



National Institute for Public Health  
and the Environment  
*Ministry of Health, Welfare and Sport*

# ConsExpo Web

## Consumer Exposure models model documentation

Update for ConsExpo Web 1.0.2





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and the Environment  
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## Colophon

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## Synopsis

### **ConsExpo Web. Consumer exposure models – model documentation**

Update with regard to new features in ConsExpo Web – version 1.0.2

RIVM has developed a manual for ConsExpo Web. This web application has been developed for use by exposure experts and risk assessors to estimate exposure to chemical substances from various products under various exposure conditions. Exposure assessments provide necessary information for the evaluation of the safety of chemical substances in consumer products. ConsExpo Web is the successor to ConsExpo 4. Using ConsExpo Web, exposure experts and risk assessors from authorities, institutes and companies can assess consumer exposure in a transparent, standardized fashion.

There is a wide variety of consumer products, ranging from cosmetics to cleaning products and pest control products. Their use (e.g. how much of the product is used and how frequently) also varies among consumers. ConsExpo Web provides a number of generally applicable exposure assessment models and a database of exposure factors. Together, the models and the database provide a basis on which exposure from a specific product can be estimated.

This document provides an overview of ConsExpo Web, an explanation of the exposure and absorption models available in ConsExpo Web and guidance for the careful analysis of the exposure assessment. ConsExpo Web is available via [rivm.nl/consexpo](http://rivm.nl/consexpo). After registration, the use of ConsExpo Web is free.

Keywords: ConsExpo, consumer products, exposure assessment, manual, mathematical models



## Publiekssamenvatting

### **ConsExpo Web. Consumenten blootstellingmodellen – documentatie**

Actualisatie naar aanleiding van nieuwe mogelijkheden in ConsExpo Web – versie 1.0.2

Het RIVM heeft een handleiding opgesteld voor het gebruik van ConsExpo Web. Deze internetapplicatie is ontwikkeld om de blootstelling aan chemische stoffen te schatten voor uiteenlopende producten en omstandigheden waaronder consumenten aan ze worden blootgesteld. De blootstellingsberekeningen geven informatie die nodig is om de veiligheid van chemische stoffen in consumentenproducten te kunnen beoordelen. ConsExpo Web is de opvolger van ConsExpo versie 4 en is bedoeld voor blootstellingsexperts en risicobeoordelaars van overheden, instituten en bedrijven. Met ConsExpo Web kunnen zij blootstellingschattingen op een transparante en gestandaardiseerde manier uitvoeren.

Er bestaat een grote verscheidenheid aan consumentenproducten, van schoonmaakmiddelen en ongediertebestrijdingsmiddelen tot verf en cosmetica. Ook de manier waarop consumenten de producten gebruiken verschilt, zoals de doseringen en de frequentie. ConsExpo Web biedt een aantal algemeen toepasbare blootstellingsmodellen en een database met gegevens over blootstellingsfactoren. Tezamen bieden zij een basis van waaruit de blootstelling van een specifiek product geschat kan worden.

De handleiding geeft een overzicht van ConsExpo Web, een uitleg van de in ConsExpo Web beschikbare blootstelling- en opname modellen en aanbevelingen om de blootstellingsschatting zorgvuldig te analyseren. ConsExpo Web is beschikbaar via [rivm.nl/consexpo](http://rivm.nl/consexpo) en is, na registratie, gratis te gebruiken.

Kernwoorden: ConsExpo, consumentenproducten, blootstellingsschatting, handleiding, mathematische modellen





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## Summary

Consumers are exposed to chemical substances in consumer products. To assess the risks of such exposures, an estimate of their magnitude is required. ConsExpo is a modelling tool that can be used to estimate consumer exposure to a wide variety of products in a wide variety of circumstances. The ConsExpo tool has been made available as a web application, ConsExpo Web. This application succeeds ConsExpo 4, a stand-alone consumer exposure modelling software tool.

This document provides user guidance and background information on the ConsExpo Web tool. ConsExpo Web provides a number of generally applicable exposure models and a database of exposure factors for a broad set of consumer products. Together, the models and the database provide the tools needed to assess exposure for a wide range of consumer products. Only basic additional information on product composition and the physicochemical properties of the substance under assessment are needed.

This report describes in detail how the ConsExpo Web tool is to be used to conduct consumer exposure assessments. It describes how to add multiple scenarios to an assessment, how to select models and how to specify model inputs. Different output measures and methods of evaluating and visualizing exposure are also discussed.

A detailed description of the ConsExpo models is also provided. ConsExpo Web contains models to estimate exposure via inhalation, dermal contact and oral ingestion. The exposure models vary in complexity, from simple screening models to more advanced, physics-based models.

Additionally, it is discussed how ConsExpo can be used to obtain insight into the factors affecting exposure to substances in consumer products by using the sensitivity analysis and probabilistic evaluation tools.



## Additions or changes to the manual – version December 2016

December 2017

Necessary additions or changes are made to this manual (Delmaar & Schuur, 2016), because of next versions of ConsExpo Web, which are published in July 2017 and December 2017.

See Appendix III for features added in ConsExpo Web version 1.0.1 and 1.0.2.

This manual is changed at:

- Section 3.1 Inclusion of a preview panel of selected models, default values including the Q-factors when a scenario is selected from the default fact sheet database
- Section 3.1. Possibility to choose default from database for body weight
- Section 3.1 Export functionality to Chesar (see separate help document, and reporting function adapted to a functionality to report to Excel
- Section 3.1.1. Possibility to duplicate scenario
- Section 3.2.2 Possibility to export graph data to Excel
- Section 3.2.2. Explanation on how to export data from graphs
- Section 3.3.1. Inclusion of an additional endpoint “peak exposure” for the inhalation models “exposure to spray” (instantaneous, spraying) and “exposure to vapour” (instantaneous release, constant release and evaporation) as a time-weighted average of 15 min.
- Section 4.1.1.2 “Limit concentration to saturated air concentration” is checked by default.
- Section 4.1.1.4. Information of mass transfer coefficient, possibility to choose default of 10 m/hr instead of using outcome of model estimation
- Section 4.1.1.4 Inclusion of the parameter dilution
- Section 4.1.2.2 15 µm included as standard default for inhalation cut off diameter
- Section 4.1.4. Possibility to choose default from database for inhalation rate



## 1 Introduction

Consumer products contain chemical substances. Consumers using these products may be exposed to these substances. To assess the risks of such exposure, an exposure estimation has to be performed. The assessment of exposure to substances in consumer products is complicated by the wide variety of consumer products and variation in the behaviour of consumers. ConsExpo Web is a web application that features a set of models that assist in the assessment of exposure to substances in consumer products.

ConsExpo Web is the successor to the ConsExpo 4 computer program. This program was initially developed at the request of the Netherlands Food and Consumer Product Safety Authority (NVWA). The ConsExpo Web application was developed with the help of the RIVM's counterpart institutes ANSES (France), BfR (Germany), FOPH (Switzerland) and Health Canada and the Netherlands Food and Product Safety Authority and the Dutch Ministry of Health, Welfare and Sport.

What is the rationale behind the exposure models in ConsExpo? Exposure to consumer products is characterized by a great diversity in the chemical composition and usage of products. The questions encountered during the process of human risk assessment are manifold. How can exposure be estimated? What exposure data are available? Are they representative of the situations in which the product is used? Which factors determining exposure are important? Which dose measure to calculate? How should multi-route exposure be assessed? How should risk be characterized? What effects cause the main risks? On what time scale are effects relevant? ConsExpo Web (hereafter referred to as ConsExpo) is designed to facilitate indoor exposure estimates for the process of exposure and risk assessment.

ConsExpo implements a range of generally applicable mathematical models describing exposure processes via inhalation, dermal contact and oral ingestion. For all routes of exposure, ConsExpo provides models of increasing complexity from simple screening models to more detailed mechanistic models. This allows the exposure assessment to be carried out using a tiered approach, starting with simple, first-order models used to estimate maximum exposure, and moving on to more detailed and complex models when the exposure estimation needs to be refined. As a rule, the more detailed the exposure assessment, the more data is needed. Whereas the simple, first-order models require only limited, general information, the more advanced models often require very specific data, which may be hard to obtain.

To assist in exposure assessments, ConsExpo is equipped with a database of default products for which exposure scenarios have been defined and a set of default values for use as model input parameters is provided. The database may serve as a starting point for the exposure assessment. The justifications for the default values are given in fact sheets for specific product categories. Fact sheets have been published on paints (Bremmer et al. 2007), pest control products (Bremmer et al.

2006a) and cosmetics (Bremmer et al. 2006b), among other products. For a complete overview and the most recent versions of the fact sheets, see the ConsExpo website ([www.consexpo.nl](http://www.consexpo.nl)).

ConsExpo outputs different measures of estimated exposure. Depending on the route of exposure, ConsExpo calculates (mean) air concentrations, external doses and internal doses. Different periods of exposure are also considered: the exposure event, the day on which exposure takes place and the average annual exposure (mean air concentration or dose). The application can produce graphs of the different exposure measures over time. In addition, ConsExpo can generate probabilistic evaluations, using distributions of input values for a (set of) parameter(s) rather than deterministic values. Furthermore, the application enables sensitivity analyses to be carried out.

ConsExpo Web consolidates to a large extent features of the ConsExpo 4 software tool. In addition, it features a model for assessing exposure to substances emitted from solid materials and a low-tier model for the assessment of exposure to substances in sprays, which was added next to the more complex spray model included in ConsExpo 4.

ConsExpo also allows the combination of multiple scenarios in a single assessment, where ConsExpo 4 allowed only the evaluation of one scenario for one substance in one product.

The aim of this report is to provide guidance on how to use ConsExpo. It includes a description of the models included in the application, as well as some important notes to enable a careful analysis of the results. The report is an update of the documentation on ConsExpo 4 (Delmaar et al. 2005).

### **Contact**

ConsExpo is accessible via [www.consexpoweb.nl](http://www.consexpoweb.nl). Information on the ConsExpo program and supporting products is available at [www.rivm.nl/consexpo](http://www.rivm.nl/consexpo). To make comments, ask questions or report problems or bugs, please contact us at [ConsExpo@rivm.nl](mailto:ConsExpo@rivm.nl).

### **Proclaimer for use of the ConsExpo Web tool**

ConsExpo Web is an online tool designed to estimate the consumer exposure to substances in several consumer products.

New knowledge or insights may lead to model changes and updates of the tool. Adjustments to the model to a new version will be clearly communicated via the website. The actual version is mentioned in the footer of the webpage.

The application of ConsExpo Web, including the evaluation and selection of data, requires expert knowledge on consumer exposure assessment and risk assessment. When used as a starting point for risk assessment adequate interpretation of the results of the model calculation is required.

RIVM is not responsible for the consequences of the operational use of ConsExpo Web.



## 2 ConsExpo framework

ConsExpo is a web application developed for the assessment of exposure of consumers to substances in consumer products. The ConsExpo tool implements a set of models that facilitate the estimation of chemical substance exposure arising from the use of consumer products.

There is a wide variety of consumer products. In order for it to be applicable to most of these products, the ConsExpo software was set up to be generic, in the sense that, rather than exposures related to specific products, it models general exposure processes that may be relevant to different types and groups of products.

Specific data on factors determining exposure are scarce. As a result exposure assessments are often based on limited data. The ConsExpo framework was designed to provide the models and the information on exposure factors needed in these situations.

### 2.1 General considerations

The level of exposure to a substance in a consumer product is determined by factors such as the use of the product and the contact with the substance after its release from the product. The assessment of the exposure starts by specifying emission of the substances from the consumer product and transport to other parts of the residential environment. Emission and transport determine the concentration–time profiles of the substances, during and after use of the product.

There are various ways in which a person can be exposed to a substance in a consumer product. For example, a volatile substance may be emitted into air that is subsequently inhaled. A product may be applied to the hands, resulting in dermal exposure to a substance in the product. By hand-to-mouth contact some of the substance can be transferred to the mouth, resulting in oral exposure. Consequently, a substance may be absorbed into the body via these different routes, resulting in an internal dose.

The user should be aware that the ConsExpo models, like all models, are only a simplified representation of reality, valid only as an approximation and only in limited conditions of application. The results of an exposure assessment obtained by modelling should always be treated with caution.

### 2.2 Definitions

ConsExpo distinguishes between external and internal exposures. External exposure within the ConsExpo framework is defined as: contact of the substance with the outer boundary of the body (i.e. skin or lung or gut wall). Internal exposure is defined as the amount absorbed over this boundary. ConsExpo implements separate models for calculating the external exposure and for assessing the absorption of the substance.

As for the time scales, ConsExpo considers exposure during the exposure event, on the day of exposure and year average exposure.

