exclusion rules, used to avoid unrealistic scenarios are detailed in Tables S4 to S7 and Fig. S1.

The determinants: cloud volume, airborne fraction, density nonvolatile and the inhalation cut-off diameter,

Table 1. Description of the determinants, their type and range of variation or values used for the ConsExpo spray model for the case of hairspray use.

Determinant[a]	Variation range	Explanation	Reference
Spray duration	Normal distribution (0.18, 0.1) in minutes.	…	Bremmer et al. (2006)
Frequency	Normal distribution (0.76, 0.68) in minutes.	…	Bremmer et al. (2006)
Weight fraction substance	Uniform distribution [0,1].	…	
Initial particle distribution	Log-normal distribution (46.5, ACV 2.1) truncated at 50 µm.	…	Delmaar and Bremmer (2009), RIVM (2010)
Exposure duration	Uniform distribution [5,15] in minutes.	The default value used in ConsExpo cosmetics fact sheet is 5 min. This parameter value is based on personal judgement.	Bremmer et al. (2006)
Room volume	Uniform distribution [10,20] in m^3.	The default value used in ConsExpo cosmetics fact sheet is 10 m^3. It is recommended to use a default value of 20 m^3 for an unspecified living area.	RIVM (2014)
Ventilation rate	Uniform distribution [0.6,2].	The default value used in ConsExpo cosmetics fact sheet bathrooms is $2h^{-1}$. It is recommended to use a default value of $0.6h^{-1}$ for an unspecified room.	RIVM (2014)
Room height	2.5 m (Standard room height).	The height has not been varied, as the room's volume depends on its surface area and height.	Bremmer et al. (2006)
Mass generation rate	Product amount divided by the spray duration.	The average amount of product applied per application for hairspray (aerosol) follows a lognormal distribution (GM = 1.84 g, GSD = 2.40 g).	U.S. EPA (2011)
Cloud volume	0.0625 m^3	The default value for cloud volume is set at 1/16 m^3.	Bremmer et al. (2006)
Airborne fraction	0.2	Determined experimentally for different sprays.	Delmaar and Bremmer (2009), RIVM (2010)
Density nonvolatile	1.5 g/cm^3	Many nonvolatile substances in cosmetics are large organic compounds with densities usually between 1.0 and 1.5 g/cm^3.	Bremmer et al. (2006)
Inhalation cut-off diameter	15 µm	The inhalation cut-off diameter is only an approximation of the complicated process of deposition of particles in the lung. In general, its value should be around 10 to 15 µm. The default value is set at 15 µm.	Bremmer et al. (2006)

[a]All determinants are numerical.

were fixed based on the default values recommended in the ConsExpo cosmetics fact sheet (Bremmer et al. 2006). Variation range limits for exposure duration, room volume and ventilation rate were randomly chosen for this proof of concept.

Modeling

The outputs of ART and ConsExpo models were expressed as external air concentrations (mg/m^3). No secondary sources were considered at the workplace, and nor in the general environment setting.

The output considered for the consumer exposure scenarios (ConsExpo) was a full day (24 h) average chemical concentration in the air (taking into account the events per day). For occupational exposure, the duration of a full-shift exposure of workers is 8 h. If the exposure scenario duration is less than 480 min, a non-exposure period was added to have a full-shift duration of 480 min. The chemical concentrations in the workplace air were normalized over 24 h to be comparable to those of ConsExpo.

The models were coded on MATLAB software (The MathWorks Inc., MATLAB Version: 23.2.0.2409890 [R2023b] Update 3) to allow the run of multiple scenarios simultaneously. To verify the correctness of the exposure estimates of the recoded models, a set of scenarios was randomly selected, and the results of the recoded model were compared with those from the original tool.

Table 2. Description of the determinants, their type and range of variation or values used for the ART model for the case of liquid surface spraying.

