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Comparison of consumer exposure modelling tools
Inventory of possible improvements of ConsExpo

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Abstract

Comparison of consumer exposure modelling tools

ConsExpo is a suitable computer software programme with mathematical models for assessing the exposure of consumers to chemicals in consumer products. This tool can be further improved by adopting certain features from other existing consumer exposure modelling tools.

In ConsExpo, different routes of exposure are taken into account, such as the route via the skin, and through inhalation and oral uptake. An important feature of ConsExpo 4.1 is that it contains a database with default values and standard exposure scenarios (who is exposed? where? how? and how often?) for a wide range of consumer product types. Examples include cosmetics, paint, cleaning products, pest control products and disinfectants. The default values and exposure scenarios are described in detail in fact sheets.

ConsExpo was compared with other existing consumer exposure modelling tools in an investigation to discover whether the tools contained any exposure scenarios, mathematical models or other features that might be useful for ConsExpo. The aim of the study was to find features that may improve this version (4.1). The investigation demonstrated that ConsExpo is very suitable for assessing exposure to chemicals in consumer products. The other tools did not contain any exposure scenarios for which assessment with ConsExpo is not possible.

Nonetheless, a number of mathematical models and other software features have been found that may be of importance to ConsExpo. For example, some tools are capable of assessing exposure to a chemical in multiple products. Assessment of this so-called ‘aggregate exposure’ will possibly play an important role in the risk assessment of chemicals in future legislation in the EU (REACH).

Keywords: ConsExpo, consumer products, exposure assessment, model, comparison

Rapport in het kort

Vergelijking van modellen om consumentenblootstelling te berekenen

ConsExpo is een geschikt computerprogramma met rekenmodellen om de mate van blootstelling van mensen aan stoffen in consumentenproducten te schatten. Het programma kan verder verbeterd worden door bepaalde elementen uit andere bestaande rekenmodellen over te nemen.

In ConsExpo wordt rekening gehouden met verschillende manieren van blootstelling: via de huid, via inhalatie en via orale opname. Bij het programma hoort een database, waarin standaardwaarden en blootstellingscenario's (wie wordt waar en hoe blootgesteld aan wat en hoe vaak) voor vele producttypen worden aangeboden (bijvoorbeeld cosmetica, verf, reinigingsmiddelen, ongediertebestrijdingsmiddelen en desinfectantia). De beschrijving van deze standaardwaarden en blootstellingscenario's wordt gerapporteerd in zogenoemde 'fact sheets'.

Om ConsExpo verder te kunnen verbeteren is een vergelijking gemaakt met andere bestaande rekenmodellen. In de inventarisatie werd gekeken of deze modellen blootstellingscenario's, wiskundige methoden of andere aspecten bevatten die een nuttige aanvulling kunnen zijn voor ConsExpo. Uit de inventarisatie bleek dat ConsExpo zeer geschikt is om de blootstelling te schatten voor stoffen in consumentenproducten. In andere rekenmodellen werden namelijk geen blootstellingscenario's aangetroffen, die niet met ConsExpo berekend kunnen worden. Wel zijn er wiskundige methoden en andere elementen gevonden die voor ConsExpo van groot belang kunnen zijn. Zo kunnen sommige rekenmodellen blootstelling aan stoffen uit meerdere producten berekenen. De berekening van deze zogenaamde 'geaggregeerde blootstelling' zal mogelijk een rol gaan spelen in de risicoschatting van chemische stoffen onder de toekomstige wetgeving in de EU (REACH).

Trefwoorden: ConsExpo, consumentenproducten, blootstellingschatting, model, vergelijking

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Samenvatting

ConsExpo is een computerprogramma met mathematische modellen die de blootstelling aan stoffen in consumentenproducten beschrijven. Het programma kan gebruikt worden in de risicoschatting van stoffen in consumentenproducten door de blootstelling aan deze stoffen te schatten. De recente aanpassing van het programma heeft de gebruikersvriendelijkheid is verbeterd en enkele modellen herzien.
In dit onderzoek is ConsExpo vergeleken met andere hulpmiddelen voor het modelleren van consumentenblootstelling. Het doel van deze vergelijking was het vinden van aspecten waarin ConsExpo aangepast en verder verbeterd kon worden. De volgende hulpmiddelen zijn in deze vergelijking opgenomen: Multi-Chamber Concentration and Exposure Model (MCCEM), Consumer Exposure Module (CEM), PRObabilistic Methodology for Improving Solvent Exposure assessment (PROMISE©), Lifeline Aggregate and Cumulative Exposure / Risk assessment Software™, Central Risk and Exposure Modelling e-solution (CREMe), Pesticide Inert Risk Assessment Tool (PIRAT), Residential Exposure Assessment Model (REx), Wall Paints Exposure Assessment Model (WPEM), Model for diffusion-controlled building materials, SprayExpo, Skin Permeation (SKINPERM) en de European Technical Guidance Document on Risk Assessment (TGD).

