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Overarching issues – ConsExpo Web and fact sheets

Authors: RIVM ConsExpo team
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National Institute for Public Health and the Environment
Postbus 1 | 3720 BA Bilthoven
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1 Introduction

The consumer exposure assessment tool ConsExpo (ConsExpo v3) has been released to the public for the first time in 2001. Since this first release, the tool has been updated several times. In 2005, an updated version 4.1 was released. The ConsExpo exposure assessment tool was made available as a web application, ConsExpo Web (www.consexpoweb.nl), in 2016. An updated version of ConsExpo Web, version 1.0.3, has been released in January 2018.
In support of ConsExpo, fact sheets have been compiled in which default models and input parameters are suggested for different product groups. Default models and input values for the products described in the fact sheets are included in the ConsExpo tool itself, where they can be used to generate standardized exposure assessments. ConsExpo and the fact sheets are continuously being developed and brought up to date. Since the release of ConsExpo 4.1 in 2005, multiple updates have been made to the product defaults in the ConsExpo tool and fact sheets, which are specified in Table 1 below.

Table 1. Timeline of updates of defaults in fact sheets and the ConsExpo tool

Year	**ConsExpo**	**Fact sheets**
2005	ConsExpo 4.1	
2006		• General • Pest control • Cosmetics • Disinfectants • Cleaning products
2007		• Do-it-yourself • Paint products
2010	Update Defaults in ConsExpo 4.1	
2014		Update General
2016	ConsExpo Web 1.0	
2018	ConsExpo Web 1.0.3	Update Cleaning products

In some instances adaptations made in a method to derive default values, have led to an update of the defaults included in the ConsExpo tool, although the fact sheet from which the defaults originated was not updated. The defaults provided in the tool may thus deviate from those in (outdated) versions of a fact sheet. Furthermore, changes in the ConsExpo Web tool and updates of methods and data that are carried through in any specific fact sheet may leave elements of other fact sheets outdated.

In this document we describe methods that are used in multiple fact sheets to derive default values. We focus on methods that have been subject to changes in the course of time and thereby have resulted in fact sheets getting outdated. As such, the document provides a centralized reference and documentation of these, so called ‘overarching issues’.

We provide an overview of the timeline of the adaptations made to these overarching issues and the impact of these adaptations on the ConsExpo default values. This timeline will indicate which fact sheets document defaults that are considered outdated.
In addition to defaults proposed in the fact sheets, the ConsExpo tool contains default assessments. These are in principle based on the defaults proposed in the fact sheets. In cases where the fact sheets have become outdated, the defaults included in ConsExpo are actualized. Thus, the latest version of the ConsExpo tool will always include the up-to-date versions of all the default values. For the outdated fact sheets, default values may therefore deviate from those presented in ConsExpo.

This document is intended to be kept up to date and to reflect the current state of affairs at all times.

2 Overarching issues – a summary

The following overarching issues are discussed in this document:

1. Spray model and defaults for mass generation rate, spray duration (inhalation) and release duration (dermal)
2. Mass transfer coefficient
3. Dilution as parameter

A summary of the adaptations regarding these issues is given below:

1. In the derivation of defaults for the spray model two different adaptations have been made:
   a. The defaults for the particle size distribution and the 'airborne fraction' have been derived from experimental data in 2010. The method is described in Delmaar & Bremmer (2009), with defaults that have been derived for all spray products (RIVM, 2010). Fact sheets that date before 2010 are to be considered outdated with respect to these parameters. The defaults in the ConsExpo tool for the earlier fact sheets have been actualized (see Table 1).
   b. In the most recent Cleaning Products Fact Sheet (Meesters et al., 2018), a different method is used to derive defaults for the 'mass generation rate' and 'spray duration' from experimental data presented earlier (Delmaar & Bremmer, 2009). Defaults for the 'mass generation rate' and 'spray duration' will be adjusted in the relevant fact sheets when these are updated in future. In the ConsExpo Web version 1.0.3, the defaults are still derived using the old method. However, since the impact of the new defaults on the estimated exposure is expected to be minimal, the old defaults for these parameters can still be used.
2. ConsExpo provides models to estimate the mass transfer coefficient in the 'exposure to vapour' model. It was suggested in all fact sheets published before 2018 to use these models by default. With the ConsExpo Web 1.0.3 release and the publication of the updated version of the Cleaning Products Fact Sheet (Meesters et al., 2018), it is proposed to use a value of 10 m/h as a default, instead. The fact sheets published before 2018 are considered outdated in this respect. The default of 10 m/h is implemented in the tool and should be used with default assessments from previous fact sheets.
3. ConsExpo Web 1.0.3 introduces a dilution parameter in the 'exposure to vapour' model. The updated version of the Cleaning Products Fact Sheet (Meesters et al., 2018) provides defaults for this parameter. Earlier fact sheets suggest emulating dilution of the product by adjusting the weight fraction of the product. This method is considered depreciated but can still be used. It leads to equivalent results as the use of the 'dilution' parameter in the updated ConsExpo tool. Defaults from earlier fact sheets have not been updated in the tool.