Determinant	Type	Variation range	Explanation
Vapor pressure	Numerical	$P = 10$ Pa	Has not been varied as the analysis was carried out on nonvolatile liquids only (vapor pressure ≤ 10 Pa). In fact, this variable is not required for the calculation of the substance emission potential.
Weight fraction	Numerical	Uniform distribution [0,1].	…
Viscosity	Categorial	Two categories are possible: low viscosity (like water) and medium viscosity (like oil).	…
Application rate	Numerical	Uniform distribution [0,50.4] in l/min.	This variable is required in categorical form (high application rate (>3 l/min), moderate application rate (0.3 to 3 l/min), low application rate (0.03 to 0.3 l/min), and very low application rate (<0.03 l/min)).
Spray direction	Categorial	Two categories are possible: spraying in any direction (including upwards), only horizontal or downward spraying, and downward only.	…
Spray technique	Categorial	Two categories are possible: spraying with high compressed air use, and spraying with no or low compressed air use.	…
Surface contamination	Categorial	Four categories are possible: default level, general good housekeeping practices, demonstrable and effective housekeeping practices, and process fully enclosed.	…
Exposure duration	Numerical	Uniform distribution [0,480] in minutes.	…
Dispersion	Categorial	Randomly varied using all the possible categories and combinations (indoor/outdoor, room volume, ventilation, use of different types of spray rooms and laminar flow booths). See Table S3.	…
Control measures	Categorial	Randomly varied using all the possible categories of control measures. Some values have been excluded as they are not encountered in spraying activities. See Table S4.	…
NF (near field) and FF (far field) zone	Categorial	Varied between NF and FF.	…
Personal enclosure (FF)	Categorial	…	Has not been varied as workers in spraying activities are usually not equipped with personal enclosures. Therefore "No personal enclosure" level was used for FF scenarios)
Segregation (FF)	Categorial	…	Has not been varied as sources are not isolated from the work environment in a separate room. Therefore, the "No segregation" level was used for FF scenarios.

Analysis

Random pairs of scenarios, representing exposure situations from the 2 exposure sources (hairspray and surface spraying) for the same individual were generated. Ten different datasets of 10^4 scenario pairs were generated and used in the analysis to quantify uncertainty in the decision regarding aggregation.

A comparison ratio (CR) between the chemical concentration in the occupational environment (C_{occ}) and its concentration in the general environment (C_{env}) was calculated for each scenario pair using the Equation (1):

$$CR = \frac{C_{occ}}{C_{cons}} \quad (1)$$

In this proof of concept, we consider the occupational exposure source as dominant, when the chemical concentration in the occupational source (C_{occ}) is at least

Table 3. Distribution of number of scenarios across the ART categorical determinants.

Determinants	Values	Number of scenarios
Source location	F1: Near field (NF)	24,986
	F2: Far field (FF)	25,014
Viscosity	V1: Liquids with low viscosity (like water)	25,013
	V2: Liquids with medium viscosity (like oil)	24,987
Spray direction	D1: Spraying in any direction including upwards	16,718
	D2: Only horizontal or downward spraying	16,611
	D3: Only downward spraying	16,671
Spray technique	T1: Spraying with high compressed air use	25,048
	T2: Spraying with no or low compressed air use	24,952
Localized controls	C1: No localized controls	43,031
	C2: Horizontal/downward laminar flow booth	897
	C3: Other enclosing hoods	869
	C4: Other LEV systems	890
	C5: Glove bags (non-ventilated)	874
	C6: Glove bags (ventilated or kept under negative pressure)	850
	C7: Low specification Glove box	884
	C8: Medium-specification glove box	865
	C9: High-specification glove box/isolator	840
Surface contamination	S1: Default level (no specific cleaning practices, no protective clothing that repel spills, process not fully enclosed)	12,529
	S2: General good housekeeping practices	12,422
	S3: Demonstrable and effective housekeeping practices	12,520
	S4: Process fully enclosed	12,529
Dispersion	L1: Indoor	7,773
	L2: Outdoor close to buildings	2,787
	L3: Outdoor far from buildings	2,798
	L4: Crossflow spray room	2,874
	L5: Down-flow spray room	2,773
	L6: Downward laminar flow booth	2,758
	L7: Downward laminar flow booth using partial screen	2,747
	L8: Downward laminar flow booth using partial screen fitted with Glove ports	2,734
	L9: Downward laminar flow booth using full screen fitted with Glove ports	2,741
	L10: Outdoor close to buildings FF (1 to 4 m)	5,084
	L11: Outdoor close to buildings FF (> 4 m)	4,986
	L12: Outdoor far from buildings FF (1 to 4 m)	4,918
	L13: Outdoor far from buildings FF (>4 m)	5,027