Het resultaat van dit onderzoek was dat ConsExpo de blootstelling kan schatten voor alle blootstellingscenario’s die in de andere hulpmiddelen aanwezig waren. Er waren echter enige onderlinge verschillen in de mathematische modellen die voor deze schatting gebruikt werden. In specifieke gevallen kunnen meer complexe mathematische modellen van andere hulpmiddelen nuttig zijn voor ConsExpo, hoewel experimentele data nodig zijn om te bevestigen of deze modellen de blootstelling werkelijk beter beschrijven dan de modellen in ConsExpo.
De onderzochte hulpmiddelen bevatten een aantal aspecten die van belang kunnen zijn voor ConsExpo, zoals aanvullende database opties en de mogelijkheid om geaggregeerde blootstellingsschattingen (blootstelling aan één stof in verschillende consumentenproducten) uit te voeren.
De algemene bevinding van de vergelijking is dat van de beschikbare hulpmiddelen ConsExpo het meest geschikt is voor het uitvoeren van blootstellingsschattingen voor stoffen in consumentenproducten in het algemeen.

Summary

ConsExpo is a computer program with mathematical models which describe the exposure to chemicals in consumer products. The program can be used in the risk assessment of chemicals in consumer products by assessing the exposure to these chemicals. The recent adaptation of the program improved the user-friendliness and updated a number of models. In this research, ConsExpo has been compared with other consumer exposure modelling tools. The goal of this comparison was to find aspects which can be used to adapt and further improve ConsExpo. The following tools have been included in the comparison: Multi-Chamber Concentration and Exposure Model (MCCEM), Consumer Exposure Module (CEM), PRObabilistic Methodology for Improving Solvent Exposure assessment (PROMISE©), Lifeline Aggregate and Cumulative Exposure / Risk assessment Software™, Central Risk & Exposure Modeling e-solution (CREMe), Pesticide Inert Risk Assessment Tool (PIRAT), Residential Exposure Assessment Model (REx), Wall Paints Exposure Assessment Model (WPEM), Model for diffusion-controlled building materials, SprayExpo, Skin Permeation (SKINPERM) and European Technical Guidance Document on Risk Assessment (TGD).

The result of this investigation was that ConsExpo can assess exposure for any of the exposure scenarios included in the other tools. However, the mathematical models used for this calculation were sometimes different. In specific cases, some more complex mathematical models in other tools may be useful for ConsExpo, although experimental data are needed to confirm whether these models actually describe the exposure better than the models contained in ConsExpo.
The tools investigated contained a number of features which can be essential for ConsExpo, such as additional database options and the possibility to perform aggregate exposure assessments (exposure to one chemical from different consumer products).
An overall finding of the comparison was that for the general purpose of performing exposure assessments for chemicals in consumer products, ConsExpo appears to be the most adequate tool currently available.

1. Introduction

A potentially important exposure pathway of humans to environmental chemicals forms the use of consumer products containing chemicals as ingredients or residues. The assessment of exposure levels via this route is not an easy task to perform. Due to the wide variety of consumer products and variation in the behaviour of consumers, representative exposure data are generally not available. In these circumstances, exposure assessors are often confined to estimating exposure levels by means of (mathematical) models. ConsExpo is such a computer program with mathematical models to assist in the exposure assessment of chemicals in consumer products (RIVM, 2006). The program was initially developed by RIVM to improve exposure assessment for consumer products, on request of the Dutch Food and Food Consumer Product Safety Inspectorate (VWA).

Features of ConsExpo are:

- mathematical models generally applicable to a large variety of non-food consumer products
- mathematical models describing exposure via inhalation, dermal contact and oral ingestion
- mathematical models of varying complexity for each exposure route
- optional use of a database with default products, related exposure scenarios and default values for their input model variables
- exposure assessment expressed as external and internal exposure
- exposure outcomes ranging from acute to chronic exposure
- different output styles of the exposure assessment such as point values or graphs
- possibility to perform probabilistic calculations, using stochastically distributed input values

Recently, the fourth version of the program, ConsExpo 4.1, has been released, in which user friendliness was significantly improved compared to previous versions. In addition, the set of mathematical models used in previous versions was reviewed and updated according to the latest insights and new experimental data (Delmaar et al., 2005).

The aim of the current report is to make an inventory of other existing consumer exposure modelling programs. By comparison of ConsExpo with features of these programs, suggestions will be made for possible improvements of ConsExpo.

2. Existing consumer exposure models

At present, only few exposure modelling programs applicable to a wide range of consumer exist. Many exposure modelling programs are designed specifically for exposure assessments for a specific group of consumer products or via a specific exposure route. Both types of models may have useful features that could serve as a basis for a revision of ConsExpo. Below, a short description of the capabilities of the different programs is given and potential useful features for ConsExpo are discussed.