### 2.3 Available models

An overview of all the models available in ConsExpo and the input parameters that apply to each model is presented in Table 1. All models and their boundary conditions are described in more detail in Chapter 4.

Table 1. Available exposure models in ConsExpo

Exposure route	Sub-models
<i>Inhalation</i>	
Exposure to Vapour	<ul style="list-style-type: none"> <li>• Instant Release</li> <li>• Constant Release</li> <li>• Evaporation</li> </ul>
Exposure to Spray	<ul style="list-style-type: none"> <li>• Instant release</li> <li>• Spraying</li> </ul>
Emission from Solid Materials	
<i>Dermal</i>	
Direct Product Contact	<ul style="list-style-type: none"> <li>• Instant Application</li> <li>• Constant Rate</li> <li>• Rubbing Off</li> <li>• Migration</li> <li>• Diffusion</li> </ul>
<i>Oral</i>	
Direct Product Contact	<ul style="list-style-type: none"> <li>• Direct Oral Intake</li> <li>• Constant Rate</li> <li>• Migration</li> </ul>
Migration from Packaging Material	

### 2.4 ConsExpo fact sheets

A number of fact sheets has been published that bring together relevant exposure information for a main category of consumer products. Currently, fact sheets are available for cleaning products, cosmetics, paint products, pest control products, disinfectant products, do-it-yourself products and children's toys (Bremmer et al. 2002; 2006a; 2006b; 2007; Ter Burg et al. 2007; Prud'homme de Lodder et al. 2006a; 2006b). These fact sheets will be updated in the coming years and extended to cover, for example, air fresheners. A General Fact Sheet (te Biesebeek et al. 2014), which deals with subjects that are relevant to several main categories, has already been updated. It gives, for instance, anthropometric data and details on residential buildings: data that are needed in all product fact sheets.

The consumer product categories consist of products for which exposure takes place in a similar fashion. For each category the relevant ConsExpo models are described, default parameter values are provided for a typical scenario and the choice of these default values is justified. When using the database, the user should always consult the corresponding fact sheet, in order to be aware of the basis of the selected parameter values and their limitations.

The default parameters are an integral part of ConsExpo. When the user selects a product, the program provides default models and input values for those models. The defaults can serve as a starting point for exposure estimation but should be used in the absence of accurate scenario data only. Whenever more detailed information for the product is available, these data should be used instead.

The fact sheets describe a high-exposure scenario in which consumers frequently use the relevant product under relatively unfavourable circumstances. The basic assumptions are: relatively frequent use, application of a relatively large amount in a small room with a low ventilation rate, and a relatively long stay in that room. However, when conservative estimates of all input parameters are made, the overall estimate may easily become unrealistically high.

For this reason, in the ConsExpo fact sheets it was decided to make somewhat less conservative assumptions for the default values for the input parameters. Whenever a distribution of data on the exposure factor is given, a 75<sup>th</sup> percentile is chosen as a value to represent the distribution of this particular exposure factor. This yields more realistic, yet still conservative, estimates of exposure. It should be noted, that also by following this approach the exact degree of conservatism applied is still unknown. This can only be revealed by including uncertainty and variability in the exposure factors explicitly in the calculations and performing probabilistic estimations (see Section 5.2 for details).



### 3 Using ConsExpo

Using ConsExpo, an exposure assessment is conducted for one substance in a single product. The exposure is assessed for a single target population. Considering multiple populations or products requires the creation and evaluation of multiple separate exposure assessments.

ConsExpo defines 'assessment' and 'scenario' data structures to organize an exposure assessment. The user may create and store multiple assessments. The assessment contains information on the substance, the product and the target population. An assessment may contain one or more exposure scenarios. An exposure scenario contains information on the frequency of occurrence of an exposure event. In addition, the scenario specifies the exposure models and parameter input that are used to estimate exposure.

Scenarios can represent exposure during different uses, or different phases of use, of the same product (e.g. preparation of a product, actual use of the product, post-application exposure), or different tiers of an iteratively refined exposure assessment.

#### 3.1 The Assessments screen

When ConsExpo is opened, the first screen is the 'Assessments' screen (see Figure 1). This screen provides an overview of all the assessments (if any have been made already) of the current user.

The user may create a new assessment, import an assessment from a file or create a new assessment using information from the fact sheets, using the 'Use Fact Sheet' button.

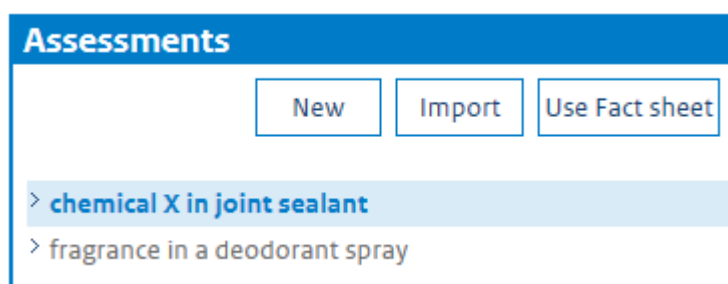


Figure 1. The ConsExpo Assessments pane gives an overview of available assessments.

In the case that an assessment is created from the fact sheet, a panel is opened on which a fact sheet, a product category, product, and scenario can be selected. After selection a preview of the selected scenario, including the input parameter defaults and Q-factors is given in a separate panel (see Figure 2).

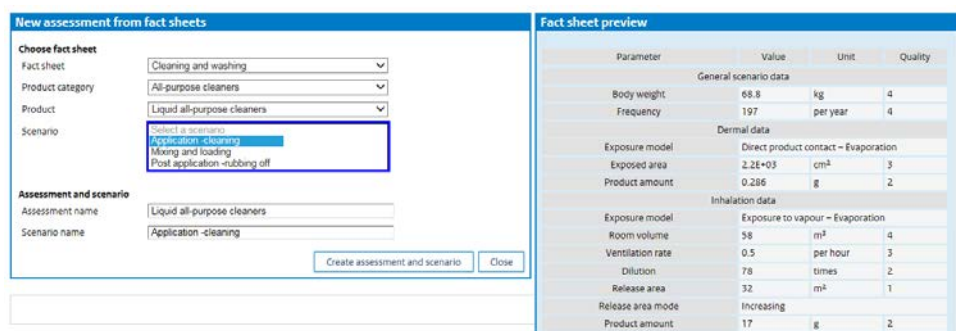


Figure 2. Fact sheet preview as shown when a fact sheet – product category – product – scenario is selected.

Selecting a specific assessment from the list of available assessments opens the 'Assessment settings' window (Figure 3). Here the user may edit substance, product and population properties.

For the population, default body weights may be selected from three available databases; Canadian (adapted by Health Canada from CCHS, 2005 and National Health and Nutrition Examination Survey (NHANES) using data from 1999-2010), ConsExpo General fact sheet (te Biesebeek et al. 2014) or EU Biocides Framework (ECHA, 2017).

The user may delete the assessment and/or export the assessment to a file that can be shared with other users.

Export is possible to a ConsExpo Web file (.ce), as export file to Chesar (see manual for export RIVM, 2017; .chr), and as report (in .csv format) to Excel.

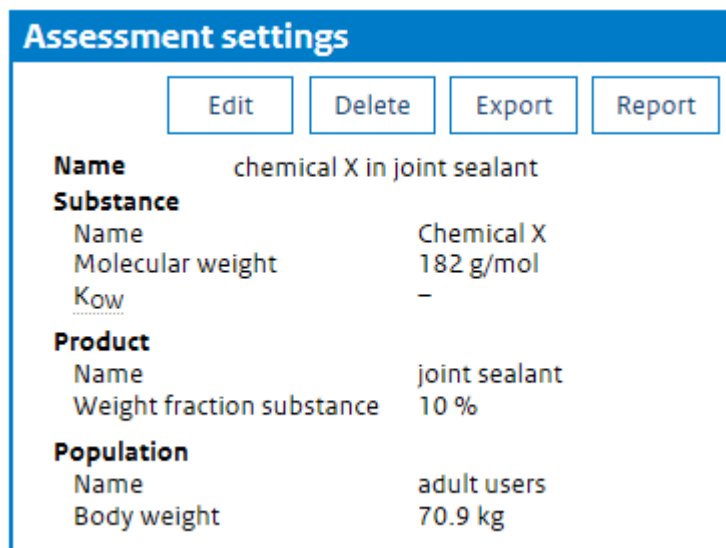


Figure 3. The Assessment settings window shows the settings for the selected assessment and allows the user to edit, delete or export the assessment to file. Additionally, if an assessment has been completely specified, a report may be generated by using the 'Report' button.

### 3.1.1 Specifying scenarios

Selecting a particular assessment opens the 'Scenarios' window. In the 'Scenarios' window (Figure 4), a list of available scenarios is displayed.

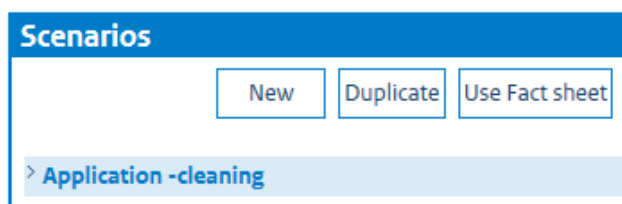


Figure 4. The Scenarios window.

From the list of scenarios the user may select an existing scenario for editing or simulation, add a new blank scenario, create a new scenario based on defaults from the ConsExpo fact sheets, or duplicate an available scenario.

Selecting a scenario or creating a new scenario brings up the 'Overview scenario' window (Figure 5), displaying a summary of the exposure scenario created or selected. It shows which routes of exposure have been included and which exposure models have been selected for simulation.



Figure 5. The Overview scenario window shows the selected routes for the scenario and the models chosen to model exposure and absorption for each route.

From the 'Overview scenario' window, the scenario may be edited (i.e. models for simulation can be selected for the scenario and input for the models can be provided), the scenario can be deleted or different aspects of the scenario can be evaluated by pressing the 'Simulate' button.

Clicking on 'Edit' opens the 'Edit scenario' window (Figure 6). Here the scenario name and the exposure frequency should be set, a description of the scenario can be provided and models to simulate exposure for the different routes (inhalation, dermal and oral) can be specified.

When a specific exposure or absorption route is to be included, the user should check the box in front of the required route.

Figure 6. The Edit scenario window allows the user to name the scenario, specify the exposure frequency and select models for each route of exposure.

### 3.1.2 Specifying input parameters

Different models require different inputs. Data input is done by specifying a single (point) value in the box after the parameter, e.g. 'Exposure duration', name and selecting the appropriate unit from the units dropdown (see Figure 7).

Figure 7. Specifying a parameter input

Alternatively, parameters may be specified as distributions rather than single, deterministic values. This enables ConsExpo to perform probabilistic evaluations by Monte Carlo simulation.

Distributions of parameter values are specified by pressing the Distributions button . This opens the Distribution editor, where a distribution type can be chosen (none, uniform, triangular, normal or log normal) and parameters to define the distribution can be specified.

Pressing the **Graph** button will show a preview of the specified distribution (Figure 8).



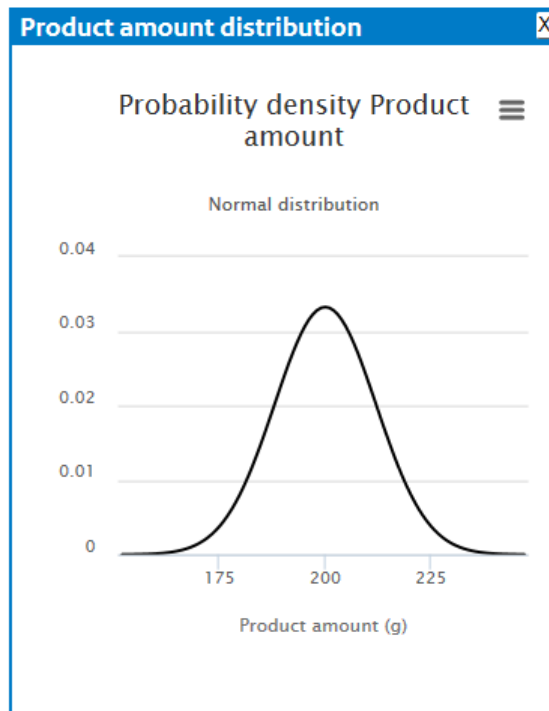


Figure 8. Specifying a distribution as parameter input rather than a deterministic value. The specified distribution is used to perform a probabilistic (Monte Carlo) simulation of the scenario.

The parameter probability distributions supported by ConsExpo are described below.