10 times greater than the concentration in the consumer exposure source (C_{cons}). This is translated by CR > 10. Conversely, when C_{cons} is at least 10 times greater than C_{occ}, translated by CR < 0.1, we consider that the consumer exposure source is dominant. Aggregation was deemed appropriate when neither the occupational nor the consumer source was dominant (0.1 < CR < 10).

Scenario pairs were classified into one of 3 aggregation classes (occupational exposure dominance, consumer exposure dominance, and aggregation) according to their CR.

The categorical determinants were analyzed 1 by 1 to assess whether the presence of a particular value in a scenario affects the CR and, consequently, the decision regarding the need for aggregation. For a given value of categorical determinant i, the occurrence of the classification of the scenario pairs containing this value in a group j is calculated using the Equation (2):

$$\text{Occurrence}_i = \frac{\text{Number of pairs}_{i,j}}{\text{Number of pairs}_i} \quad (2)$$

For example, to assess the influence of the value "spraying with high compressed air use" of the categorical determinant "spray technique" on the "occupational exposure dominance" class, we calculated the ratio of the number of pairs that include this value and belong into this class, to the total number of pairs that include this value.

The continuous determinants were analyzed using iterations with a step defined as the maximum value/100, to determine the value that classifies the scenarios into one of the 3 classes defined by the CR. For a given value corresponding to a value k of the determinant i,

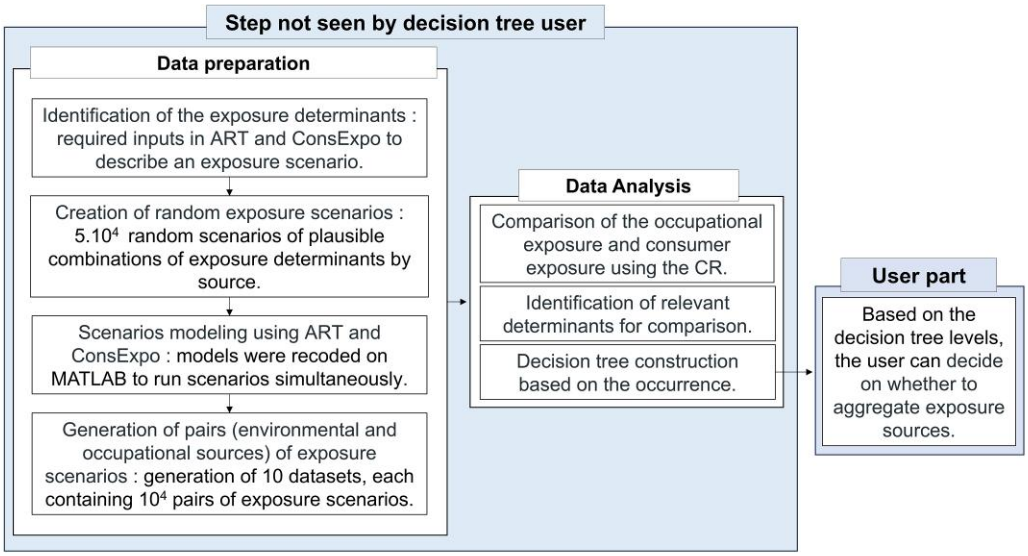

Fig. 1. A summary of the decision tree construction methodology.

the occurrence of the classification of the scenario pairs in a group *j* is calculated using the Equations (3) and (4):

$$\text{Occurrence}_{i \geq k} = \frac{\text{Number of pairs}_{\ i \geq k,\ j}}{\text{Number of pairs}_{\ i \geq k}} \tag{3}$$

$$\text{Occurrence}_{i < k} = \frac{\text{Number of pairs}_{\ i < k,\ j}}{\text{Number of pairs}_{\ i < k}} \tag{4}$$

For example, to determine the weight fraction value in hair spray that classifies a scenario pair into the "occupational exposure dominance" class, we used the values (k) that weight fraction can take between 0 and 1 in increments of 0.01. We calculated then the ratio of pairs with a weight fraction below k that belong to this class, relative to the total number of pairs with a weight fraction below k. We performed similar calculations for pairs with a weight fraction above k.