2.1 Multi-Chamber Concentration and Exposure Model

The Multi-Chamber Concentration and Exposure Model (MCCEM) was developed on behalf of the Office of Pollution Prevention and Toxics (OPPT) of the US Environmental Protection Agency (US-EPA) to aid in the evaluation of new and existing chemicals (US EPA, 2006a). The program models time varying indoor air concentrations and inhalation exposures in different chambers of a residence.

Features of MCCEM are:

- mathematical model describing exposure via inhalation only, expressed as external (potential) exposure
- optional use of database with zone descriptions, volumes and airflows for one-story, two-story and three-story residences in different states of the United States
- exposure levels of four different zones within a residence can be simulated
- exposure assessments expressed as acute (peak concentrations and single day doses) and chronic (lifetime average daily doses) outcomes
- distributed input values possible for a limited number of parameters

2.1.1 Mathematical models

Compared to ConsExpo, this program simulates inhalation exposure by means of a more complex mathematical model. Multiple sources in multiple zones of the house can be defined, along with effects of reversible or irreversible sinks. Exposure is calculated taking into account the air exchange between different chambers (zones) in the residence and the activity pattern of the exposed individual which needs to be defined by the user.
The more complex mathematical model may describe exposure to a chemical more accurately than the inhalation models included in ConsExpo, because it takes into account more factors that may influence the exposure. However, this has not been demonstrated by experimental data and a disadvantage of the more complex model is that it needs much more specific input. For example, the user must specify how the chemical is emitted from the source, by selecting

a constant, single exponential or incremental emission rate model or by means of data entry. Information on the course of the emission of a chemical from a source can be determined based on data from environmental chamber testing, but this information will unlikely be available for every chemical in every product. In addition, activity patterns of the exposed person need to be defined, i.e. in which room the exposed person is located throughout the day of use. This type of information is generally not readily available to the exposure assessor. However, this model may be useful specifically for scenarios where a source is emitting chemicals during a longer period of time, e.g. carpets or plywood.

2.1.2 Useful features

Features of MCCEM that may be useful for ConsExpo are:

- the possibility to select default values for individual model input variables such as room volume and ventilation rate from a database
- the possibility to include more than one source emitting the same chemical during the same exposure period, which may be particularly useful for aggregate exposure assessments[1]
- the possibility to specify more complex exposure scenarios in terms of frequency of exposure, such as multiple exposure events per day during a specific season of the year
- the possibility to enter notes in the program, for example to describe the exposure scenario, assumptions or other remarks that may be important for the interpretation of the results, which will be included in the output report

2.2 Consumer Exposure Module (CEM)

The Consumer Exposure Module (CEM) was designed on behalf of the OPPT of the US-EPA to aid in the evaluation of new and existing chemicals (US EPA, 2001). CEM is an interactive model which calculates conservative estimates of potential inhalation exposure and potential and absorbed dermal exposure to consumer products. CEM is available as a module within the Exposure and Fate Assessment Screening Tool Version 2.0 (E-FAST V2.0).

Features of CEM are:

- screening-level exposure assessments expressed as acute potential dose rates, and average and lifetime average daily dose rates
- built-in databases on human exposure factors, default values for use amounts for 9 preset scenarios, activity patterns for residents in the home and common chemical components of consumer products with associated typical weight fractions

[1] Although several definitions of aggregate exposure exist, this report uses the term ‘aggregate exposure’ for the total exposure to one chemical that arises from multiple sources via different pathways

2.2.1 Mathematical models

Consumer inhalation exposures modelled in CEM use the same approach and calculations as scenarios depicted in the former Screening -Level Consumer Inhalation Exposure Software (SCIES). Dermal exposures are modelled using the same approach and equations as the former DERMAL Exposure Model. These two models were originally developed as separate screening level, exposure assessment tools but are now available only as integrated tools in the E-FAST CEM module. The approach and calculations of the higher tier tool MCCEM discussed above are also included in CEM, although the effect of indoor sinks is not included. The dermal model of CEM uses a film-thickness approach which assumes that exposure occurs from a thin layer of the consumer product on a defined skin surface area to determine potential exposure.
The film thickness approach is also included in the dermal loading mode ‘diffusion’ of the ConsExpo dermal model. Contrary to the CEM model, the ConsExpo model also takes into account the diffusion coefficient - a value that accounts for the fact that the compound in the layer is not in direct contact to the skin, but first needs to diffuse through the layer to the skin. The potential added value of the inhalation models for ConsExpo has been discussed in the previous section on MCCEM. The dermal model included in CEM has no apparent added value for ConsExpo.

2.2.2 Useful features

The CEM software is in many ways quite similar to the ConsExpo software. Both CEM and ConsExpo contain databases with default scenarios for a number of consumer products and related default values for the model input variables. The default values contained in CEM have been extracted directly from the US-EPA exposure factor handbook (US EPA, 1997). The default exposure factor values in ConsExpo originate from different sources instead of from one widely accepted (European) data source. A (limited) European exposure factor sourcebook is available through ExpoFacts, but momentarily does not contain data on frequency and amount of consumer product use (University of Kuopio, 2006).
A feature of CEM that may be valuable for ConsExpo is the database containing common chemical components of consumer products with associated ‘typical’ weight fractions.