In the following sections these overarching issues are discussed in more detail.

3 Overarching issues – discussion in detail

3.1 Spray model and defaults

The ConsExpo spray model and the defaults provided for it have undergone multiple changes in different fact sheets in the course of time. Since the release of ConsExpo 4.1 in 2005, changes have been made with respect to the following three aspects:

1) The way in which defaults for the **particle size distribution** are derived.
   This adjustment impacts the 'particle size distribution' parameters (median and C.V) and the 'airborne fraction' parameter (in effect since 2009, described in Delmaar & Bremmer, 2009).
2) The way the parameter 'spray duration' is assumed to be used in a simulation.
   This change impacts both the **'spray duration' and 'mass generation rate'** parameters (in effect since (Meesters et al., 2018)).
3) The '**weight fraction non-volatile'** parameter has been removed from the model.
   This has no impact on the calculated exposure (implemented in the release of ConsExpo Web 1.0, 2016).

Defaults in the relevant fact sheets from before the time the method to derive defaults was introduced have not been altered. The defaults will be updated in the updated versions of the fact sheets in future. Also the latest version of the ConsExpo tool, ConsExpo Web version 1.0.3 includes the updated default values.

Below we describe shortly the changes in the defaults and model (points 1-3 above).

3.1.1 Adjustment particle size distribution

In 2005, defaults have been set based on experimentally determined particle size distributions. In 2009, defaults have been adjusted in order to give a better description of the respirable particles in the distribution (i.e. particles with diameter < 22.5 µm). The method is described in detail in Delmaar & Bremmer (2009). It has been applied in the analysis of additional product data (RIVM, 2010).

The 'airborne fraction' parameter describes the fraction of the sprayed respirable particles that becomes airborne and is available for inhalation. In 2005, defaults for the airborne fraction were derived from fitting the model to air concentration measurements arising during simulated use of spray products. In 2009, defaults for the 'airborne fraction' have been adjusted to incorporate adjustments to the defaults for the particle size distribution. I.e. it now also includes a normalisation factor for the adjusted particle size distribution. Hence, the 'airborne fraction' has become an aggregate parameter that is obtained from two parameters fitted from experimental data. Defaults based on this method have been derived for multiple products (RIVM, 2010). These defaults are included

in the latest version of the tool and will be used in the relevant fact sheets when they are updated.

3.1.2 Adjustment of the default for 'spray duration' and 'mass generation rate'

To quantify the total mass of substance released when using a consumer spray, ConsExpo uses two parameters: the 'spray duration' and 'mass generation rate', the product of which is the total mass of product sprayed during use.
Defaults for the mass generation rate are based on experimentally determined information (Delmaar & Bremmer, 2009).
For defaults derived between 2005 and 2018, the spray duration accounted for the total time the spray was used, including the 'dead time' between intermittent applications of the spray. The ConsExpo spray model assumes that mass is released at a constant (mass generation) rate during the spray duration. To compensate for the over-estimation of the total mass released during the use of a spray, the default for the 'mass release rate' was derived by lowering measured release rates from actual sprays so that:

[*Mass generation rate default] x [Spray duration default]*
=
[Mass generation measured] x [Actual spray duration]

Since the publication of the updated Cleaning Products Fact Sheet (Meesters et al., 2018), the default for spray duration is given for the net spraying time, not accounting for 'dead time' between spraying. The default for the mass generation rate is derived directly from the measured release rates for the different sprays. All other fact sheets will be adapted on this point with the future updates. The impact of using the older default values on the calculated exposure (in the meantime) is expected to be minimal.