A determinant value is considered relevant for decision tree construction when it is associated CR falls within the same aggregation class in more than 80% of the scenario pairs (occurrence ≥ 80%) where that determinant value is present. The mean of the occurrences in the 10 datasets was used to select the discriminating determinant values (Equation 5). The confidence in the observed occurrence rates was assessed by calculating corresponding 95% confidence intervals.

$$\text{Average occurrence} = \frac{1}{10}\sum_{i=1}^{i=10} \text{Occurrence}_i \tag{5}$$

For example, to evaluate whether the presence of the determinant value "C9: high-specification glove box or isolator" in a scenario pair is associated with the dominance of the consumer exposure source, we used the following equation:

$$\text{Occurrence}_{C9} = \frac{\text{Number of pairs}_{\ C9,\ \text{consumer exposure dominance}}}{\text{Number of pairs}_{\ C9}}$$

This occurrence is calculated for the 10 datasets. If the average occurrence is higher than 80%, then the determinant value "C9: high-specification glove box or isolator" is considered relevant for decision tree construction.

For illustrative purposes of the decision tree, only 3 levels were considered. The levels were built following a decreasing order of the occurrences. For example, a determinant value that enables the discrimination of the dominant exposure source in 90% of cases will be positioned in 1 level higher in the decision tree than a determinant value that allows for the discrimination of the dominant source in 80% of cases.

A summary of the decision tree construction is shown in Fig. 1.

Results

Modeling

Categorical determinants were represented approximately equally in the 5.10^4 scenarios. Table 3 shows the distribution of number of scenarios across the ART categorical determinants. The determinants of ConsExpo (Table 1) are all numerical.

The high number of scenarios with no localized controls is due to the fact that localized controls are not

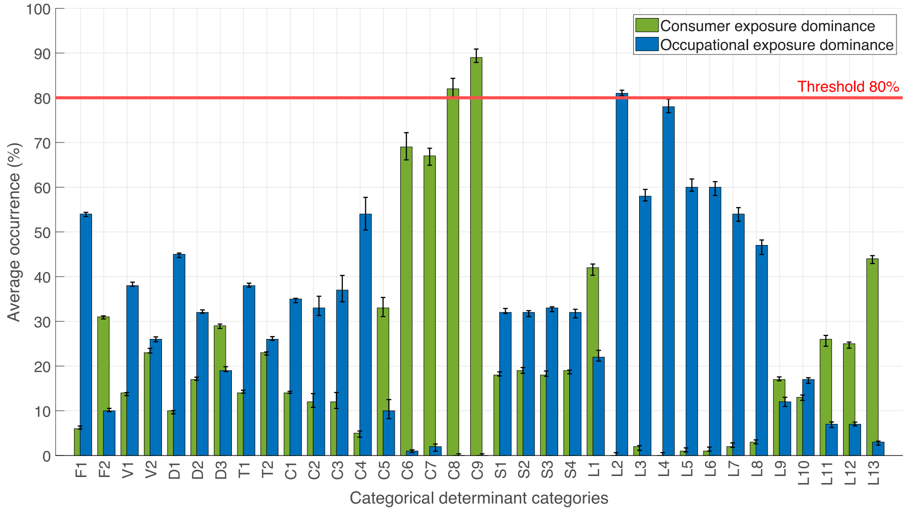

Fig. 2. Average occurrence with 95% confidence interval for hairspray exposure and surface spraying exposure dominance when each of the categorical determinants values is present in a scenario.

assigned to scenarios whenever booths and spray rooms are used or for outdoor activities, as shown in Fig. S1.

For categorical determinants, the number of scenarios per value depends on the number of determinant values. A small number of values per determinant leads to a higher number of scenarios per value.