2.3 Probabilistic methodology for improving solvent exposure assessment (PROMISE©)

PROMISE© is a software tool developed for the Solvents Council of the American Chemistry Council to assist in the exposure assessment of industrial chemicals (American Solvents Council, 2005). PROMISE© is primarily designed for estimating single exposure events in occupational settings and in certain consumer-type applications. The program is best suitable for chemicals that have some volatility and exist either in the pure form or in a formulation. Features of PROMISE© are:

- designed specifically to perform probabilistic exposure assessments

- mathematical models describing exposure via inhalation, dermal contact and oral ingestion
- optional use of library containing default values for many model input variables
- use of model input variable ranges and distributions rather than single value point estimates. The user has a choice of up to 15 different types of distributions
- output in the form of a distribution of dose from the defined scenario can be evaluated, visualized, analyzed, documented, saved and directly compared to alternative scenarios, alternative exposure and uptake models, and different similar scenarios using alternative values for the model input variables

2.3.1 Mathematical models

The mathematical models of PROMISE© are based on existing models such as those in ConsExpo version 2.0 and the Environmental Protection Agency (EPA) dermal transport model for ACC's American Solvents Council. In the ConsExpo 4 version, mathematical models in ConsExpo 2.0, such as the dermal diffusion uptake model have been modified and updated according to the most recent information. The mathematical models in PROMISE© are therefore not considered useful for an improvement of ConsExpo.

2.3.2 Useful features

Features of PROMISE© that may be useful for ConsExpo are:

- a database with referenced data for many of the model input variables, including distributions
- direct comparison of outputs between exposure scenarios using alternative values for model input variables
- possibility to calculate any desired percentage or percentile as output of stochastic exposure assessments
- a greater choice of distribution types (15)
- Possibility to enter textual comments at several points throughout the exposure assessment, for example description of variable input values

2.4 Lifeline Aggregate and Cumulative Exposure / Risk assessment Software™.

LifeLine™ Software Version 4.3 is a tool to characterize population-based aggregate and cumulative exposures and risks from pesticide residues (The LifeLine Group, 2006). The sources of exposure included in the program are diet, home environments, drinking and tap water, residential pesticide products, pesticide users or an aggregate of all of these sources. The software provides a tool to understand the relative contributions from these sources, and how they vary across individuals' lives. Although not a consumer exposure program as such,

this program is included in this report because non-food consumer products, namely residential pesticide products, is one of the exposure sources included in LifeLine™.

Features of LifeLine™ are:

- probabilistic model of aggregate and cumulative exposures to pesticides and other chemicals
- applicable to the general US and Canadian populations and selected sub-populations
- routes of exposure considered in the model are: inhalation, dermal penetration and oral from diet, or from child's mouthing behaviours
- database of activity patterns, body weight and length, skin surface area of hands and whole body, inhalation rates, residential details, and diets of US and Canadian population
- possibility to assess the history of each individual's exposures to a pesticide from all sources, the patterns of exposure for populations at different ages, the distribution of exposure across a population at any age and season, and the corresponding risks for acute and chronic non-cancer toxic effects associated with those exposures, as well as lifetime cancer risks

2.4.1 Mathematical models

Lifeline™ is a very complex program needing a lot of input from the user on characteristics of the population of interest. The mathematical models used to assess an individual's exposure to substances from non-food consumer products are not described and as such are hard to evaluate for the purpose of comparison with ConsExpo.

2.4.2 Useful features

Some features of Lifeline™ that may be useful to ConsExpo:

- possibility to assess aggregate and cumulative exposure
- possibility to perform risk evaluation by including toxicity data input
- possibility to create custom files with default population groups such as general populations, pregnant females, children and elderly with related activity patterns that can serve as input for different exposure assessments
- possibility to create custom files with default product or chemical properties that can serve as input for different exposure assessments

2.5 Central Risk and Exposure Modelling *e*-solution (CREM*e*)

CREM*e* is an exposure assessment tool specializing in the areas of population exposure assessment to consumer products, food and environmental concerns (CREM*e* Ltd., 2006b).

The CREM*e* tool is delivered as a web service with access to high performance computing (HPC). Currently, there are several different CREM*e* exposure tools: for additives, pesticides, food packaging, novel foods and cosmetics and personal care. Especially the latter is useful for comparison with ConsExpo.