#### *Normal*

Specify the mean  $\mu$  and standard deviation  $\sigma$ . The distribution is defined by the probability density function:

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

#### *Log Normal*

Specify the median  $\mu$  and arithmetic coefficient of variation C.V. The probability density is defined as:

$$P(x) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\ln(x) - \ln(\mu)}{\sigma}\right)^2\right)$$

and

$$C.V. = \sqrt{e^{\sigma^2} - 1}$$

#### *Uniform*

Specify a lower bound  $x_0$  and an upper bound  $x_1$  of the distribution. The probability density is defined as:

$$P(x) = \frac{1}{x_1 - x_0}$$

#### Triangular

Specify (a) location (minimum), (b) scale (maximum) and (c) shape (maximal probability). The probability density varies between the minimum and maximum values and has maximum probability at the 'shape'. It is defined as:

$$P(x) = \frac{2(x-a)}{(b-a)(c-a)}; a \leq x \leq c$$

$$P(x) = \frac{2(b-x)}{(b-a)(b-c)}; c \leq x \leq b$$

## 3.2 Simulation

From the 'Scenario overview' window, the user may evaluate different aspects of the specified models for the selected scenario.

### 3.2.1 Results

If the user has specified single (point) values for all model parameters, clicking the 'Simulate' button will generate a deterministic calculation. ConsExpo displays the results in the 'Output scenario' window (Figure 9) with an overview of calculated point values for all specified end points (see Section 3.3 for an overview of the calculated end points in ConsExpo).

Output scenario Application		
Results	Graphs	Sensitivity analysis
<b>Inhalation</b>		
Mean event concentration	1.1 × 10 <sup>-25</sup> mg/m <sup>3</sup>	
External event dose	1.5 × 10 <sup>-28</sup> mg/kg bw	
Internal event dose	1.5 × 10 <sup>-28</sup> mg/kg bw	
Chronic internal dose	3.1 × 10 <sup>-28</sup> mg/kg bw/day	
<b>Dermal</b>		
Dermal load	2.6 × 10 <sup>-1</sup> mg/cm <sup>2</sup>	
External event dose	4.3 × 10 <sup>-1</sup> mg/kg bw	
<b>Integrated</b>		
External event dose	4.3 × 10 <sup>-1</sup> mg/kg bw	


Figure 9. The Output scenario window features three sub-sections: 'Results', 'Graphs' and 'Sensitivity analysis'. The 'Results' section displays end point estimates of exposure for all included routes.

### 3.2.2 Graphs

Clicking on 'Graphs' shows the exposure during a single event via graphs of the time course of the exposure (Figure 10). The time axis will

automatically be set to the exposure duration specified by the user. For models that do not depend on time, the graph option is not available.



Figure 10. The Graphs section of the Output scenario window shows the results of the simulation of exposure during the exposure event. A plot of the time series for a selected end point is made against exposure duration. From the graph options, it is possible to export the data to Excel. This can be done by left-mouse clicking the  icon in the upper right corner of the graph's panel. The dropdown menu features a 'Download Excel' option, which downloads the graph data in a comma separated file.

### 3.2.3 Sensitivity analysis

Sensitivity analysis allows the user to investigate graphically the sensitivity of the model outcome to changes in one single parameter (Figure 11). The user should select the required calculation end point (exposure measure), select the parameter for which the sensitivity analysis is to be performed from the 'Parameter' drop-down list and set the range of variation and the units for the requested parameter. A graph is plotted showing the outcome of the calculations for the range of values given for the chosen parameter.

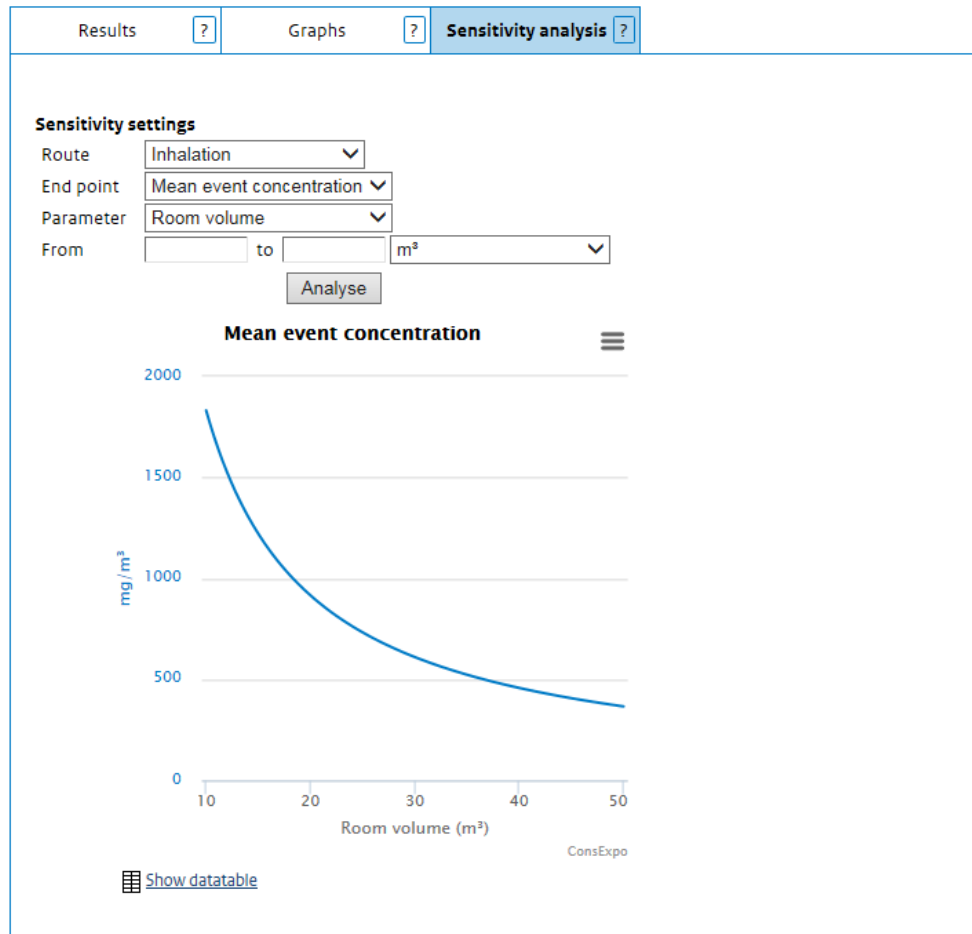


Figure 11. The Sensitivity analysis section in the Output scenario window enables the assessment of sensitivity of the selected model(s). The parameter value is shown for the specified range of values of the parameter, giving insight into the change in the end point with changes in the input parameter considered.

### 3.2.4

#### Probabilistic results

If the user has specified at least one parameter as a distribution, ConsExpo will perform a probabilistic evaluation. When simulating a probabilistic scenario, the user is asked to specify the number of random samples that will be taken in the Monte Carlo simulation (Figure 12). Currently, the number of samples (or 'iterations') that can be chosen in ConsExpo varies from 1,000 to 50,000.

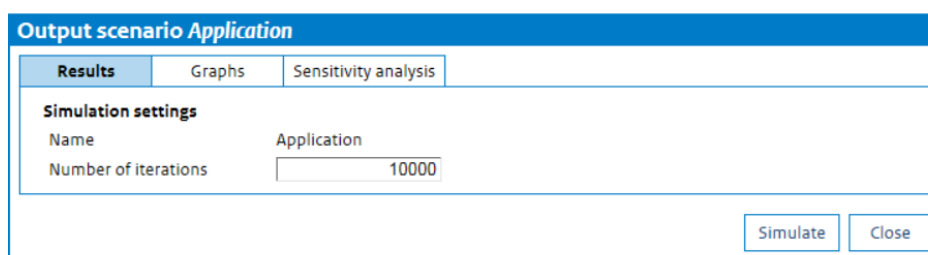


Figure 12. When a user specifies a distribution for an input parameter rather than a single, deterministic value, a probabilistic evaluation is conducted. When simulating the scenario by pressing the 'Simulate' button in the 'Overview

*Scenario' window, the user is first asked to specify the number of samples (or 'iterations') that are to be taken in the probabilistic simulation. After specification of the number of iterations and pressing the 'Simulate' button again, a probabilistic evaluation is conducted.*

When the user presses the 'Simulate' button again, a Monte Carlo simulation is run. The 'Results' tab on the output window summarizes the resulting distributions of probabilistic end points. For these the mean, median, standard deviation and 90<sup>th</sup> and 99<sup>th</sup> percentiles are presented. A complete plot of the distribution as a frequency histogram and a cumulative probability distribution can be viewed by pressing 'Plot distribution'.

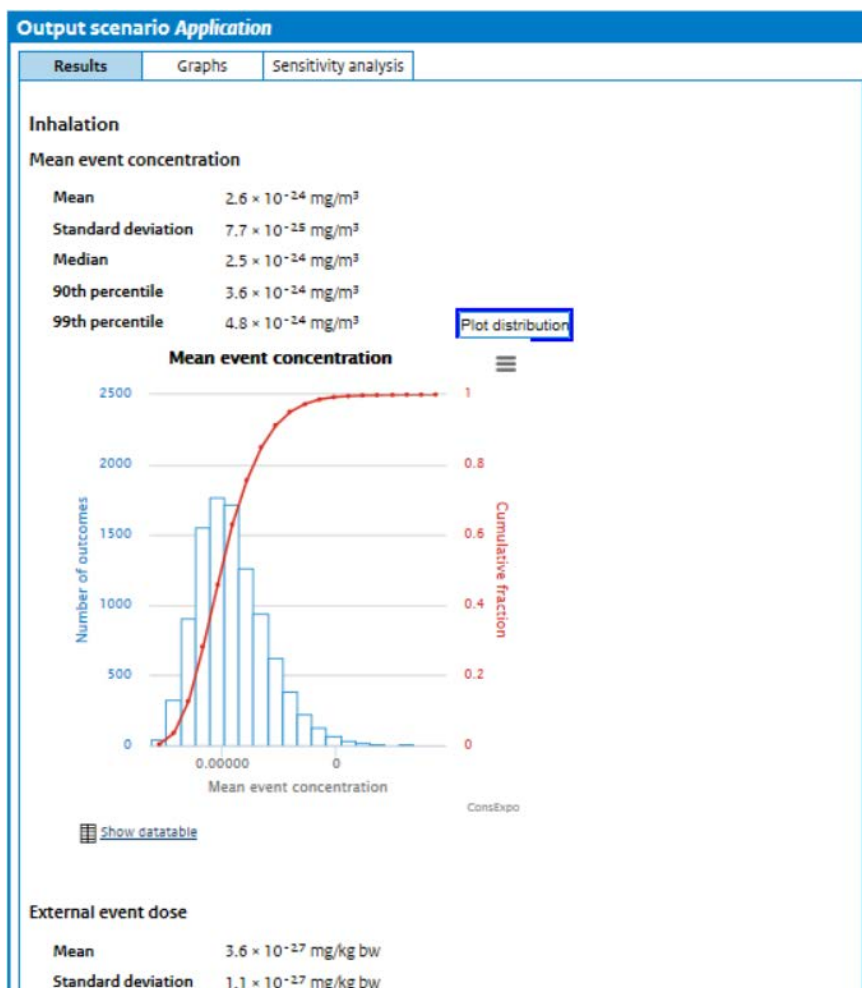


Figure 13. The results of a probabilistic assessment, including a histogram and cumulative plot of the distribution of exposure.

### 3.3 Output measures

ConsExpo calculates various measures for each route of exposure. Integrated doses (i.e. doses summed over various routes) are also evaluated if absorption models are used in the assessment.

### 3.3.1 *Inhalation*

For the inhalation route the following exposure measures are given:

- **Mean event concentration:** average air concentration on exposure event. Note: depends strongly on chosen exposure duration;
- **Peak concentration:** peak concentration is the 15 minute time weighted average of the air concentration around its maximum. In case the exposure duration is less than 15 minutes, the mean event air concentration is given instead.
- **Mean concentration on day of exposure;** average air concentration over the day (accounts for the number of events on one day)
- **Year average exposure;** mean daily air concentration averaged over a year
- **External event dose:** the amount that can potentially be absorbed by inhalation per kg body weight during one event.
- **External dose on the day of exposure:** the amount that can potentially be absorbed per kg body weight during one day. The external doses for multiple events that take place on the same day are added.
- **Internal event dose:** absorbed dose per kg body weight during one event.
- **Internal dose on day of exposure:** the absorbed dose per kg body weight during one day Note: these can be higher than the 'event dose' for exposure frequencies larger than 1 per day.
- **Internal year average dose:** daily absorbed dose per kg body weight averaged over a year.