Daily average concentrations in air for hair spray scenarios ranged from 2.10^{-5} to 1.72 mg/m^3. While concentrations for surface spraying ranged from 7.10^{-9} to 206 mg/m^3.

Decision tree construction

In this example, "Dispersion" and "Control measures" were the determinants that discriminated the dominance of one source over another while meeting the 80% occurrence criterion. Figure 2 shows the average occurrences and their 95% confidence intervals of hairspray exposure (consumer exposure) dominance and surface spraying (occupational exposure) dominance, respectively, for each determinant value shown in Table 3.

In our case, aggregation should be considered when the surface spraying scenario does not include high or medium glove box use, which provide permanent encapsulation of the emission source, combined with effective local exhaust ventilation (Fransman et al. 2013), and when spraying is not performed outdoors near buildings. In fact, when combining hairspray exposure and surface spraying exposure, with the latter restricted to scenario's use of "High-specification glove box/isolator" and "Medium-specification glove box," the results suggest that hairspray exposure is typically dominant over surface spraying exposure. These findings were observed on average in 89% (95% confidence interval [CI]: 87.89% to 90.90%) and 82% (95% CI: 80.21% to 84.34%) of scenarios where these determinant values were present respectively. An "Outdoor close to buildings" activity leads to the dominance of surface spraying exposure over hairspray exposure on average in 81% (95% CI: 80.47% to 81.68%) of the scenarios where this level was present. The results for the 10 datasets analyzed separately are presented in Figs. S2 and S3.

The use of crossflow spray rooms showed a trend toward surface spraying exposure dominance. The occurrence of this finding ranged between 75% and 81%. The average occurrence was 78% (95% CI: 76.66% to 79.70%). For numerical determinants, only the weight fraction in the hairspray showed an occurrence close to 80% in 2 data sets (79.31% and 79.21%). A chemical substance representing less than 2% of the hairspray composition suggests the dominance of surface spraying exposure on average in 74%. The occurrence of this finding ranged between 67% and 79% of cases. These determinants are not considered in the decision tree construction as the average occurrences of the source dominance does not exceed 80%.

The decision tree is shown in Fig. 3. The probability of the aggregation decision being right decreases as the levels decrease. The decision tree levels are independent from each other, and the order is interchangeable. Scenarios not satisfying 1 level are not excluded in the next level. Reading of the decision tree can start at any level and the order of the levels of the decision tree is based on decision relevance (in descending order of occurrence).

We plotted the concentration distributions for the 2 exposure sources for illustrative purposes to show their overlap. The greater the overlap, the higher the probability of encountering scenario pairs with a CR