Features of CREM*e* cosmetics and personal care are:

- probabilistic model calculating dermal external exposure from cosmetics and personal care products
- web based system which allows large data set management
- possibility to share input and output data, reports and files, within and outside the institution

2.5.1 Mathematical models

The mathematical model underlying CREM*e* cosmetics and personal care is simple, as it only calculates external exposure: frequency x amount / body weight. This model is analogous to the 'instant application' dermal mode included in ConsExpo. The CREM*e* tool is capable of performing stochastic exposure assessments using large data sets, in which variables can be correlated. The assessments are comparable to the way dietary intake studies perform probabilistic intake exposure assessments. When considering external dermal exposure, the calculation is relatively simple compared to, for example, external inhalation exposure, since the parameters for external dermal exposure (frequency, amount and body weight) are easy to collect. Should this concept be used for inhalation exposure, more complex parameters, such as ventilation rates and particle size have to be collected, which is a very resource intensive task.

2.5.2 Useful features

Some features of CREM*e* that may be useful to ConsExpo:

- possibility to insert (large) data sets for input variables for use in probabilistic exposure assessments
- possibility to correlate variables

2.6 Pesticide Inert Risk Assessment Tool (PIRAT)

The Pesticide Inert Risk Assessment Tool (PIRAT) provides screening level estimates of exposure and risk to pesticide inert ingredients that are used in a residential setting, i.e. ingredients other than the active ingredients in pesticide products (US EPA, 2006b). The tool is developed by Versar, Inc. for the US-EPA's Office of Pesticide Programs (OPP) and is currently available in its beta version.

Features of PIRAT are:

- deterministic assessment of either dermal or inhalation route during application for adults
- deterministic assessment of either dermal, inhalation or oral exposure route after application for adults or children (toddlers, 3 years of age)
- assessment of both indoor and outdoor residential uses of pesticide products
- assessment of acute and chronic risks
- Pesticide Handlers Exposure Database (PHED) containing default values for amounts of exposure per amount of active ingredient handled (PHED unit exposure value). PHED is a software system consisting of two parts - a database of measured exposure values for workers involved in the handling of pesticides under actual field conditions and a set of computer algorithms used to subset and statistically summarize the selected data. Users select criteria to subset the PHED database to reflect the exposure scenario being evaluated. The data generated as such are then used as surrogate values for residential exposure. The sub-setting algorithms in PHED are based on the central assumption that the magnitude of handler exposures to pesticides are primarily a function of activity (e.g. mixing/loading, applying), formulation type (e.g. wettable powders, granulars), application method (e.g. aerial, ground boom), and clothing scenarios (e.g. gloves, double layer clothing).

2.6.1 Mathematical models

The mathematical models used in PIRAT rely on OPP's PHED residential SOP's (Keigwin, 1998). To calculate the potential dose rate during application for most scenarios, the model variables used are the PHED unit exposure value for that specific activity, the application rate, the inert weight fraction, the amount used, and the body weight of the exposed individual. The mathematical models to calculate potential dose rates for post application scenarios are slightly more complicated in that the variables included in the model change for each activity. For example surface area and ingestion rate are included in calculations of exposure from hand-to-mouth activities.

The mathematical models in ConsExpo cover all scenarios included in PIRAT, both during and after application, although the mathematical models used in PIRAT used to calculate exposure for these scenarios may sometimes differ slightly from those in ConsExpo. For example, the mathematical models for inhalation exposure in PIRAT do not take into account ventilation rates in the room of exposure. The models for dermal and oral exposure are based on similar assumptions as those in ConsExpo. Therefore, these models appear to be of no added value to ConsExpo.

2.6.2 Useful features

Features of PIRAT that may be useful for ConsExpo are:

- database with weight fraction data based on a review of residential-use pesticide labels
- database with defaults for unit exposure values (amount exposed to per amount handled) based on measured data and exposure scenario criteria

- possibility to assess outdoor residential use of consumer (pesticide) products by means of using unit exposure values
- display the mathematical algorithm upon selection of the exposure scenario, and/or in the output
- possibility to include toxicity data and evaluate the risk
- possibility to view multiple exposure assessments in one window, for example separate columns with results for adults and children

2.7 Residential Exposure Assessment Model (REx)

The Residential Exposure Assessment Model (REx) is a spreadsheet EXCEL based model to estimate exposure and associated risk from residential use(s) of pesticides (Infoscientific.com, 2006). The model was developed by Infoscientific.com on commission of the US-EPA and according to the TGD was intended to be included in the Cumulative and Aggregate Risk Evaluation System (CARES). As an individual spreadsheet, REx is no longer used by the US-EPA.

Features of REx are:

- aggregating one or more (up to six) product use scenarios (from US EPA SOPs) with either simple deterministic or complex stochastic exposure and dose assessments
- receptors (exposed subjects) are adults and three categories of children (< 1 year, 1 year < age < 6 years, and age > 6 years)
- aggregation can be done for scenarios during use and post application
- use of the Pesticide Handlers Exposure Database (PHED) containing default values for amounts of exposure per amount of active ingredient handled (PHED unit exposure value). More information on PHED can be found under section 2.6, describing the PIRAT software

2.7.1 Mathematical models

Similar to the PIRAT software, the mathematical models in the REx spreadsheet rely on OPP's PHED residential SOPs (Keigwin, 1998). These have been discussed under section 2.6.