3.1.3 Weight fraction non-volatile

This parameter was included in the ConsExpo spray model from 2005. The value of the parameter does not impact the outcome of the exposure evaluation, however. It is therefore removed from the (updated) spray model implemented in ConsExpo Web, from version 1.0 onward.

Situation in ConsExpo Web and Fact Sheets – October 2018:
In Table 2 below the current status of fact sheets on the method that are used to derive defaults for the particle size distribution and spray duration, are summarized. In this table, 'Method 2005' refers to the "old" method employed since the release of ConsExpo 4.1. 'Up-to-date' refers to the "newer" methods described above.

Table 2. Overview of update status of the different RIVM ConsExpo product category fact sheets

Fact sheet	Year of publication	Update status	
		particle size distribution/ airborne fraction	spray duration/mass generation rate
Cleaning products	2018	up-to-date	up-to-date
Cosmetics	2006	method 2005	method 2005
Disinfectant products	2006	method 2005	method 2005
Do-it-yourself	2007	method 2005	method 2005
Paint products	2007	method 2005	method 2005
Pest control products	2006	method 2005	method 2005

ConsExpo Web 1.0.3 defaults are considered to be up-to-date and can be used without adjustments. The method to derive the spray particle size distribution and airborne fraction are all in line with the method proposed in Delmaar & Bremmer (2009). For the 'spray duration' and 'mass generation rate' an updated method is used in the updated version of the Cleaning Products fact sheet (Meesters et al., 2018) which is not yet implemented for the defaults derived in the other fact sheets. However, the impact of the defaults derived with the new method on the exposure assessment is expected to be minimal.

3.2 Mass transfer coefficient

Default value for the mass transfer coefficient

The ConsExpo inhalation model 'exposure to vapour: evaporation' requires an estimate of the mass transfer coefficient as input. The mass transfer coefficient determines the transfer of an evaporating substance from the product surface across a 'boundary layer' of stagnant air in contact with the product, into bulk indoor air. The mass transfer coefficient determines the rate of evaporation of the substance from the product.

The mass transfer coefficient depends on the diffusion coefficient of the substance through air, the speed of air moving over the product's surface, and the surface area of the product. In both ConsExpo 4.1 and ConsExpo Web two different, relatively crude methods to estimate the mass transfer coefficient are provided: Langmuir's and Thibodeaux's models. For the update of ConsExpo Web to version 1.0.3 (January 2018), both these models have been evaluated by considering other data and models for comparison.

On the basis of this evaluation, it was concluded that the estimates provided by the models seem to be systematically too high and that, instead of the use of these models, the use of a default mass transfer coefficient of 10 m/h is recommended.

Below, we discuss the Langmuir's and Thibodeaux's default models including their limitations. Next, alternative information and more representative models to estimate the mass transfer coefficient are introduced. These models are applied to a set of substances for which the necessary physical-chemical information is given. In a range of representative scenarios, the mass transfer coefficient is estimated. On the basis of the range of estimated values and information on published

data, we propose a default value of the mass transfer coefficient in ConsExpo and the fact sheets.

ConsExpo 4.1 and ConsExpo Web default methods

Langmuir

Langmuir's equation (Langmuir, 1913) describes the evaporation into vacuum. It essentially ignores the resistance by the boundary layer. In this way, it represents the absolute maximum of transfer, but the calculated values will not be representative of realistic indoor conditions.

$$h_m = (RT/(2\pi M))^{0.5}$$

Thibodeaux

Thibodeaux's method as implemented in ConsExpo was taken from Jayjock (1994). This reference in turn quotes a method reported in (US-EPA, 1981), based on Thibodeaux (1979). The method relies on the extrapolation of a measured transfer coefficient from one substance ('1') to another ('2'), based on the molecular weight. Here, it is assumed that the diffusion coefficient D scales with the molecular weight M as:

$$\frac{D_1}{D_2} = (\frac{M_2}{M_1})^{0.5}$$

The US-EPA (1981) used a measured mass transfer rate of water and a number of default assumptions to arrive at (in m/h)

$$h_m = 30 \times (\frac{18}{M})^{1/3}$$

for a substance with molecular weight M (g/mol).

The conditions under which the mass transfer rate of water has been measured are unknown (i.e. indoors or outdoors, the size of the source, temperature, et cetera). It is unclear how representative the measured mass transfer rate is for indoor residential settings.