### 3.3.2 *Dermal*

The following dermal exposure measures are given:

- **Dermal load:** the amount of substance per cm<sup>2</sup> of exposed skin.
- **External event dose:** the amount that can potentially be absorbed per kg body weight during one event.
- **External dose on day of exposure:** the amount that can be absorbed per kg body weight on the day exposure occurs. The external doses for multiple events that take place on the same day are added.
- **Internal event dose:** absorbed dose per kg body weight during one event.
- **Internal dose on day of exposure:** absorbed dose per kg body weight during one day. Note: these can be higher than the 'event dose' for exposure frequencies larger than 1 per day.
- **Internal year average dose:** daily absorbed dose per kg body weight averaged over a year.

### 3.3.3 *Oral*

Oral exposure measures given by ConsExpo are:

- **External event dose:** the dose that can be absorbed orally per kg body weight during one event.
- **External dose on day of exposure:** the dose that can be absorbed orally per kg body weight on the day exposure occurs.
- **Internal event dose:** the absorbed dose per kg body weight during one event.

- **Internal dose on day of exposure:** the absorbed dose per kg body weight on the day exposure takes place.
- **Internal year average dose:** the absorbed dose per kg body weight averaged over a year.

#### 3.3.4 *Integrated*

The integrated doses are the sums of the corresponding doses per route. These are given only for internal exposure (i.e. when absorption is included in the calculation). Measures given are:

- **Internal event dose:** the total absorbed dose per kg body weight during one exposure event.
- **Internal dose on day of exposure:** the absorbed dose per kg body weight during one day. Note: these can be higher than the 'event dose' for exposure frequencies larger than 1 per day.
- **Internal year average dose:** the daily absorbed dose per kg body weight averaged over a year.

### 3.4 **Report**

A report of the assessment is generated by pressing the 'Report' button in the 'Assessment settings' pane (see Figure 3). The ConsExpo report gives a complete (textual) overview of the exposure calculation. It displays all parameter values and the calculated exposures. The text can be exported as a .csv file, which can be imported in Excel.





## 4 The models

ConsExpo includes exposure and absorption models for each exposure route. This chapter describes in more detail the available models and their parameters.

In the description of the model equations the units of the parameters are given according to the standard S.I. system. These units are used only for description purposes. The user can choose more appropriate units when using the program.

### 4.1 Inhalation route

Many consumer products contain substances that may reach the body via the inhalation route. A simple example is a spray containing a volatile substance. After spraying, the substance may be present in the air inhaled by the product user or by other people. Subsequently, a substance may enter the body by absorption in the lungs. Three exposure models – Exposure to Vapour, Exposure to Spray and Emission from Solid Materials – and one absorption model are available in ConsExpo to describe indoor inhalation exposure to substances in consumer products.

#### 4.1.1 *Exposure to Vapour model*

The Exposure to Vapour model describes a situation in which a substance evaporates from a liquid product into the room air. Examples include the evaporation of substances from an open tin of paint or from a freshly painted wall. The substance may comprise 100% of the product, or be part of a mixture of substances.

The concentration of the substance in the room air will depend on the amount of substance present in the room, the room size, the ventilation of the room air, the vapour pressure of the substance and the rate at which the substance is released into the air.

Depending on the information available on the use of the product, different modes of release of the substance from the product can be selected to calculate the release of the substance into the room air. The different release modes are the Instantaneous Release, Constant Rate and Evaporation.

In some cases, the amount that actually is released into indoor air is limited by the saturated vapour pressure of the substance. The resulting air concentration will depend on this vapour pressure, the substance's molecular weight and the temperature during application. The latter may represent typical room conditions, but may also be the temperature at which the substance is handled (e.g. the temperature of a solvent), which may be higher than room temperature. In all cases, care should be taken that the vapour pressure is specified at the temperature at which the substance is handled. For example, if a substance is solved in water of a temperature of 40 °C, the vapour pressure at this temperature should be specified.

## 4.1.1.1 General parameters

Parameters that are used for all options within the Exposure to Vapour model are:

- **Exposure duration:** the total time the exposed person is in the room where the substance is being released.
- **Product amount:** the amount of product used in one event.
- **Weight fraction substance:** the fraction of substance in the product.
- **Room volume:** the volume of the room in which the exposure occurs.
- **Ventilation rate:** the number of total air changes in the room per unit of time. For example, if it takes 20 minutes for all the air in the room to be exchanged, the ventilation rate is 3 times per hour.

## 4.1.1.2 Exposure to Vapour: Instantaneous Release

The Instantaneous Release mode is the mode of release that will usually result in a relatively high exposure, and can therefore be used as a first tier to establish the upper level of exposure. The scenario assumes that all substance is released from the used product at once into the room and is subsequently removed by ventilation.

The air concentration of the substance at time  $t$  for the Instantaneous Release mode is calculated as:

$$1. \quad C_{air} = \frac{A_o \times w_f}{V} \times e^{-qt}$$

where:

$C_{air}$	concentration of substance in the room air	[kg/m <sup>3</sup> ]
$A_o$	product amount	[kg]
$w_f$	weight fraction of the substance in the total product	[fraction]
$V$	room volume	[m <sup>3</sup> ]
$q$	ventilation rate of the room (number of air changes per time unit)	[1/s]
$t$	exposure duration	[s]

In reality, there is a limit to how much of the substance can evaporate in the air, depending on its vapour pressure. By default, the checkbox in front of the phrase 'Limit concentration to saturated air concentration' is checked. When the box is checked, air concentrations as calculated by the Instantaneous Release mode are limited by the saturated air concentration of the pure substance.

This air concentration,  $C_{sat}$ , is calculated from the saturated vapour pressure using the ideal gas law:

$$2. \quad C_{sat} = MP_{sat} / RT$$

where:

M	molecular weight of the substance	[kg/mol]
P <sub>sat</sub>	saturated vapour pressure	[Pa]
R	universal gas constant	[J/mol/K]
T	temperature	[K]

#### 4.1.1.3 Exposure to Vapour: Constant Rate

In contrast to the Instantaneous Release mode, which describes the release of a substance into the air at once, the Constant Rate mode describes the release of a substance at a constant rate over a certain period. During this time, the substance may be removed from the air by ventilation of the room.

This mode of release can be used if information on the evaporation properties of the substance is not available, but the period during which the substance evaporates can be estimated. In addition to the parameters used in the Instantaneous Release mode, the Constant Rate mode uses the 'emission duration' parameter: a reasonable estimate of the time during which the substance is released.

The air concentration of the substance at time  $t$  for the Constant Rate release mode is calculated as:

$$3a. \quad C_{air} = \frac{A_o \times w_f / t_r}{qV} \times (1 - e^{-qt})$$

For exposure  $t < t_r$  (i.e. during release)

$$3b. \quad C_{air} = \frac{A_o \times w_f / t_r}{qV} \times (1 - e^{-qt_r}) \times e^{-q(t-t_r)}$$

For exposure  $t > t_r$  (i.e. after release)

In the case of no ventilation (i.e.  $q=0$ ) these equations reduce to

$$3c. \quad C_{air} = \frac{A_o \times w_f}{V} \times \frac{t}{t_r}$$

For exposure  $t < t_r$  (i.e. during release)

$$3d. \quad C_{air} = \frac{A_o \times w_f}{V}$$

For exposure  $t > t_r$  (i.e. after release)

where:

$C_{\text{air}}$	concentration of substance in the room air	[kg/m <sup>3</sup> ]
$t_r$	emission duration	[s]
$A_o$	amount of product used	[kg]
$w_f$	weight fraction of the substance in the product	[fraction]
$V$	room volume	[m <sup>3</sup> ]
$q$	ventilation rate of the room (number of air changes per time)	[1/s]

#### 4.1.1.4 Exposure to Vapour: Evaporation

The Evaporation mode describes the release of the substance from the surface of the product by a physics based description of evaporation.

The Evaporation mode explicitly models the evaporation of the substance from the product. Evaporation is driven by the difference between the vapour pressure in the room air and the saturated vapour pressure of the substance. The rate of evaporation is proportional to this pressure difference and depends on the surface area of the product and the mass transfer coefficient. This mass transfer coefficient is a measure of how fast the evaporated substance is transferred from the product surface into the room air. It accounts for the fact that emission from a product is limited due to the presence of a stagnant layer of air over the product's surface through which the substance diffuses to reach indoor air. The mass transfer coefficient depends on a number of factors including the diffusivity of the substance through air (dependent on molecular weight), the air flow over the product, and the surface roughness of the product.

Estimating the mass transfer coefficient

ConsExpo offers two models that give an approximate estimate of this mass transfer coefficient. The first is Langmuir's method (Zemansky and Dittman 1984), which consists in ignoring all transport-limiting processes such as diffusion. It provides an upper limit of the rate of release for any system and will in general result in a high over-estimation of the peak concentrations in the room air. The other method is that of Thibodeaux (1979) and is a simplification of the more complicated Slater two-layer model, which describes the release of a substance from water into air. Mass transfer coefficients calculated using this model will be lower than the ones calculated by Langmuir's method, but it should be remembered that this method is only an approximation of a specific system (evaporation of a solute from water outdoors) and has limited validity outside the domain for which it was derived.

Several alternative models have been developed and used to estimate mass transfer in indoor environments.

Weschler and Nazaroff (2008) use a particle deposition model to derive typical mass transfer rates for SVOCs from flat surfaces indoors to indoor air. This model uses information on the range of typical diffusivities of substances in air indoors to describe the mass transfer. They conclude that for the substances they considered the mass transfer coefficient ranges from 2.5 to 3.9 m/h.

The US EPA Consumer Exposure Model (CEM) user's guide (US-EPA, 2016) proposes a method to estimate the mass transfer coefficient as

$$4. \quad h_m = 46.8 \times \frac{3.3}{(2.5 + MW^{1/3})^2}$$

$h_m$  is the mass transfer coefficient in m/h and MW the molecular weight in g/mol.

This model takes only diffusivity of the substance (which depends on the molecular weight MW) into consideration. Using this model, based on variation in the molecular weight, a range of mass transfer coefficients can be estimated:

Molecular weight (g/mol)	mass transfer coefficient (m/h)
20	5.7
100	3.0
300	1.8
600	1.3

Delmaar (2010) reviews a number of models to estimate the mass transfer coefficient for a flat surface. This review shows that these different models predict the mass transfer coefficient to be in a range of 2 to 16 m/h depending on the model used, the diffusivity of the substance in air (thus molecular weight) and the air flow over the surface.

Default value for use in ConsExpo

The different methods and models applied in literature indicate that the mass transfer coefficient is in the order of 1 to 10 m/h, where the previously used default methods (the models of Langmuir and Thibodeaux) result in much higher estimates.

Therefore, a generic default value of 10 m/h is selected in ConsExpo.

This generic default is usable for a situation where specific properties of the substance, the product and the indoor environment are not known.

Another aspect of the model that needs to be specified is the release area, the area of the product from which the substance evaporates. The release area will change during the application of the product. Values for two input parameters need to be given:

- **Release area:** the total surface area on which the product is applied.
- **Application duration:** the period during which the product is applied.

Two modes are available for the release area:

- **Constant.** This option is appropriate if the substance is released from a surface area that remains the same size over time; for example, the surface area of a bucket containing the product or the area of a board treated with a wood preservative.
- **Increases over time.** This option is appropriate when the area from which the substance is released is not of a constant size. For example, when a wall is being painted, the surface area covered with paint from which the substance is released increases over time.

The release rate of the substance is determined by the temperature, substance properties and the mass transfer coefficient. Input is needed on:

- **Temperature:** the temperature at which the product is applied.
- **Molecular weight and vapour pressure:** the physicochemical properties of the substance in question.
- **Mass transfer coefficient:** the rate at which the substance is transferred between the product and the air. ConsExpo offers two models to approximate this rate: Langmuir's method and Thibodeaux's method (see above).

Langmuir's equation for the mass transfer coefficient is:

$$5a. \quad K = \sqrt{R \times T / (2\pi \times M)}$$

where:

K	mass transfer coefficient	[m/s]
M	molecular weight of the substance	[kg/mole]
R	universal gas constant	[J/mol/K]
T	temperature	[K]

Thibodeaux's equation for the mass transfer coefficient is:

$$5b. \quad K = \frac{1}{2} \times \sqrt[3]{0.018/M/60}$$

where:

K	mass transfer coefficient	[m/s]
M	molecular weight of the substance	[kg/mole]

Molecular weight of the matrix: this parameter needs to be defined if the substance in question is not in its pure form, but part of a product. It is the average molecular weight of the rest of the total product (the product minus the substance in question). It is derived from the concentrations and molecular weights of the components of the product as:

$$6a. \quad \frac{C_{rest}}{M_r} = \frac{(1-w_f) \times \rho}{M_r} = \sum_i \frac{C_i}{M_i} = \sum_i \frac{w_i \times \rho}{M_i}$$

from which

$$6b. \quad M_r = \frac{(1-w_f)}{\sum_i \frac{w_i}{M_i}}$$

where the summation index  $i$  is over all substances in the mixture except for the substance in question ( $i^{\text{th}}$  component).  $M_i$  is the mol weight of the  $i$ -th component and  $M_r$  is the mol weight of the (rest of the) matrix. If the product consists largely of a single component (e.g. water) the mol weight matrix is roughly equal to the molecular weight of that component (e.g. 18 g/mol for water).