2.7.2 Useful features

Features of REx that may be useful for ConsExpo are:

- possibility to perform aggregate exposure assessments
- possibility to insert toxicology data and compare this to the exposure assessment
- default distributed values for model variables instead of default point values only

2.8 Wall Paints Exposure Assessment Model (WPEM)

The Wall Paints Exposure Assessment Model (WPEM) estimates the potential exposure of consumers and workers to the chemicals emitted from wall paint which is applied using a roller or a brush (US EPA, 2006c).

Features of WPEM are:

- mathematical models developed from small chamber data to estimate the emissions of chemicals from oil-based (alkyd) and latex wall paint
- database with detailed use, workload and occupancy data (e.g. amount of time spent in the painted room, etcetera)
- six default scenarios describing adult, child or professional exposure to paint
- output evaluated in a home used by EPA for testing purposes
- exposure assessment output expressed as Lifetime and Average Daily Doses, Lifetime and Average Daily Concentrations, and peak concentrations

2.8.1 Mathematical models

The mathematical models underlying WPEM is based on experimental small chamber data. The models are very specific for latex and alkyd wall paint and are not applicable to other consumer products. The output of WPEM was evaluated in a home used by EPA for testing purposes. In general, the experimental values were within a factor 2 compared to the modelled values.
For an in-depth exposure assessment of chemicals in paint, this model is very useful. However, as such it falls outside the scope of the ConsExpo software, which provides general, broadly applicable models for a diverse group of consumer products.

2.8.2 Useful features

A feature of WPEM that may be useful for ConsExpo is that it contains a database of chemicals often contained in paint, with physicochemical properties.

2.9 Model for diffusion-controlled building materials

A model describing the rate of absorption and desorption of volatile organic chemicals (VOCs) by diffusion-controlled building materials was developed by Kumar and Little (2003). Diffusion-controlled materials may act both as sources and as sinks for VOCs, depending on the relative magnitudes of the gas- and material-phase concentrations. The model has been validated by chamber experiments with phenol and *n*-dodecane and showed a good prediction of the source and sink behaviour of the building materials.

2.9.1 Mathematical models

A main difference with the evaporation model in ConsExpo is that the model described by Kumar and Little also factors in the possible sink function of materials for VOCs. The latest published version of the model also includes a non-uniform initial material-phase concentration and a time-dependent function describing the gas-phase influent VOC concentration, allowing for a more realistic modelling of indoor environment conditions. The model has been validated only for diffusion-controlled building materials and for the purpose of assessing exposure from these materials, the model may be useful for ConsExpo. In addition, it could be investigated whether the current evaporation model in ConsExpo could be extended with a sink model.

2.10 SprayExpo

SprayExpo is a deterministic model to predict the inhalation and dermal exposure during spray application of biocidal products (BAuA, 2006). It was developed by the Fraunhofer Institute for Toxicology on commission of the German Federal Institute for Occupational Safety and Health (BAuA). SprayExpo calculates the airborne concentration of the respirable, the thoracic and the inhalable, or any other meaningful size fraction of aerosols containing biocidal substances in indoor environments originating from the release of liquid biocidal sprays. The model is based on a simulation of the motion of released droplets taking into account gravitational settling, turbulent mixing with the surrounding air, and droplet evaporation.

Features of SprayExpo are:

- short term exposure model covering time scales typical for the release process. Long term emissions of vapours from walls and other surfaces are not included
- applicable to biocidal product composed of a non volatile active substance dissolved in a solvent with known volatility
- inhalation as well as the dermal exposure from spray applications can be assessed
- explicit modelling of the spatial distribution of the exposure concentration
- possibility to differentiate between inhalable, thoracic, respirable, total or dermal dose

2.10.1 Mathematical models

The mathematical model underlying SprayExpo is in its basic assumptions similar to the spray model in ConsExpo. A difference with the model in ConsExpo is that SprayExpo differentiates between five different release patterns (wall line, wall area, ceiling, floor or room) instead of the two release patterns in ConsExpo (spraying towards exposed person or not). In addition, contrary to ConsExpo, the mathematical model in SprayExpo takes into account the turbulence difference and the spray angle.

2.10.2 Useful features

Features of SprayExpo that may be useful for ConsExpo are:

- possibility to calculate exposure concentrations over time after spraying multiple times
- possibility to distinguish exposure assessments for different regions of the respiratory tract
- possibility to assess dermal exposure after spraying

2.11 Skin Permeation (SKINPERM)

Skin Permeation (SKINPERM) is a software program that estimates the skin permeation coefficient of a chemical from aqueous solutions using the physicochemical properties such as molecular weight and the octanol-water coefficient as independent parameters (Ten Berge, 2006).