Alternative models to estimate mass transfer indoors

In addition to the methods presented above, other models and information on the mass transfer coefficient are available. Below, a brief overview of these methods is given.

Boundary layer ('Kiil' model)

Aerodynamics provides a fundamental method to calculate the mass transfer from surfaces, the so-called 'boundary layer' theory (see, for example Welty, 2007). Based on this theory, Kiil (2006) provides an equation to estimate the mass transfer coefficient that takes into account the diffusion of the substance in air D, the air velocity over the surface v, and the size of the emitting source, characterized by the 'characteristic length' L. Equation 21 in Kiil (2006) expresses the convective mass transfer over a surface in the dimensionless Reynolds (Re) and Schmidt (Sc) numbers as,

$$h_m = 0.664 \frac{D}{L} Re^{\frac{1}{2}} Sc^{\frac{1}{3}}$$

with

$$Re = L \frac{v}{\mu}$$

and

$$Sc = \frac{\mu}{D}$$

we obtain

$$h_m = 0.664 \times D^{\frac{2}{3}} / \mu^{\frac{1}{6}} \times (\frac{v}{L})^{0.5}$$

Here is μ the kinematic viscosity of air, 1.50x10^{-5} m^2/s.
Using this equation, the units of h_m are the same as used to express D and L (e.g. m/h if D is in m^2/h and v is in m/h).

Sparks
Sparks et al. (1996) determined the experimental correlation between Nusselt, Reynolds and Schmidt numbers (Nu, Re and Sc) for a cylindrical cup filled with pure p-dichlorobenzene. Schmidt, Reynolds and Nusselt numbers were determined for a range of indoor air velocities over the surface of 0.05 – 0.6 m/s. The authors suggest the following experimental correlation to predict the mass transfer coefficient:

$$h_m = 0.33 \times D \times Re^{0.67} / L$$

With the expression for the Reynolds number Re given above, this becomes

$$h_m = 0.33 \times D \times (L \times v/\mu)^{0.67} / L$$

Here, the units of the calculated h_m are the same as used to express D and L.

US-EPA AMEM method
US-EPA provides a method in the AMEM (Arthur D. Little Polymer Migration Estimation Model; (US-EPA, 1990)) to estimate the mass transfer coefficient. This method is also implemented in Consumer Exposure Model (CEM) (US-EPA, 2016), . AMEM gives an expression for the diffusion coefficient in air, (Eq 4.21 in (US-EPA, 1990))

$$D = 3.3/(2.5 + M^{\frac{1}{3}})^2$$

Here, M is the molecular weight of the substance in g/mol. The diffusion coefficient D is calculated in cm^2/s.

For the mass transfer coefficient under general ambient air conditions (US-EPA, 1990, eq 4-35) suggests

$$h_m = 1.3 \times D$$

as a generic estimate of the mass transfer coefficient. Combining these two equations and converting from cm/s to m/h, leads to

$$h_m = 46.8 \times \frac{3.3}{(2.5 + M^{1/3})^2}$$

Information on mass transfer coefficient in literature
In addition to the calculation methods for the mass transfer presented above, measured values of the mass transfer coefficient are given in literature. Weschler and Nazaroff (2008) provide a review of data on emission factors for SVOCs from solid materials indoors. Data they considered covered a span of 2.5-3.9 m/h. Based on this, the authors indicate a range of 1-10 m/h as a typical range of values for this parameter.

Comparing estimates of the mass transfer coefficient
In this section, we provide a comparison of the different methods discussed to estimate the mass transfer. This was done by evaluating the different methods in a range of scenarios representative of indoor consumer exposure conditions. Indoor conditions and product properties influence the estimate of h_m via the air velocity v and the product 'characteristic length' L respectively.
According to a review by McCready and Fontaine (2010) there is limited information on the air velocity indoors. But the information that is available indicates that 0.05 m/s is a typical median value for indoor conditions and 0.1 m/s represents a somewhat high, but still representative value.
For the emission surface we consider moderately small dimensions as a smaller source dimension tends to lead to higher estimates of the mass transfer. For the scenarios we adopted as indicative the values of 0.3 and 1 meter respectively. For many products the surface area will be larger, for some smaller, but we consider the range taken in the scenarios to provide a reasonable indication of a fairly small source.
In summary, the following scenarios are evaluated:

Table 3. Overview scenarios with characteristic length L and air velocity v

Scenario	L(m)	v(m/s)
I	1	0.1
II	1	0.3
III	0.3	0.3

Scenarios I and II are expected to provide relatively high but representative values of the mass transfer coefficient. Scenario III is expected to represent a situation where emission is faster than for typical indoor conditions and most sources.