The evaporation of a substance from a layer of product is described by a set of two coupled differential equations:

$$7a. \quad \frac{dA_{air}}{dt} = K \times S \times \frac{M}{RT} \times (P_{eq} - P_{air}) - Q \times V_{room} \times C_{air}$$

$$7b. \quad \frac{dA_{prod}}{dt} = -K \times S \times \frac{M}{RT} \times (P_{eq} - P_{air}) + A_{tot}/T_{app} \times w_f$$

where:

$A_{prod}$	mass substance in the product	[kg]
$P_{eq}$	equilibrium vapour pressure	[Pa]
$P_{air}$	actual vapour pressure	[Pa]
$V_{room}$	room volume	[m <sup>3</sup> ]
$Q$	room ventilation rate (number of air changes per time)	[1/s]
$A_{tot}$	total amount of product used	[kg]
$T_{app}$	application time	[s]
$w_f$	weight fraction substance in product	[fraction]
$K$	the mass transfer coefficient defined above	[m/s]
$S$	surface area of the product	[m <sup>2</sup> ]

Equation 7a describes the amount of substance evaporating from the product into the air (first term) and the subsequent removal of the substance by ventilation of the room air (second term). The evaporation is driven by the difference between the vapour pressure in the room air  $P_{air}$  and the equilibrium vapour pressure of the substance in the product  $P_{eq}$ . If the product is (applied in) a mixture, the latter is approximated by Raoult's law:

$$8. \quad P_{eq} = \left( \frac{P_{vap} C_v}{C_v + C_r \frac{M}{M_r}} \right),$$

where:

$P_{vap}$	saturated vapour pressure of the substance	[Pa]
$M$	molecular weight of the substance	[kg/mole]
$C_v$	concentration of the substance in the product	[kg/m <sup>3</sup> ]
$C_r$	concentration of the rest of the material in the product	[kg/m <sup>3</sup> ]
$M_r$	average molecular weight of the rest of the material	[kg/mole]

Note that Raoult's law is valid only for ideal, non-interacting liquids and constitutes only an approximate description of a real situation.

If the product is the substance in a pure form, the  $P_{eq}$  is equal to the saturated vapour pressure of the substance itself. Equation 7b describes the change of substance in the layer of product. It consists of two terms. The first term describes the amount of product evaporating from the product into the room air and is minus the source term in equation 7a. The second term describes the increase in the amount of product due to application of the product, if applicable. When

a surface area is covered with an amount  $A_{tot}$  of product in a time  $T_{app}$ , the amount of product applied per unit time is given by:

$$9. \quad \frac{dA_p}{dt} = A_{tot} / T_{app}$$

Multiplication by the fraction  $w_f$  of substance in the product gives the increase in substance in the product layer.

If the surface area from which the substance evaporates is constant, as in the case of evaporation from an open can or from a previously treated surface, the second term is zero.

To simulate emission and exposure from a product used in dilution an additional factor is introduced: the dilution.

Dilution is expressed in 'times': the number of times a substance is diluted (on weight basis). The equation that should be used to calculate the dilution is:

$$10. \quad dilution_{times} = \frac{solvent_{amount} + product_{amount}}{product_{amount}}$$

where:

$dilution_{times}$	dilution	[times]
$solvent_{amount}$	amount of solvent	[g]
$product_{amount}$	amount of product applied in the solution	[g]

When dilution is used, the 'product amount' parameter is interpreted as the amount of diluted product applied on a surface. The dilution is used to calculate the weight fraction  $wf_{solution}$  in the solution from the weight fraction  $wf$  in the product as:

$$11. \quad wf_{solution} = \frac{wf}{dilution_{product}}$$

The air concentration of the substance is evaluated by numerical integration of the system of equations 6a) and b). In case the product is the substance in pure form, equation 6a) become uncoupled of 6b) and emission is not automatically limited by the depletion of the substance from the liquid phase. In this case, the mass balance is checked in the numerical evaluation and emission is forced to be zero when the available substance has been depleted.

#### 4.1.2 Exposure to Spray model

The Exposure to Spray model describes the indoor inhalation exposure to slowly evaporating or non-volatile substances in droplets or particles that are released from a consumer spray. For volatile substances, the Exposure to Vapour model is more appropriate even when the substance is released by a spray application. The Exposure to Spray model may also be used to describe products that give rise to airborne particulate matter inhalation, such as dusts or powders.



The Exposure to Spray model distinguishes between two release modes to model the release and distribution of the spray product in the indoor environment: the Instantaneous Release and Spraying modes.

#### 4.1.2.1 Exposure to Spray: Instantaneous Release

In the Instantaneous Release mode, the sprayed material is assumed to be distributed homogeneously over the room air immediately upon release. After release, the substance is assumed to be removed by ventilation only.

The air concentration of the substance at time  $t$  for the Instantaneous Release mode is calculated as:

$$12. \quad C_{air} = \frac{A_o \times w_f}{V} \times e^{-qt}$$

where:

$C_{air}$	concentration of substance in the room air	[kg/m <sup>3</sup> ]
$A_o$	released mass of the spray	[kg]
$w_f$	weight fraction of the substance in the total product	[fraction]
$V$	room volume	[m <sup>3</sup> ]
$q$	ventilation rate of the room (number of air changes per time unit)	[1/s]

#### 4.1.2.2 Exposure to Spray: Spraying

The Spraying mode of the Exposure to Spray model was developed on the basis of the results of experimental work (Delmaar and Bremmer 2009). This mode takes into account the distribution of aerosol particles from spraying and the subsequent removal of these particles by deposition and ventilation.

Of particular interest in the case of inhalation exposure to aerosols is the region in the respiratory tract where the aerosol particles are deposited. This deposition depends on many factors, such as the size of the particles, the breathing pattern and human physiology. Particles that are deposited in the higher airways (extrathoracic and tracheobronchial regions) are cleared by a system of cilia and mucous via the gastrointestinal tract, which leads to exposure via the oral route. Only the particles that are deposited in the alveolar region will reach the lung–blood barrier and give rise to inhalation exposure.

General exposure parameters needed for this model are:

- **Spray duration:** the net spraying time between start and finish of spraying, not counting time between sprays.
- **Exposure duration:** the amount of time spent in the room where the spraying is taking place.
- **Room volume:** the volume of the room where the spraying is taking place.
- **Room height:** the height of the room where the spraying is taking place.
- **Ventilation rate:** the number of total air changes in the room per unit time.

- **Spraying towards person option.** This option is included to account for situations in which a person is inside the spray cloud, as is the case in using hairsprays and deodorants. When selecting the model option 'spraying towards person' the user is given the option to specify the initial volume of the cloud. This volume is defined to be the volume of the cloud after 1 second.

Air concentrations may be inhomogeneous because the spray is released in a cloud. The exposure of a person will depend on his or her position relative to the cloud and the dispersion of the cloud.

The dispersion of the cloud depends on ventilation of the room, thermal sources in the room and movement of people through the room (displacing the air inside it). In general, dispersion is in the order of a few minutes or less. As a simplification, in the ConsExpo Spray model the volume of the cloud after 1 second is assumed to further increase linearly in time until spraying stops or the cloud volume equals the volume of the room. It is assumed that during the use of the spray (the actual spraying) the breathing zone of the exposed person is located inside this volume. After spraying, the sprayed material is assumed to be homogeneously dispersed over the entire room.

The model requires values for the following product-specific parameters:

- **Mass generation rate:** the amount of substance that will be released from the spray container during the spraying per unit of time.
- **Aerosol diameter distribution:** the (mass-based) diameter distribution of the aerosol particles or droplets immediately after they are sprayed. The user has a choice of two parametric distribution functions: normal and log normal. For both distributions an average particle diameter (mean or median) and a width (standard deviation or coefficient of variation) have to be specified. In addition, the maximal particle diameter that is produced by the spray has to be given. This maximal particle diameter should not be set too high (preferably  $<50 \mu\text{m}$ ), since only inhalable particles are relevant.
- **Airborne fraction:** the fraction of the non-volatile material that becomes airborne after spraying as droplets. The airborne fraction will depend on the way in which the product is being used – i.e. in treating a surface (paint, wood preservative) or sprayed into the air (fly spray) – as well as on the aerosol diameter distribution that has been specified.
- **Weight fraction substance:** the fraction of the substance in question in the product.
- **Density non-volatile:** the mass density of the total of non-volatile substances.
- **Inhalation cut-off diameter:** the diameter below which the sprayed particles can be inhaled and reach the lower areas of the lungs (the alveolar region). Aerosol particles with a diameter larger than this cut-off are assumed to be deposited in the higher parts of the respiratory tract and cleared via the gastrointestinal tract, leading to oral exposure. The inhalation cut-off diameter is only an approximation of the complicated process of deposition of particles in the lung. In practice, its value is suggested to be set at

around 10–15  $\mu\text{m}$ . Currently, in the tool a default is provided of 15  $\mu\text{m}$ .

Particle diameter distributions are in practice determined by a standardized method determining the light-scattering profile of the spray at some distance (often 30 cm) from the spray nozzle. It is assumed that at this point all of the substance has evaporated from the smaller particles (diameter <50  $\mu\text{m}$ ). This assumption seems to be adequate for these particles and for substances of moderate volatility. For larger particles and for less volatile substances such as water, this approximation will not be valid. It is therefore advised to specify particle diameter distribution functions for particles up to about 50  $\mu\text{m}$ , which constitute the inhalable fraction of the particles.

The change in air concentration over time depends on the size of the sprayed particles, and calculations are performed for (size) distributions of particles.

The mass of particles with diameter  $\delta$  is given by:

$$13. \quad M_{\delta}(t) = M_{tot} \times P(\delta, t) d\delta$$

The particle mass distribution function  $P(\delta, t)$  is determined from the initial distribution specified by the user  $P(\delta, 0)$ .

In the ConsExpo Spray model the airborne particles are assumed to contain only non-volatile components, since moderately volatile substances will evaporate quickly from the smaller (inhalable) aerosol particles.

The total amount of material in the airborne particles is a combination of the fraction of non-volatile material that is contained in the specified particle distribution and the fraction of these particles that becomes airborne during application. This latter fraction will depend on the way the product is used, i.e. whether it is sprayed on a surface or directly into the room air. Thus, the total mass of the substance in particles that is being released from a spray per unit of time is given by:

$$14. \quad R_{release} = R_{spray} \times w_f$$

where:

$R_{release}$	rate of release of mass in aerosol particles	[kg/s]
$R_{spray}$	rate of release of sprayed product	[kg/s]
$w_f$	weight fraction of the substance in the product	[fraction]

From this, a fraction

$$15. \quad R_{airborne} = R_{release} \times f_{airborne}$$

becomes actually airborne and available for inhalation. Here:

$f_{airborne}$	airborne fraction of material	[fraction]
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Multiplying this mass generation rate of airborne particles by the normalized initial distribution yields the mass release rate per particle diameter.

$$16. \quad R_{airborne}(\delta) = R_{release} \times f_{airborne} \times P(\delta, 0) d\delta$$

The particles that are released from the spray are assumed to be evenly distributed over a volume  $V$ , which can be either the cloud volume or the room volume.

Particles with diameter  $\delta$  are removed from the room air by gravitational precipitation and by ventilation of room air.

The velocity  $v_s$  at which particles fall to the floor is given by Stokes settling velocity:

$$17. \quad v_s = \frac{g \rho_{droplet} \delta^2}{18\eta} \times SC$$

where:

G	gravitational acceleration	[m/s <sup>2</sup> ]
$\rho_{droplet}$	(average) mass density of the particle	[kg/mole]
H	air viscosity	[N s/m <sup>2</sup> ]
SC	Cunningham slip correction factor, which is only important for particles with a diameter of <1 $\mu\text{m}$ . It is taken to be 1 in the model	

Within a time  $dt$  the number of particles that reach the floor (and are thus removed from the air) is given by:

$$18. \quad C_{air}(\delta) \times S \times v_s(\delta)$$

where:

$C_{air}(\delta)$	concentration of mass of particles with diameter $\delta$	[kg/m <sup>3</sup> ]
S	surface area of the floor onto which the particles fall	[m <sup>2</sup> ]

The mass that is being removed by ventilation per unit of time is given by:

$$19. \quad C_{air}(\delta) \times V \times q_{vent}$$

where:

$q_{vent}$	ventilation rate of the room in number of air changes per unit time	[1/s]
V	volume of the room	[m <sup>3</sup> ]

During spraying the mass of particles with diameter  $\delta$  generated is given by  $R_{airborne}$ .