2.11.1 Mathematical models

An older version of the SKINPERM Quantitative Structure Activity Relationship (QSAR) used in this software is already included in ConsExpo, along with other QSARs. Since 2003, an adapted version of the QSAR is used in SKINPERM, which according to the developer Ten Berge is more in line with QSARs for aqueous diffusivities and provides a better fit. Momentarily, Ten Berge is working on an even newer model for skin permeability which, based on personal communication, appears to be very promising. Expectations are that this model will be available for insertion in ConsExpo in the near future.
It should however be noted that no accepted, validated method currently exists to estimate dermal uptake of chemicals.

2.11.2 Useful features

The software in itself contains no features that are of apparent added value to ConsExpo.

2.12 European Technical Guidance Document on Risk Assessment (TGD)

Although not an exposure assessment software tool as such, the European Technical Guidance Document on Risk Assessment (TGD) contains information that may be useful for ConsExpo.
As discussed in section 2.11, currently no validated method exists to estimate uptake of chemicals through the skin. The same applies to uptake via the respiratory and gastrointestinal tract. Nevertheless, any information on the uptake of a chemical may greatly improve the (systemic) exposure assessment. Risk assessors often resort to using experimental data, or assume a 100% uptake. The EU Technical Guidance Document on Risk

Assessment (TGD) gives some general guidance on whether uptake of a chemical following exposure might occur (ECB, 2003). Table 1 below presents an overview of quantitative chemical properties reported in the TGD that potentially lead to high or low uptake of a substance via the three main exposure routes. The values in the table can serve as a general guidance, which could potentially also be included in ConsExpo.

Table 1 Quantitative properties of a chemical or product that may influence potential uptake via different exposure routes

Exposure route	Chemical/product property	Potential uptake	
		High	Low
Inhalation	Vapour pressure (KPa)	> 25	< 0.5
	Particle size (µm)	< 1-5	> 100
	Log P	> 0	
Oral	Molecular weight	< 500	> 1000
	Particle size	< 1 nm	> 100 µm
	Water solubility (mg/L)		< 1
	Log P	0-4	> 4
Dermal	Molecular weight	< 100	> 500
	Water solubility (mg/L)	> 10.000	< 1
	Log P	1 - 4	< 0, > 6
	Vapour pressure (Pa)	< 100	
	Surface tension (mN/m)	< 10	

3. Conclusions and recommendations for improving ConsExpo

For the general purpose of performing exposure assessments for chemicals in consumer products, ConsExpo appears to be the most adequate program currently available. Other exposure modelling programs discussed in this report have often been designed for more specific purposes such as aggregate exposure assessments for pesticides from different sources or exposure assessments for chemicals in paint. However, these programs are sometimes equipped with features that would also be useful to ConsExpo. Based on these features, some potential useful modifications of ConsExpo can be suggested.

3.1 Mathematical models

The exposure modelling tools discussed in this report contained no consumer product use scenarios for which exposure assessment is not possible with ConsExpo. Therefore, the mathematical models currently included in ConsExpo appear capable of modelling exposure for most consumer products. Moreover, the majority of exposures can be assessed with more than one mathematical model, differing in complexity. Nevertheless, alternative models exist for the same exposure scenarios. For certain scenarios (multiple chamber inhalation exposure, exposure from wall paint), more complex models are available, but due to lack of experimental data it is often unknown whether these models describe the actual exposure better or worse than the models in ConsExpo. In addition, such more complex models often also require more specific input data, although default values are sometimes provided.
Some useful additions to models in ConsExpo can be given:

- ConsExpo's current exposure to spray model does not contain a simple, first tier mode which estimates a worst case exposure based on minimum input of data. As all other exposure models in ConsExpo do contain such a first tier mode, it would be appropriate to include a simple mode in the spray model as well.
  An additional improvement of the spray model would be the ability to distinguish between exposed doses in different respiratory regions. This information may for example be useful for chemicals that exert local effects in specific regions of the respiratory tract. Assessment of dermal exposure after a spray application would also be useful.
- The source/sink model for diffusion-controlled building materials by Kumar and Little (2003), or components thereof, may be a useful addition to ConsExpo's evaporation model.
- To provide more guidance on the extent of dermal, inhalation and oral uptake of chemicals, incorporation of the physicochemical related uptake properties of chemicals reported in the TGD could be considered. However, it should be kept in mind that the

uptake of chemicals is influenced by many factors simultaneously. For example, a chemical with high water solubility would suggest a high dermal uptake, but if the chemical has a Log P (octanol/water) below 0, it may be too hydrophilic to cross the lipid rich environment of the stratum corneum and dermal uptake will be low. In addition, chemical-specific membrane carriers or barriers may supersede the influence of physicochemical properties. It may therefore be difficult to provide a general model for uptake which takes into account all such factors.