The mass transfer coefficient is estimated in these three scenarios for a number of substances for which the necessary physical chemical properties (molecular weight and diffusion in air) are given. The data was taken from (US_EPA 1990), see Table 4.

Table 4. Substances and their physical properties used in the evaluation of models to estimate the mass transfer coefficient

Substance	Molecular weight (g/mol)	Diffusion coefficient in air (m^2/s)
Benzene	78.11	0.00000732
Hexane	86.17	0.00000932
Benzyl acohol	108.13	0.00000712
Trichloroethylene	131.4	0.00000875
Pentachloroethane	202.31	0.00000673
Hexachlorobenzene	284.8	0.000012
Diisooctyl phthalate	390.56	0.00000377

Results and discussion

In the figure below the calculated mass transfer coefficients using different methods in different scenarios have been plot. The molecular weight of the different substances was used as the independent variable on the x-axis.

It should be noted that the evaluation of the Langmuir model was left out of the plot as values calculated using this model are typically several orders of magnitude higher.

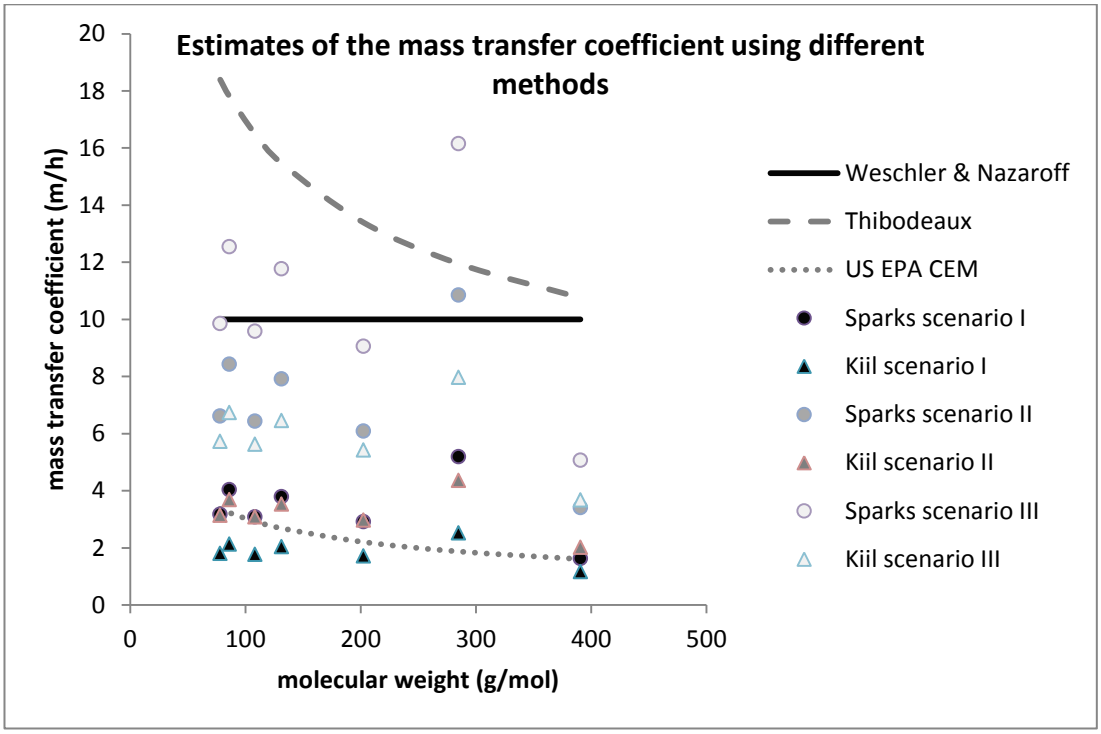

Figure 1. Comparison of the different methods to calculate the mass transfer coefficient in a set of representative indoor emission scenarios (I-III).