Therefore, the change in mass  $A_{air}(\delta)$  of the airborne particles with diameter  $\delta$  during spraying is given by:

$$20a. \quad \frac{dA_{air}(\delta)}{dt} = -q_{vent} \times A_{air}(\delta) - v_s(\delta) \times S \times \frac{A_{air}}{V} + R_{airborne}(\delta)$$

and after spraying by:

$$20b. \quad \frac{dA_{air}(\delta)}{dt} = -q_{vent} \times A_{air}(\delta) - v_s(\delta) \times S \times \frac{A_{air}}{V}$$

Under the simplifying assumption that the cloud disperses immediately through the room, these equations reduce to:

$$20c. \quad \frac{dA_{air}(\delta)}{dt} = -(q_{vent} + \frac{v_s(\delta)}{h}) A_{air} + R_{airborne}(\delta)$$

during spraying, and

$$20d. \quad \frac{dA_{air}(\delta)}{dt} = -(q_{vent} + \frac{v_s(\delta)}{h}) A_{air}$$

after spraying. In these equations:

H	room height	[m]
---	-------------	-----

From this it follows that the amount of substance in the air  $A_{air}$  during spraying is:

$$21a. \quad A_{air}(\delta, t) = \frac{R_{airborne}(\delta)}{q_{vent} + \frac{v_s(\delta)}{h}} (1 - \exp(-(q_{vent} + \frac{v_s(\delta)}{h})t))$$

After spraying, that is when  $t > T_{spray}$ , the mass of particles with diameter  $\delta$  in the room air is determined as:

$$21b. \quad A_{air}(\delta, t) = \frac{R_{airborne}(\delta)}{\gamma(\delta)} (1 - e^{-\gamma(\delta) \times T_{spray}}) \times e^{-\gamma(\delta) \times (t - T_{spray})}$$

where we introduced:

$$\gamma(\delta) = q_{vent} + \frac{v_s(\delta)}{h}$$

The total concentration of the substance follows from integration over the entire particle distribution:

$$22. \quad C_{air}(t) = \frac{1}{V} \int A_{air}(\delta, t) d\delta$$

## 4.1.2.3

## Non-respirable oral exposure

The material in aerosol particles with a diameter larger than the inhalation cut-off is assumed to be deposited in the higher regions of the respiratory tract and lead to oral exposure. ConsExpo offers the option 'include oral non-respirable material exposure'. If this option is checked, ConsExpo adds an oral route model to the exposure scenario and accounts for the non-respirable fraction of the inhaled spray.

## 4.1.3

*Emission from Solid Materials*

The levels of indoor air concentration that result from the emission of substances from solid materials are determined by various processes. On the one hand, the substance is emitted from the material into the bulk air. On the other hand, the substance is removed from the air. The first process is determined by diffusion of the substance to the surface of the material and subsequent mass transfer from the surface into the air. The removal of the substance from air is a result of different mechanisms, such as ventilation, degradation and sorption of the substance by indoor surfaces such as walls, furniture and dust.

The Emission from Solid Materials model included in ConsExpo describes a simplified situation (see Figure 14). It includes diffusion in the product and transfer into air, but it neglects indoor sinks other than ventilation. As a consequence, the air concentrations estimated using this model will usually over-estimate the real air concentrations for less volatile substances, for which other sinks are potentially important. The sorption of less volatile substances to skin and clothing may also give rise to dermal exposure, which may be comparable to or even higher than the exposure due to inhalation of the substance. This dermal absorption route is currently not included in ConsExpo.

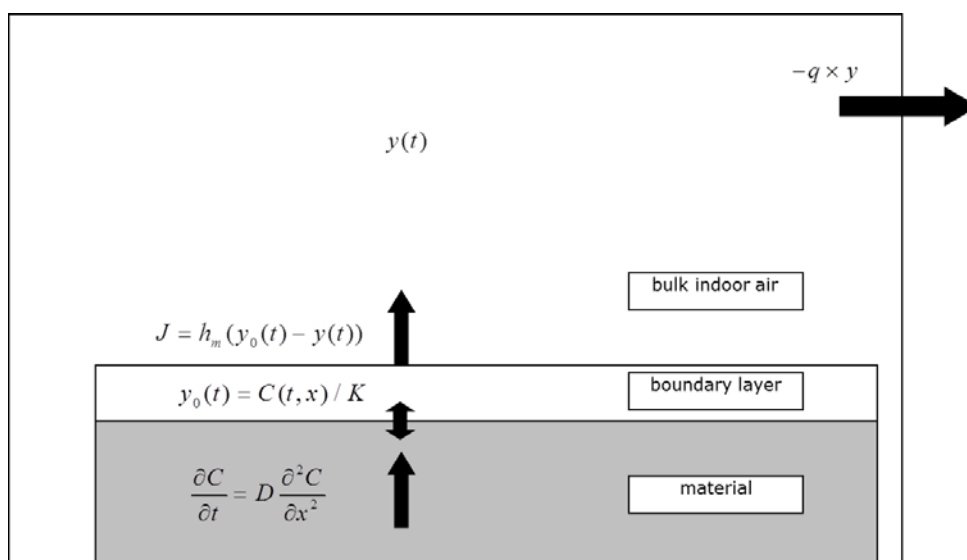


Figure 14. The processes included in the model describing the emission of substances from solid materials.

The Emission from Solid Materials model requires the following inputs:

- **Product surface area:** the surface area of the product.
- **Product thickness:** the thickness of the product.
- **Product density:** the density of the product.

- **Diffusion coefficient:** the diffusion coefficient of the substance in the material.
- **Weight fraction substance:** the weight fraction of the substance in the material.
- **Product/air partition coefficient:** This describes the affinity of the substance to the material. The partition  $P_{a,b}$  coefficient between two media a and b is defined as the ratio between the concentrations in media a and b when the distribution is in equilibrium.
- **Mass transfer coefficient:** the rate at which a substance is transferred between the product and the air. For a discussion of estimating this parameter and a justification of the default value of 10 m/h, see paragraph 4.1.1.4.
- **Ventilation rate:** the rate of removal of air from the room
- **Inhalation rate:** the volume of air inhaled by the exposed person per unit of time.
- **Total emission period:** the total duration of emission.
- **Start exposure:** the time after onset of emission (at 0 by definition) that exposure starts.
- **Exposure duration:** The time a person is present in the room where the emission takes place.

In the model, the material (product) is modelled as a slab of thickness  $L$ . With the assumptions described above, the concentration  $C$  in the material is determined by a one-dimensional diffusion equation:

$$23. \quad \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

where  $t$  is the time,  $x$  is the depth in the material and  $D$  the diffusion coefficient.

To evaluate the concentration in the material, this equation should be solved with appropriate boundary conditions. In most practical applications the initial concentration  $C_0$  can be assumed to be homogeneous (i.e.  $C_0(x) = \text{constant}$ ). Its numerical value has to be specified as model input.

It is further assumed that emission only takes place from the top side and that at the bottom (or at the sides) of the material there is no flux of substance out of or into the material:

$$24. \quad \left. \frac{\partial C}{\partial x} \right|_{x=0} = 0$$

At the material air surface ( $x=L$ ) there is an outflux  $J$  of the substance:

$$25a. \quad J = D \left. \frac{\partial C}{\partial x} \right|_{x=L}$$

This flux of substance from the material surface equals the flux through the stagnant boundary layer in the air above the surface:

$$25b. \quad J = D \left. \frac{\partial C}{\partial x} \right|_{x=L} = h_m (y_o(t) - y(t))$$

Under isothermal conditions, the air concentration  $y_0$  directly above the surface is assumed to be proportional to the material concentration  $C(x=d)$ :

$$26. \quad y_0 = \frac{C|_{x=L}}{K}$$

The mass transfer coefficient  $h_m$  describes the transport velocity of the substance from the material surface to the bulk indoor air  $y$ . The bulk air concentration is assumed to be homogeneous (well mixed). It is determined by the emission from the material and the removal by ventilation:

$$27. \quad \frac{dy}{dt} = \frac{S}{V} \times h_m \times (y_0 - y) - q \times y$$

The diffusion model with the given boundary conditions is solved numerically using a Runge-Kutta scheme.

To summarize, in the equations above the following parameters are used:

S	product surface area	[m <sup>2</sup> ]
L	product thickness	[m]
C	concentration of the substance in the product	[kg/m <sup>3</sup> ]
D	diffusion coefficient of the substance in the product	[m <sup>2</sup> /s]
$h_m$	mass transfer coefficient	[m/s]
q	ventilation rate	[1/s]
K	material air partition coefficient of the substance	[-]

#### 4.1.4 Modelling inhalation and absorption

ConsExpo implements a single absorption model: the Fixed Fraction absorption model, in which it is assumed that a certain fraction of the inhaled substance enters the systemic circulation through the lung alveoli:

$$28. \quad A_{abs} = f_{abs} \times C_{air} \times Q_{inh} \times t$$

where:

$F_{abs}$	absorption fraction, assumed to be known from experimental studies. Set to 1 as worst case, if no information is available	[fraction]
$C_{air}$	concentration of the substance in the (inhaled) air	[kg/m <sup>3</sup> ]
$Q_{inh}$	inhalation rate of the exposed person	[m <sup>3</sup> /s]
T	exposure time	[s]

To model inhalation and absorption the following input is needed:

- **Absorption fraction:** the fraction of the inhaled substance that enters the blood through the lung wall. If no information is available, the value should be set to 1, as the worst case.
- **Inhalation rate:** the inhaled volume per unit of time. In the absence of information on the inhalation rate, a default value can be selected from a database; Canadian (US EPA, 2011) or EU Biocides Framework (ECHA, 2017). Or it can be calculated in the program based on body weight and degree of activity (see also the ConsExpo General Fact Sheet; te Biesebeek et al. 2014).



This default inhalation rate value is based on empirical formulae (Freijer et al. 1997):

sleep:

$$Q_{inh} = 0.8 \times B_w^{0.6}$$

rest:

$$Q_{inh} = 1.05 \times B_w^{0.6}$$

light exercise:

$$Q_{inh} = 2.3 \times B_w^{0.65}$$

heavy exercise:

$$Q_{inh} = 11.0 \times B_w^{0.45}$$

## 4.2 Dermal route

ConsExpo's dermal model estimate exposure resulting from substances that, during or after product use, come into contact with the skin. Dermal contact with consumer products occurs, for example, when products are directly applied to or spilled on the skin or when the skin is immersed in water in which a product is dissolved. At present only one dermal model is implemented: the Direct Contact with Product model.

### 4.2.1 *Direct Contact with Product model*

This model comprises a set of application modes, all describing the situation in which a substance or a product comes into direct contact with the skin. The modes distinguished are: Instant Application, Constant Rate, Rubbing Off, Migration, and Diffusion.

A parameter that needs to be defined for all modes is the 'exposed area'. This refers to the surface area of the skin that is exposed to the product.

#### 4.2.1.1 Direct Contact with Product: Instant Application

The Instant Application mode assumes that all substance in the applied product comes directly in contact with the skin. The model can be used as a first-tier worst case approach if details of how the skin is exposed to the substance are not known. The model simply calculates exposure as the amount of product per surface area of skin (dermal load) or kg of body weight (external dose).

The two essential parameters used for this mode are:

- **Weight fraction substance:** the fraction of the substance in the total product.
- **Amount product:** the amount of total product applied to the skin.

The dermal load is calculated as:

$$29. \quad L_{derm} = A_{prod} \times wf / S_{exp}$$

And the external dose as:

$$30. \quad D = A_{prod} \times wf / W_{body}$$

where:

$A_{prod}$	amount of product applied to the skin	[kg]
$w_f$	weight fraction of the substance in the product	[fraction]
$S_{exp}$	surface area of the exposed skin	[m <sup>2</sup> ]
$W_{body}$	body weight of the exposed person	[kg]

#### 4.2.1.2 Direct Contact with Product: Constant Rate

Like the Instant Application mode, the Constant Rate mode assumes that all substance in the applied product comes into contact with the skin. The difference from the previous mode is that information on the contact time can be input. The mode calculates dermal exposure over a period. Therefore, if a good estimate can be made of the time during which the substance is applied on the skin, this mode can be used instead of the Instant Application mode.