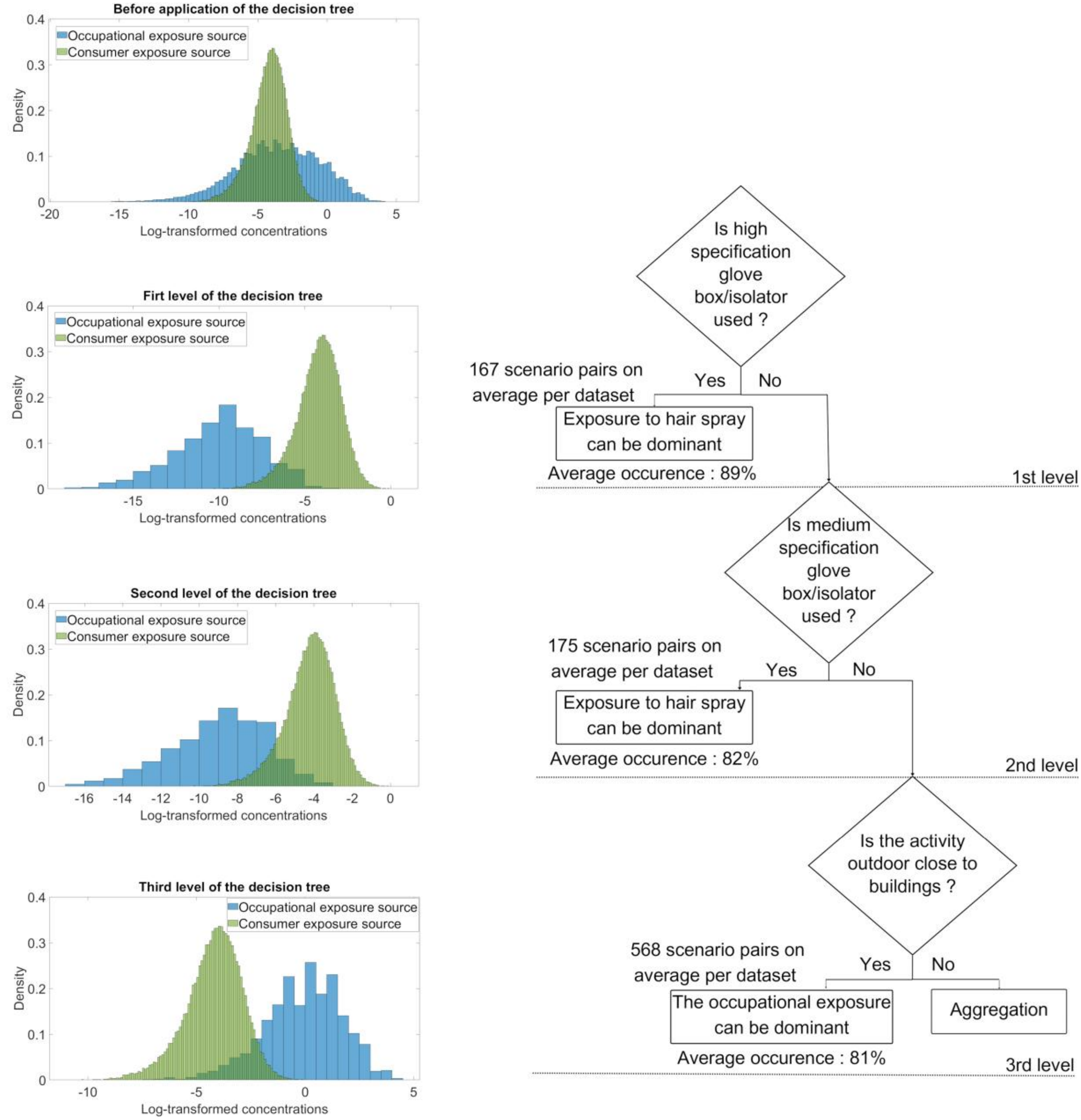

Fig. 3. Decision-making flowchart for aggregating exposure sources and distributions of chemical concentrations in the air for hairspray and surface spraying exposure.

between 0.1 and 10. The overlap between the 2 distributions was estimated using kernel density functions. Before applying the decision tree, the overlap was found to be 58% (meaning that no decision can be made regarding which source is dominant, therefore aggregation is always considered). At the first level of the decision tree, the distribution of air concentrations in surface spraying scenarios using high-specification glove boxes/isolators (840 scenarios) was compared with the 5.10^4 scenarios of hair spray exposure. This overlap was reduced to 13% (meaning that aggregation can be avoided; the distributions show that concentrations for hairspray exposure are higher than those for surface spraying).The same finding for the second level where the overlap between the distribution of air concentrations in surface spraying scenarios with medium-specification glove boxes (865 scenarios) and the 5.10^4 hair spray exposure scenarios was 21%. At the third level, the overlap between the distribution of air concentrations in occupational scenarios where the activity takes place outdoors near buildings (2,787 scenarios) and the 5.10^4 hair spray exposure scenarios was 17% (meaning that aggregation can be avoided; the distributions show that concentrations for surface spraying are higher than those for hairspray).

Discussion

The current study is situated strictly within an exposure assessment framework, aimed at comparing 2 exposure sources. Therefore, these findings should not be interpreted as direct indicators of health risk. Instead, they are intended to support the identification of key contributors to overall exposure.