From the range of evaluated mass transfer coefficients it can be seen that:

1) The Thibodeaux model produces estimates that are considerably higher than most other methods for especially the smaller molecules

2) All methods except Thibodeaux's method provide estimates that are below or up to the upper bound of 10 m/h reported in Weschler and Nazaroff (2008) in the scenarios I and II
3) Only in scenario III the Sparks method estimate mass transfer that exceeds the 10 m/h

The Sparks and Kiil models consider most of the fundamental aspects of the mass transfer, such as the boundary layer thickness, influenced by the air speed over the surface and the surface dimensions. In contrast, the US-EPA model, that quotes a method proposed in AMEM (US-EPA, 1990), describes a situation of typical indoor and typical source conditions. The dependency on v and L is not included but replaced by an estimate of typical values. It is not clear whether these estimated values are suitable as a conservative default as is required for use as a default in ConsExpo.
In (almost) all cases, the Thibodeaux method predicts higher mass transfer coefficients than the other methods available. The over-prediction is pronounced for lighter molecules. Predictions for the molecules of molecular weight of about 200 g/mol and more, the degree of over-prediction becomes less significant.

Conclusion
The scenario based comparison using the more realistic indoor air models (Kiil and Sparks) provide a range of estimates for the mass transfer from about 1 to 17 m/h. The values above 10 m/h are estimated in a scenario that is thought to represent conditions of very high emission. The more moderate (bust still high) emission scenarios yield estimates below the 10 m/h. Combined with the reported range of values from Weschler and Nazaroff (2008), a value of 10 m/h is deemed to be a conservative estimate for most conditions and substances. This estimated value is considerably less conservative than Thibodeaux's method for lower weight molecules. For this reason, and also because the representativeness of Thibodeaux's method for indoor conditions cannot be asserted, we propose to use the value of 10 m/h as a default in ConsExpo and the ConsExpo fact sheets, instead of the Langmuir and Thibodeaux methods.

Situation in ConsExpo Web and Fact Sheets – October 2018:
Based on the above situation, a default for the mass transfer coefficient of 10 m/h is prefilled for all product categories, in ConsExpo Web version 1.0.3 (January 2018).
The explanation for this is updated in the Cleaning Products Fact Sheet, and provided in this document, but not yet updated in the other product category fact sheets.

3.3 Dilution as a parameter

Inhalation exposure

Some consumer products are typically used in solution; the initial product amount (of the undiluted product) is diluted to acquire the functional solution of the product, which is then applied by the consumer, e.g. an all-purpose cleaner which is diluted in a bucket of water. In ConsExpo fact sheets that were published before 2018, a method was described to 'emulate' dilution. This method, in short,

suggested to adapt the 'weight fraction' of the substance in the product in proportion to the dilution.
However, in the new version of ConsExpo Web 1.0.3 a 'dilution' factor is added to the inhalation model "exposure to vapour- evaporation". This 'dilution factor' is also referenced in the updated Cleaning Products Fact Sheet (Meesters et al., 2018)).
The equation to calculate the dilution times is:

$$dilution = (A_{solvent} + A_{product})/A_{product}$$

Dilution: dilution as 'times'; $A_{solvent}$: amount (mass) of solution (g); $A_{product}$: amount of pure product (g).
Thus, the dilution is calculated as the inverse of the weight of the amount (mass) of pure product used divided by the total mass of the diluted product (i.e. the sum of the pure product and the solution).
As an example, consider a squeeze of dishwasher detergent of 7 g is diluted in a bowl with 5 l water. The product amount then equals the squeeze of dishwasher detergent (7 g). The solvent is the water in the bowl, which has a density of 1000 g/l, a volume of 5 l and thus an amount of 5000 g. The amount of solution used represents the sum of the solvent amount and the product amount, which is in the example 5000 g + 7 g = 5007 g. The weight fraction of the product amount in the amount of solution used is then 7 g / 5007 g = 0.0014. The number of dilution times is the inverse of this weight fraction, 1/0.0014 = 715 times.

Situation in ConsExpo Web and Fact Sheets – October 2018:
In ConsExpo Web 1.0.3 a possibility is included to use a dilution factor for a product used in a dilution. For the Cleaning Products Fact Sheet (Meesters et al., 2018), this dilution factor is included in the defaults database. For all defaults from the other product category fact sheets, a value of 1 is specified. The ConsExpo user is supposed to adapt this for his own use and purpose.

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