Apart from the weight fraction substance parameter described above, two more parameters are required for this mode:

- **Contact rate:** the rate at which the product is applied to the skin, in volume per time unit.
- **Release duration:** the time during which the substance is applied.

The dermal load is calculated as:

$$31. \quad L_{derm} = R \times t \times w_f / S_{exp}$$

And the external dose as:

$$32. \quad D = R \times t \times w_f / W_{body}$$

where:

R	rate at which the product is applied to the skin	[kg/s]
T	loading time	[s]
$w_f$	weight fraction of the substance in the product	[fraction]
$S_{exp}$	surface area of the exposed skin	[m <sup>3</sup> ]
$W_{body}$	body weight of the exposed person	[kg]

#### 4.2.1.3 Direct Contact with Product: Rubbing Off

The Rubbing Off mode describes a secondary exposure situation. Instead of direct application of a product to the skin, it describes a situation in which a surface (table top, floor) is treated with a product and dermal exposure arises from skin contact with the treated surface.

The parameters used in this mode are:

- **Transfer coefficient:** the surface area treated with product that is in contact with the skin per unit of time.
- **Dislodgeable amount:** the amount of product applied on a surface area that may be wiped off, per unit of surface area. An example is when 100 mg of a powder is applied to 20 cm<sup>2</sup> of carpet, and 10% of the powder is wiped off during the rubbing of the carpet. If 10 cm<sup>2</sup> was rubbed, 10% of 50 mg is 5 mg product that is wiped off. The dislodgeable amount in this example is 0.5 mg/cm<sup>2</sup>.
- **Contact time:** the period during which a treated surface is rubbed.
- **Rubbed surface:** the area of the treated surface that is rubbed. In some cases the rubbed surface may be smaller than the treated surface, for example, when part of the treated surface is not accessible.
- **Weight fraction substance:** the fraction of the substance in the product.

The dermal load is calculated as:

$$33. \quad L_{derm} = S_{area} \times F_{dislodge} \times w_f / S_{exp}$$

And the external dose as:

$$34. \quad D = S_{area} \times F_{dislodge} \times w_f / W_{body}$$

$$35. \quad S_{area} = \max(R_{trans} \times t, S_{max})$$

where:

$S_{area}$	total area rubbed during exposure, determined by the transfer coefficient $R_{trans}$ , limited by $S_{max}$ , the total contaminated surface	[m <sup>2</sup> ]
$F_{dislodge}$	dislodgeable amount	[kg/m <sup>2</sup> ]
$S_{max}$	maximal area that can be rubbed during exposure, for instance the surface area of the entire floor of the room where exposure takes place	[m <sup>2</sup> ]
$w_f$	weight fraction of the substance in the product	[fraction]
$S_{exp}$	dislodgeable amount of substance that can be rubbed off per unit surface area	[kg/m <sup>2</sup> ]
$W_{body}$	body weight of the exposed person	[m <sup>2</sup> ]
$R_{trans}$	area rubbed per unit time	[m <sup>2</sup> /s]
T	exposure duration	[s]

#### 4.2.1.4 Direct Contact with Product: Migration

The Migration mode describes the migration of a substance from a material to the skin when dermal contact with the material occurs. This mode can be used for instance in the case of exposure to dyes in clothing, in which case the dye leaches to the skin.

Values for the following parameters are required:

- **Leachable fraction:** the amount of substance that migrates to the skin per unit amount of material.
- **Product amount:** the amount of material that is in direct contact with the skin.
- **Skin contact factor:** a factor that can be used to account for the fact that the material is only partially in contact with the skin.

The dermal load is calculated as:

$$36. \quad L_{derm} = A_o \times S_{contact} \times F_{leach} / S_{exp}$$

And the external dose as:

$$37. \quad D = A_o \times S_{contact} \times F_{leach} / W_{body}$$

where:

$F_{leach}$	leachable amount of substance that migrates to the skin per unit amount of product	[fraction]
$A_o$	amount of product in contact with skin	[kg]
$S_{contact}$	skin contact factor: a factor that can be used to account for the fact that the product is only partially in contact with the skin	[fraction]
$S_{exp}$	surface area of the exposed skin	[m <sup>2</sup> ]
$W_{body}$	body weight of the exposed person	[kg]

#### 4.2.1.5 Direct Contact with Product: Diffusion

Like the Constant Rate mode, the Diffusion mode describes the direct application of a substance in a product to the skin; for instance, in the case of a cream that is applied to the skin. After application, the substance diffuses through the product to the skin. The diffusion mode can be used if the diffusion coefficient of the substance in the product is known or can be estimated.

The mode requires the following parameters:

- **Substance concentration:** the concentration of the substance in the product.
- **Diffusion coefficient:** the rate at which the substance is diffused in the product.
- **Layer thickness:** the thickness of the layer of the product applied to the skin.
- **Exposure time:** the time that the product is in contact with the skin.

The concentration in the product on the skin is described by the equation:

$$38. \quad \frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2}{\partial x^2} C(x,t)$$

where:

D	diffusion coefficient of the substance inside the product	[m <sup>2</sup> /s]
C(x,t)	substance concentration in the product at depth x and time t	[kg/m <sup>3</sup> ]

The equation above is integrated numerically with the following options for the boundary conditions.

At the product–air surface the flux of substance is assumed to be zero, assuming no evaporation, so:

$$39. \quad D \frac{\partial C(x,t)}{\partial x} = 0$$

At the product–skin interface the boundary condition is determined by the flux into the skin. This flux is determined by the dermal absorption model. If the Fixed Fraction absorption model (see Section 4.2.2.1) is being used, the permeability of the skin is assumed to be infinite in the calculations and the flux of substance into the skin is limited by the diffusion of the substance out of the product. The potential amount of substance that can be taken up is calculated using the flux

$$40. \quad F_{skin} = D \frac{\partial C(x,t)}{\partial x}$$

at the skin–product interface, where the concentration in the skin is assumed to be zero.

After calculation of the potential amount taken up, this amount is adjusted using the experimental absorption fraction  $F_{abs}$ .

If the Diffusion Through Skin absorption model (see Section 4.2.2.2) is being used, the skin permeability is used to derive the flux into the skin as:

$$41. \quad F_{skin} = P \frac{\partial C(x,t)}{\partial x}$$

And equation 37 is integrated using this boundary condition.

#### 4.2.2 Dermal absorption models

In ConsExpo, the dermal absorption of a substance can be estimated using two different models: the Fixed Fraction Absorption model, and the Diffusion Through Skin model.

##### 4.2.2.1 Fixed Fraction absorption model

The Fixed Fraction model is a simple model for which the only parameter required is the absorption fraction. The absorption fraction can be obtained from experimental results or it can be estimated. For a worst case estimation, the value can be set to 1, implying that all of the substance is taken up through the skin.

Dermal absorption ( $A_{abs}$ ) of the substance is calculated as:

$$42. \quad A_{abs} = f_{abs} \times A_{derm}$$

where:

$F_{abs}$	absorption fraction	[fraction]
$A_{derm}$	amount of substance in contact with the skin	[kg]

##### 4.2.2.2 Diffusion Through Skin absorption model

The Diffusion Through Skin absorption model can be used when the substance in contact with the skin is in an aqueous solution. This model can only be used in combination with the dermal exposure modes Instant Application or Diffusion.

The parameters required for this model are:

- **Concentration:** the concentration of the substance in the product.
- **Permeability skin:** the permeability of the skin to the substance.
- **Contact time:** the period of dermal contact with the product.

The absorption is calculated as:

$$43. \quad A_{abs} = A_{skin} \times \left(1 - \exp\left(-\frac{P \times S}{V} \times t\right)\right)$$

where:

$A_{skin}$	amount of substance on the skin	[kg]
P	permeability of the skin	[m/s]
V	volume of the substance on the skin (follows from the concentration and the amount on the skin)	[m <sup>3</sup> ]
S	exposed skin area	[m <sup>2</sup> ]
t	exposure time	[s]

### 4.3 Oral route

ConsExpo provides two models to estimate oral exposure: the Direct Product Contact model and the Migration from Packaging model. Exposure is calculated as the amount potentially taken up per kg body weight and the actual dose (amount absorbed per kg body weight), using a user-provided absorption fraction.

#### 4.3.1 *Direct Product Contact model*

The model includes three modes, describing exposure through direct ingestion of the product containing the substance: through direct intake of the product, through intake at a constant rate, and through migration of the substance from the product to the saliva during product mouthing.

##### 4.3.1.1 Direct Product Contact: Direct Intake

The Direct Intake mode describes exposure to a substance from a product that is swallowed at once. This mode can be used as a first tier (screening) model if details of the exposure process are unknown.

The parameters used in this mode are:

- **Weight fraction substance:** the fraction of the substance in the product.
- **Amount ingested:** the amount of total product swallowed.

The external dose is calculated as:

$$44. \quad D = A \times w_f / W_{body}$$

where:

A	amount of product swallowed	[kg]
$w_f$	weight fraction of the substance in the product	[fraction]
$W_{body}$	body weight of the exposed person	[kg]

##### 4.3.1.2 Direct Product Contact: Constant Rate

The Constant Rate mode describes a scenario in which the substance is taken in over a period. This mode can be used to estimate, for instance, (secondary) exposure originating from dermal contact with the hands and subsequent hand–mouth contact.

The parameters used in this mode are:

- **Weight fraction substance:** the fraction of the substance in the product.
- **Ingestion rate:** the amount of total product ingested per unit of time.
- **Exposure time:** the amount of time during which the product is ingested.

The external dose is calculated as:

$$45. \quad D = R \times w_f \times t / W_{body}$$

where:

R	ingestion rate of the product	[kg/s]
$w_f$	weight fraction of the substance in the product	[fraction]
t	time during which the product is being ingested	[s]
$W_{body}$	body weight of the exposed person	[kg]

#### 4.3.1.3 Direct Product Contact: Product Mouthing

The Product Mouthing mode describes a scenario in which oral exposure occurs through the leaching of a substance from a product to the saliva in the mouth.

The parameters used in this mode are:

- **Exposure time:** the time during which the product is mouthed.
- **Product amount:** the total amount of product that is mouthed.
- **Weight fraction substance:** the fraction of the substance in the product.
- **Contact area:** the surface area of the product that is mouthed.
- **Initial migration rate:** the amount of the substance migrating from the product per unit of time.

The external dose is calculated as:

$$46. \quad D = A \times w_f \times (1 - \exp(-\frac{R_m \times S}{A \times w_f} \times t)) / W_{body}$$

where:

A	total amount of product that is mouthed	[kg]
R <sub>m</sub>	rate at which the substance migrates from the product (per unit area)	[kg/m <sup>2</sup> .s]
S	surface area of the product that is mouthed	[m <sup>2</sup> ]
w <sub>f</sub>	weight fraction of the substance in the product	[fraction]
t	mouthing time	[s]
W <sub>body</sub>	body weight of the exposed person	[kg]

#### 4.3.2 Migration from Packaging Material model

This exposure model calculates the exposure to substances from food packaging material via food.

The migration of the substance into food is calculated from the concentration of the substance in the packaging material, the contact area between the packaging and the food, and the migration rate. The oral exposure resulting from consumption of the food is subsequently calculated by assuming that the migrated substance is homogeneously distributed over the food and that the intake of the substance is therefore proportional to the fraction of packaged food consumed.

The parameters needed to assess this type of exposure are:

- **Substance concentration:** the concentration of the substance in the packaging material.
- **Thickness package:** the thickness of the packaging material.
- **Contact area:** the area of contact between packaging material and food.
- **Packaged amount:** the amount of food packaged.
- **Ingested amount:** the amount of food consumed.

If no information is available on the release of the substance from the packaging material, the option 'instantaneous' can be selected to describe the release of all the substance at once. The amount of substance available for migration is calculated as:



$$47. \quad A_{comp} = C_{prod} \times S_{cont} \times d$$

where:

$A_{comp}$	total amount of substance that can migrate from the packaging material	[kg]
$C_{prod}$	concentration of the substance in the packaging material	[kg/m <sup>3</sup> ]
$S_{cont}$	area of contact between the packaging material and the food	[m <sup>2</sup> ]
$d$	thickness of the packaging material	[m]

If information is available, the option 'constant rate' can be selected and values for the following parameters need to be defined:

- **Migration rate:** the migration rate of the substance from the material to the food.
- **Storage time:** the storage time of the packaged food.

