Regulatory Toxicology and Pharmacology 94 (2018) 240–244

Contents lists available at ScienceDirect

Regulatory Toxicology and Pharmacology

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

Impact of exposure factor selection on deterministic consumer exposure assessment

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ARTICLE INFO

Keywords:
Consumer product
Exposure assessment
Deterministic
Exposure factor

ABSTRACT

Deterministic exposure assessment has uncertainty about the selection of input parameters on the resulting estimates. The purpose of this study was to compare inhalation exposures estimated by a specific percentile of each of the three exposure factors in deterministic assessment with population exposure. Exposure to nine household care products, namely a deodorizer, six cleaning products, and two disinfectants were investigated. The population exposures were individually calculated for three exposure factors (frequency of use, amount of use, and duration of use) from an existing database of 3333 participants representing the national population. Deterministic exposure assessment was conducted according to various percentiles of exposure factors. 99th percentiles of population exposure in all nine consumer products were 1.3–2.4 times greater than the 95th percentiles. Inhalation exposures based on the 75th percentiles of each of the three exposure factors in deterministic assessment were much lower than the 95th percentiles of the population exposure. Deterministic exposure estimates using 85th to 99th percentiles of each of the three exposure factors were closer to the 95th percentiles of the population exposure. We concluded that exposure factors in deterministic assessment should be greater than the 75th percentile to more precisely estimate exposure of at-risk groups.

1. Introduction

Exposure to chemicals in consumer products (CPs) is often estimated by indirect assessment using exposure scenarios. Model-based exposure assessments of chemicals in CPs have been conducted using probabilistic and deterministic methods. Probabilistic approaches consider probability distributions in input variables and predict the distribution of exposure in a target population (Cullen and Frey, 1999). Deterministic methods use point estimates of input parameters to provide a single worst-case value (IPCS, 2005). Deterministic methods are often used to screen CPs for hazardous exposures.

Despite the allure of the apparent simplicity of deterministic methods, outcome may be strongly dependent on the selection of the percentile of the distribution of exposure factors. Although exposure factors can be obtained through surveys, behavioral observation, or activity models (Parmar et al., 1997), information on exposure factors is often limited. In order to estimate exposure with exposure factors, knowledge of the type of distribution (ie, normal, log-normal, other) is important, especially when estimating higher ranges of exposures (Hakkinen et al., 1991). However, it is difficult to find the exact patterns of distribution of exposure factors through the small samples. Even though the pattern of distribution on actual population determined by sample, which percentile is chosen as an input value may affect the uncertainty of the results. Deterministic methods can overestimate exposure levels because they use extreme values for the parameters (Fryer et al., 2006). The multiplication of several high percentiles together may result in the unrealistic estimates. In addition, the uncertainty of a result represented by a single value is not quantitatively considered in exposure estimation (Ferrier et al., 2002).

There are some guidelines of selection exposure factors to estimate exposure to CPs by deterministic methods. The Consumer Exposure and Uptake Model (ConsExpo) of the Dutch National Institute for Public Health and The Environment (RIVM) is an example of a CP exposure model (van Veen, 1995). ConsExpo 4.0 recommended that the specific percentile value of each exposure factor's distribution could be used to estimate exposure levels by deterministic approaches (Delmaar and Schuur, 2016; Höglund et al., 2012). To avoid unrealistically high estimates and to maintain conservative exposure estimates, they selected a 75th percentile as a representative value for each parameter (Delmaar and Schuur, 2016). In ConsExpo fact sheets, the 75th percentile of

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https://doi.org/10.1016/j.yrtph.2018.02.007
Received 7 November 2017; Received in revised form 8 February 2018; Accepted 9 February 2018

exposure factors (frequency, amount, spray duration, and exposure duration) have been chosen as the default values for CPs such as cosmetics, cleaning products, and disinfectant products (Bremmer et al., 2006; Prud'Homme de Lodder et al., 2006a; Prud'Homme de Lodder et al., 2006b). One study conducted deterministic exposure assessment for CPs using ConsExpo's defaults (Gosens et al., 2014).

The European Center for Ecotoxicology and Toxicology of Chemicals developed the Targeted Risk Assessment (TRA) tool for first tier assessments of consumer exposure (Ecetoc, 2009). Many default exposure factors in TRA were obtained from the RIVM fact sheets. When specific information was not available, values were derived using expert judgment. The United States Environmental Protection Agency (US EPA) developed the Consumer Exposure Model (CEM) for cleaning products (EPA, 2017). CEM provided the exposure factors by three classes of high, medium and low.

Although a certain percentile was proposed in the selection the exposure factor in deterministic assessment the precise degree of uncertainty remained unknown. Errors associated with the selection of a specific percentile for an exposure factor need to be determined. The purpose of this study was to compare inhalation exposures estimated by a specific percentile of each of the three exposure factors in deterministic assessment with population exposure. Population exposure was calculated by exposure factors of 3333 participants representing the national population.