This proof of concept is based on 2 randomly chosen exposure sources (hairspray exposure and surface spraying exposure), from 2 different environments: occupational and consumer, which were modeled using ART and ConsExpo. The chosen exposure sources could be described by multiple scenarios. 5.10^4 different scenarios were created for each source. The size of this dataset was chosen to cover a maximum number of different scenarios and ensure efficient computation time. For future use of this methodology, restricting the number of scenarios used could potentially be reduced by additional information and thorough understanding of the exposure scenarios. For instance, information of the variation range of the weight fraction of the substance in the product used (hair spray) can reduce the size of the dataset of scenarios to be compared and increase the decision accuracy.

The creation of paired scenarios allowed for the comparison of the 2 sources by considering a multitude of exposure situations. The CR enabled the classification of the pairs into one of 3 aggregation classes: occupational exposure dominance, consumer exposure dominance, or aggregation. The determinants that led to this classification, and met the chosen occurrence threshold of 80%, were identified and used in the construction of the decision tree. For this proof of concept, only 3 categories satisfied the 80% criterion (use of high-specification glove box, use of medium-specification glove box and activities conducted outdoors near buildings). This threshold was arbitrary and was chosen specifically to illustrate this proof of concept. The temporal dimension was considered in the exposure scenarios as a determinant within the utilized models (ART and ConsExpo). Consequently, when a determinant category such as the use of a glove box is identified as influencing whether environmental exposure is dominant over occupational exposure, this conclusion remains valid regardless of the duration of occupational exposure.

The CR is a parameter we used to compare the 2 sources. Thresholds for this ratio were arbitrary and specific to illustrating this proof of concept. There is currently no common practice for judging the dominance of an exposure source over another, specifically across different exposure environments. Additionally, the accuracy of decision on aggregation relies on the accuracy of the models (ART and ConsExpo) estimates, as well as the size of the dataset for comparison, whether it covers all possible exposure scenarios or not.

The substance-specific approach to decision-making on aggregation requires the analysis of all available information on the substance and its exposure scenarios. This process can be resource-intensive, especially when data on the substance are scarce or incomplete. In contrast, the decision tree approach simplifies the assessment process by providing a standardized framework that allows for prior exclusions based on available data. This approach will be tested in case studies carried out within the framework of the European PARC.

The objective behind this proof of concept is to create a tool that enables authorities and practitioners, based on simple questions, similar to those presented in Fig. 3, to decide on whether or not to aggregate exposure sources and routes, thereby making informed decisions for health protection. The prospects for developing a decision-support tool for aggregation are broad. The tool is intended to be flexible and user-friendly, enabling the refinement of the dataset used in the analysis, on the basis of prior knowledge. It would also allow users to define the occurrence threshold on the basis of regulatory standards or internal guidelines, as well as the CR at which 1 source is considered to be dominant in relation to another.

The exposure routes and sources to be compared will consist of those whose exposure can be modeled by currently available exposure models, such as the exposure scenarios that can be modeled by ART and ConsExpo. The number of sources to be compared using few determinants while ensuring a reasonable calculation time, as well as the comparison of exposure routes, would be subject for future research.

Conclusion

This study provides an extensive analysis of the determinants influencing occupational and consumer exposure to chemicals in surface spraying and hair spray, respectively. The created scenarios cover a wide range of exposure situations, allowing for a data-driven assessment. Key findings indicate that the use of high- or medium-specification glove boxes results in occupational exposure that is negligible compared with the exposure from hair spray. In contrast, activities conducted outdoors near buildings show a significant trend toward occupational exposure dominance.

This proof of concept demonstrates the feasibility of developing a decision tree to aid decision-making on the exposure aggregation and prioritization of 2 exposure sources, thereby aiding authorities and practitioners in making informed decisions for health protection.

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Author contributions

Writing original draft: H.C. Conceptualization, methodology, analysis, and results interpretation: H.C. and D.V. Results discussion, writing-review, and editing: H.C., D.V., N.V. G., K.D. B., A.C., I.B.O., and C.B.

Supplementary material

Supplementary material is available at *Annals of Work Exposures and Health* online.

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Conflict of interest

The authors declare no competing interests.

Data availability

All data used in this study were synthetic (generated in silico). The synthetic datasets can be reproduced using the methods described in the manuscript. No external datasets were used.

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