The amount of substance available for migration is then calculated as:

$$48. \quad A_{food} = \max(R_{migr} \times t, A_{comp})$$

From this the external exposure is calculated:

$$49. \quad D_{extern} = A_{food} \times \frac{A_{cons}}{A_{pack}} / W_{body}$$

where:

$A_{comp}$	total amount substance that can migrate from the packaging material	[kg]
$C_{prod}$	concentration of the substance in the packaging material	[kg/m <sup>3</sup> ]
$S_{cont}$	area of contact between the packaging material and the food	[m <sup>2</sup> ]
$D$	thickness of the packaging material	[m]
$T$	storage time of the packaged food	[s]
$R_{migr}$	migration rate of the substance from the material to the food	[kg/s]
$A_{food}$	amount of substance in the packaged food	[kg]
$A_{cons}$	amount of food consumed	[kg]
$A_{pack}$	amount of food packaged	[kg]
$W_{body}$	body weight of the exposed person	[kg]

#### 4.3.3

##### *Oral absorption model*

ConsExpo calculates the oral absorption of the substance with a fraction model. The only required parameter in the fraction model uses is the absorption fraction: the fraction of the substance that is absorbed from the lumen of the gut into the blood. For a worst case estimate, the value should be set to 1.

Oral absorption is calculated as:

$$50. \quad A_{abs} = f_{abs} \times A_{ing}$$

where:

$f_{abs}$	absorption fraction	[fraction]
$A_{ing}$	amount of substance ingested	[kg]



## 5 Analysis of the results

There are different reasons why exposure to substances in consumer products needs to be assessed: for example, to estimate the health effects in a population after an exposure event has occurred, or to set limits on substance concentrations in products to safeguard a population of users. In all cases, the exposure assessor has to deal with the high variability within the population for which the assessment is made. Parameters such as body weight, exposure duration, and use amount of product may vary significantly between individuals. For other parameters, information may be scarce or unreliable. Lack of information on variability and uncertainty of the values may lead to under- or overestimations of exposure levels and, consequently, of risk. ConsExpo offers a number of tools that help assessors to gain insight into the variability and uncertainty of the estimated exposure levels.

### 5.1 Worst case estimates

For some exposure assessments, the available information on the product use, the substance in question and/or the exposed consumer may be very limited. In these cases, a worst case exposure can be estimated by using first-tier screening models, which require a minimum amount of information. The required parameters can also be filled out using worst case single point values; for example, a high-percentile value from a distribution when data is available. However, it is important to recognize that the use of high-percentile single point values in an exposure assessment may lead to a cumulative worst case estimate of the exposure, which may quickly become unrealistic if many parameters are involved.

### 5.2 Distributions

Exposure assessments are (either explicitly or implicitly) conducted for a population. In a deterministic assessment (in which single or point values are used for all input parameters), the exposure is assessed for a person that represents a larger population. This person may represent either an average person or a typical highly exposed person in this population. Such a deterministic assessment summarizes the exposure in a single number for the entire population. In reality, however, any assessment of population exposure includes a measure of variation. This is either due to the fact that factors determining exposure vary from person to person (variability) or due to the fact that the value of exposure factors is not exactly known (uncertainty). Variation in input parameters due to variability or uncertainty may be modelled in ConsExpo by specifying distributions for input values rather than simply deterministic numbers.

#### 5.2.1 *Parametric distributions in ConsExpo*

There are four distribution functions available in ConsExpo: normal, log normal, uniform and triangular distribution (see Section 3.1.2). If specified, these distributions are used to calculate the distributions of external exposure and internal dose.

If distributed values are given for one or more parameters, ConsExpo uses Monte Carlo simulation to evaluate the distribution of the results. Samples of parameter values are randomly drawn from the specified distribution functions. For these samples, exposure is calculated and in this way a distribution of the exposure is constructed.

The resulting distribution of the results of the different endpoints in the exposure assessment can be inspected graphically in the 'Results' section. The mean, median, standard deviation and 90<sup>th</sup> and 99<sup>th</sup> percentile values of the exposure assessment are presented. This distribution represents either the variability or the uncertainty in the estimated exposure for the defined population.

In ConsExpo the user can determine the number of Monte Carlo samples that is drawn. It should be noted that a higher number of samples in general leads to a more representative distribution of the exposure, but that this is at the cost of more calculation time. For this reason, the number of samples in ConsExpo Web is limited to 50,000.

For an introduction to Monte Carlo techniques, see for instance Morgan and Henrion (1990) and Cullen and Frey (1999).

Probabilistic modelling allows the user to gain more insight in the exposure results. The exposure level is expressed as a range of values with their associated frequencies of occurrence, rather than a single average point value. This allows the user to determine whether extremely high or low exposure levels occur and what the most frequent exposure levels are.

One note of caution should be made here. In performing the Monte Carlo simulations ConsExpo randomly draws values from all specified distributions without considering possible correlations between parameters. This may lead to unrealistic combinations of parameter values and thus to unrepresentative exposure levels. For example, the inhalation rate and body weight of a person are correlated. Drawing from a distribution of inhalation rates and body weights without taking into account their correlation may lead to unrealistic combinations of high inhalation rate with low body weight and vice versa.

Although ConsExpo does not take into account correlations between parameters, it does consider the validity boundaries of parameters, excluding, for example, negative values from the sampling if a parameter is required to be positive-valued.

### 5.3 Sensitivity analysis

A sensitivity analysis of the model can be performed by investigating the effect of a range of values of one parameter on the estimated exposure levels. If a large change of a parameter value results in only a minor change of the outcome, the model is said to be insensitive to that parameter. If, on the other hand, a small change in a parameter value causes a large change in the outcome, the model is said to be sensitive to that parameter.

The sensitivity of a model can be investigated using the 'Sensitivity analysis' in the Output section of ConsExpo. A range of values for a parameter can be specified and their effect on an end point of the exposure can be plotted in a graph.

Apart from investigating the sensitivity of a model, the sensitivity analysis allows the user to investigate to what extent certain factors affect exposure levels to a substance in a consumer product. This is an important tool in determining the relative importance of uncertain parameters and in guiding the exposure assessor towards possible improvements in the exposure assessment.



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## Appendix I. Adaptations with respect to ConsExpo 4

ConsExpo Web is an update of the ConsExpo 4 tool developed in 2005. ConsExpo Web is a web application, and incorporates most of the features of ConsExpo 4. In addition, a number of improvements have been made.

First, ConsExpo Web permits multiple scenarios within a single assessment. These scenarios may, for example, represent different use phases of the product or different tiers in an iterative exposure assessment. The exposure estimates of the separate scenarios are not added, however.

Second, a model has been added to assess the exposure due to emissions from solid materials (products or articles). This model was previously released as a separate tool ('RIVM emission tool').

Third, a first-tier (screening level) model for exposure to non-volatile substances in sprays was added to the 'Exposure to Spray' model.

Finally, the terminology has been updated and the calculated exposure outputs have been adjusted. The terminology and updated exposure outputs are described in Appendix II.

## Appendix II. Updated terminology

Some of the evaluated exposure metrics have been updated in ConsExpo Web as compared with ConsExpo 4. The table below lists the exposure metrics used in ConsExpo 4 and the corresponding metric in ConsExpo Web.

ConsExpo 4.1	ConsExpo Web	Unit	Explanation / comments
<b>Inhalation</b>			
mean event concentration	mean event air concentration	mg/m <sup>3</sup>	average air concentration on exposure event Note: depends strongly on chosen exposure duration
mean concentration on day of exposure	mean air concentration on day of exposure	mg/m <sup>3</sup>	average air concentration over the day (accounts for the number of events on one day)
air concentration year average	year average air concentration	mg/m <sup>3</sup>	mean daily air concentration averaged over a year
n.a.	external event dose	mg/kg bw	amount that can be absorbed per kg body weight
n.a.	external dose on day of exposure		amount that can be absorbed per kg body weight
acute (internal) dose	internal event dose	mg/kg bw	amount absorbed during one event per kg body weight
n.a.	internal dose on day of exposure	mg/kg bw/day	daily absorbed dose per kg body weight averaged over a day Note: this can be (at frequencies >1x per day) higher than the 'event dose'.
chronic (internal) dose	internal year average dose	mg/kg bw/day	daily absorbed dose (per kg body weight) averaged over a year Note: this can be higher than the 'event dose' for exposure frequencies >1 per day.
<b>Dermal</b>			
dermal load	dermal load	mg/cm <sup>2</sup>	amount per cm <sup>2</sup> on the skin
external dose	external event dose	mg/kg bw	amount that can be absorbed per kg body weight during one event
n.a.	external dose on day of exposure	mg/kg bw/day	amount that can be absorbed per kg body weight during one day

<b>ConsExpo 4.1</b>	<b>ConsExpo Web</b>	<b>Unit</b>	<b>Explanation / comments</b>
acute (internal) dose	internal event dose	mg/kg	absorbed dose (per kg body weight) during 1 exposure event
n.a.	internal dose on day of exposure	mg/kg bw/day	absorbed dose (per kg body weight) during 1 day Note: this can be (at frequencies >1x per day) higher than the 'event dose'.
chronic (internal) dose	internal year average dose	mg/kg bw/day	daily absorbed dose (per kg bw) averaged over a year
<b>Oral</b>			
external dose	external event dose	mg/kg bw	amount that can be orally absorbed per kg body weight during one event; external exposure measure
n.a.	external dose on day of exposure	mg/kg bw/day	amount that can be orally absorbed per kg body weight during one day; external exposure measure
acute (internal) dose	internal event dose	mg/kg bw	absorbed dose (per kg body weight) during 1 exposure event
n.a.	internal dose on day of exposure	mg/kg bw	absorbed dose (per kg body weight) during 1 day
chronic (internal) dose	internal year average dose		daily absorbed dose (per kg bw) averaged over a year
<b>Integrated</b>			
acute dose (in output)	internal event dose	mg/kg bw	total absorbed dose (per kg body weight) during 1 exposure event; internal exposure
n.a.	internal dose on day of exposure	mg/kg bw/day	absorbed dose (per kg body weight) during a day
Chronic dose (in output)	internal year average dose	mg/kg bw/day	daily absorbed dose (per kg bw) averaged over a year

### Appendix III. Update features ConsExpo Web version 1.0.2

Below we summarize features added and issues addressed in ConsExpo Web after its release in October 2016.

Feature	description
<i>ConsExpo Web 1.0.2 - December 2017</i>	
Peak exposure	For the inhalation models "exposure to spray" (instantaneous, spraying) and "exposure to vapour" (instantaneous release, constant release and evaporation) the estimation of the time-weighted average for 15 min at peak exposure is included.
Excel report	The copy function for the report is replaced by the functionality to download the input and output data as .csv file (which can be opened in Excel).
Population characteristics	For the population characteristics body weight and inhalation rate, a 'select default' possibility is included. A selection can be made from Canadian defaults, ConsExpo fact sheet and EU Biocides Framework.
Defaults from updated Cleaning Products FS	The Cleaning Products Fact Sheet (Meesters et al. 2017, in preparation) is being updated. The adapted or new defaults are already included in the ConsExpo Web Fact Sheet default database. This includes the addition of a parameter for dilution in the "exposure to vapour – evaporation" model.
Duplicate scenario	Addition of the possibility to copy a scenario.
Preview of fact sheet defaults	Addition of a preview of the model and default values including the Q-factors are provided in a panel (as was in ConsExpo 4.1).
Further features	<ul style="list-style-type: none"> <li>- 15 µm included as standard default for inhalation cut off diameter (as was in ConsExpo 4.1)</li> <li>- Setting of the mass transfer coefficient as default to 10 m/hr</li> <li>- Inclusion of CAS nr at substance properties</li> <li>- Panel with assessments set at maximum size , with scroll bar</li> <li>- Possibility to include text in a comment box per exposure route (included as information in the report as well as in the export to Chesar)</li> </ul>
<i>ConsExpo Web 1.0.1 – July 2017</i>	
Export functionality to Chesar	Creates output file which can be imported in Chesar
Various minor bugs	<ul style="list-style-type: none"> <li>- Error message invalid lognormal distribution</li> <li>- Add units to x-axis distribution graphs</li> <li>- Error in emission model when using a distribution for product-air partition coefficient</li> <li>- Un caught error when using distribution for body weight</li> <li>- Runtime error when using spray model in</li> </ul>

	combination with oral ingestion without specification of inhalation rate
Set 'limit concentration to saturated air concentration' default true in exposure to vapour instant release	Is the most appropriate default behaviour
Round-off errors when using distribution of very small particles in spray model	Solved by more refined sampling of the diameter distribution (not always over – 0-max diameter, but from mean – 3 sd's to mean + 3 sd's)
Exporting graphs to Excel	Export of graphs of the air concentration to Excel was required for further manipulation outside ConsExpo as suggested by Recommendations of the Ad hoc Working Group on Human Exposure for the exposure assessment of, for example, disinfectants.

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