2. Methods

This study utilized use patterns of 9 CPs collected from 3333 participants. In a previous study, exposure factor data for 9 CPs such as a deodorizer (fabric deodorizer), cleaning products (dishwashing detergent, bathroom cleaner (bottle and trigger type), toilet rim cleaner, glass cleaner, and floor cleaner), and disinfectants (household bleach and mold stain remover) were collected (KNIER, 2012). Detailed information pertaining to data collection has been reported elsewhere (Park et al., 2015). Briefly, the nationwide survey was conducted in 15 metropolitan areas and provinces in Korea. The surveyed population included those age 15 years and older. The three exposure factors (frequency of use, amount of use, and duration of use) for the 9 CPs were obtained through face-to-face interviews.

The characteristics and percentage of usage of the 9 CPs are presented in Table 1. Exposure factors were obtained from only users of each products (a range of participants: 442-2741 depending on CPs). The percentage of people using dishwashing detergent was the largest (82%) among the 3333 participants, and the percentage of people using floor cleaner was the lowest (13.3%). The survey population is referred to as 'parent population' in the following text.

Table 1
Characteristics and percentage of usage for the 9 consumer products.

Product[a]	Container type	The percentage of users (%)	The number of users
Dishwashing detergent	Pump	82.2	2741
Household bleach	Bottle	56.4	1881
Fabric deodorizer	Trigger	36.1	1204
Bathroom cleaner (Bottle)	Bottle	20.8	693
Bathroom cleaner (Trigger-type)	Trigger	18.3	609
Toilet rim cleaner	Bottle	17.7	590
Mold stain remover	Trigger	16.0	532
Glass cleaner	Trigger	14.4	480
Floor cleaner	Bottle	13.3	442

[a] The formulation of all products was liquid. Reorganized from a previous report (KNIER, 2015).

Table 2
Input parameters for inhalation exposure assessment.

Parameter	VR (/h)	V (m^3)
Product		
Dishwashing detergent	2.5[b]	24.5[b]
Household bleach	2[a]	9.3[a]
Fabric deodorizer	0.5[c]	33.3[c]
Bathroom cleaner (Bottle)	2[a]	9.3[a]
Bathroom cleaner (Trigger-type)	2[a]	9.3[a]
Toilet rim cleaner	2[a]	9.3[a]
Mold stain remover	2[a]	9.3[a]
Glass cleaner	0.5[c]	33.3[c]
Floor cleaner	0.5[c]	33.3[c]

Abbreviations: VR, ventilation rate; V, volume of space.
[a] Ventilation rate and volume of the bathroom from KNIER (2015).
[b] Ventilation rate and volume of the kitchen from KNIER.
[c] Ventilation rate and volume of the living room from KNIER.

2.1. Exposure estimation

This study considered daily exposure to 9 CPs via inhalation. Exposure estimate was daily exposure when the product was used. Daily inhalation exposure to each product was estimated using Equation (1) based on a model suggested by the National Institute of Environmental Research (KNIER) in Korea (KNIER, 2015):

$$DE_i = \frac{A_p \times W_f \times \exp(-\mathrm{VR} \times t) \times \mathrm{IR} \times abs \times D \times n}{V \times \mathrm{BW}} \tag{1}$$

where DE_i is daily exposure via inhalation (mg/kg/day), A_p is the amount of product used (mg), W_f is the fraction of a specific chemical in the product (unitless), VR is the ventilation rate (h^{-1}), t is the duration of consumer product use (h), IR is the inhalation rate (m^3/h), abs is the absorption rate (unitless), D is the exposure duration (operation period) (h/event), n is the frequency of product use (event/day), V is the volume of space in use (m^3), and BW is body weight (kg).

The input parameters based on the exposure scenarios for each product are given in Table 2. The value of W_f was assumed to be 0.01 (1%). abs was assumed to be 1. By using an assumed weight fraction of 1%, the resulting value can be scaled by the actual weight fraction, when obtained. The IR was assumed to be 0.6 m^3/h, which was the mean inhalation rate of the Korean adult population taken from the default database of the Korean exposure factors handbook (Jang et al., 2007). D was assumed to be 82 min, which was the duration of housework from the Korean exposure factors handbook. BW was assumed to be 64.2 kg, which was the mean weight of a Korean adult, as reported in the default database of the KNIER exposure assessment tool (KNIER, 2015). A_p, t, and n were based on survey data.

2.2. Data analysis

To obtain the exposure distribution of the parent population, the individual exposure of each product user was estimated using exposure factors for the 9 CPs. The exposure of one subject was calculated by three exposure factors (frequency of use, usage amount, and duration of use) from the subject. Based on a deterministic approach, the exposures were estimated using the same percentiles of the three exposure factors. The exposures were calculated with the 50th, 75th, 85th, 95th, and 99th percentiles of each exposure factor, while other factors were based on values previously defined in *2.1. Exposure estimation* and Table 2. The point estimates of the exposure values were compared to the exposure distribution of the parent population. R version 3.3.2 (64-bit), an open-source statistical software programming language, was used for calculating median and range of the three exposure factors for the 9 CPs and the differences in exposures between samples and the parent population.