- The dermal uptake model in development by Ten Berge may be a useful update of the current dermal uptake model in ConsExpo.
- It would be useful to extend to possibilities of specifying the frequency of exposure events for more complex exposure scenarios. Currently, in ConsExpo, exposure for one event is calculated, and frequency can be specified to define how often this exposure event takes place. This frequency is then also used to estimate chronic exposure (per year). However, sometimes exposure scenarios are more complex. For example, an insecticide may be used several times in one day, but only on a limited number of days during a certain season of the year. Calculating exposure during those days is probably more meaningful than the chronic exposure assessment.

3.2 Aggregate exposure assessments

A number of programs discussed in this report are capable of performing simple aggregate exposure assessments (i.e. one chemical in multiple products). This feature would be highly useful to ConsExpo, as many chemicals are used in more than one consumer product. For a more complete risk assessment of a particular chemical, exposure resulting from all simultaneously used consumer products containing the chemical should be taken into account. The ability to perform aggregate exposure assessments will likely become more important with the upcoming EU REACH regulations. Information on chemical composition of consumer products will become available to producers or risk assessors and aggregate exposure assessments will be more feasible and may even be required for some chemicals.

3.3 Stochastic exposure assessments

ConsExpo already features possibilities to perform stochastic exposure assessments by means of Monte Carlo calculations. However, a number of adaptations increase the possibilities and improve the results of such assessments:

- A major improvement of the stochastic exposure assessment in ConsExpo would be to enable the correlation of model variables. Some model variables may be correlated, i.e. if the value of one variable increases, then the value for another variable also increases or, in case of inversely correlated variables, the other variable decreases. When performing a Monte Carlo calculation, a random value is drawn from the pool of distributed values for

that variable and this is combined with a random value for another variable. Currently, ConsExpo's Monte Carlo calculations do not take into account that these variables may be correlated. For example, it could draw a high value for both amount of shampoo used and frequency of shampoo use, whereas studies have shown that the amount of shampoo applied declines with frequency of use (CREMe Ltd., 2006a). Not taking into account correlations between variables causes inappropriate variation in the exposure assessment results.

- Currently ConsExpo contains a choice of four distributions to describe input data for a variable: normal, lognormal, triangular and uniform. Including more distribution types may be advantageous in certain cases, to better describe the data, although it may negatively affect the user-friendliness of ConsExpo.
- In some cases it may be beneficial to the user to have the possibility to include data sets as input for model variables. If the user has a data set available for a particular variable, but does not know its distribution, it may be useful to allow the user to insert the complete data set. With this possibility, the user would not have to insert a single point value, in which case much information would be lost.
- The default values for the model input variables currently contained in ConsExpo are all point values. To further expand the possibilities to perform stochastic exposure assessments, it would help to include default distributed values for certain model input variables as well.
- In ConsExpo, the output of a stochastic exposure assessment is presented in a graph, and only the mean, median, 90^{th} and 99^{th} percentile are presented as numerical values. Other values can be calculated only by exporting the data to Excel. The possibility to calculate any desired percentile as output of a stochastic exposure assessment within ConsExpo would be useful.

It needs to be pointed out that a stochastic exposure assessment is not always favoured over a deterministic exposure assessment. However, this discussion is out of the scope of this project and will be addressed elsewhere (RIVM report in preparation, to be published in 2007).

3.4 Databases

Currently, ConsExpo only contains a database with consumer product types and default values for model input variables related to these consumer product types. The exposure assessment tools discussed in this report frequently contained databases of a different calibre that may also be useful for ConsExpo. Some examples are:

- Databases of values for individual input model variables, such as room volumes, ventilation rates, body weights, etcetera. In ConsExpo, the user cannot select default values for individual model input variables. The databases included in the exposure assessment tools discussed above are sometimes accompanied by references such as US

EPA's exposure factor handbook. Such linked databases and references would be of great value to ConsExpo.
- Databases with common chemical components of consumer products with associated typical weight fractions.
- Database with defaults for unit exposure values (amount exposed to per amount handled) based on measured data and exposure scenario criteria, similar to the PHED database for pesticides discussed in section 2.6.

The downside of incorporating any database is that it requires frequent updates of the information, which may be a laborious exercise.
An alternative way to use default values would be the possibility to link data files of, for example, frequently used populations with their respective characteristics such as body weight and activity patterns, or houses with room volumes and ventilation rates. These files can be customized by the user and then be linked to ConsExpo and used for multiple exposure assessments.

3.5 Useful software features

The exposure assessment software programs discussed in this report frequently contained a number of features that may be useful for the ConsExpo software:

- A feature that would be useful for the interpretation of the exposure assessment is the possibility to enter comments accompanying different input fields, e.g. a textual description of exposure scenario or a justification for the choice of a particular value for a model input variable.
- Currently, ConsExpo is not able to run more than one exposure assessment file at once. To better compare results, it would be useful to simultaneously visualize outputs of different exposure assessments in one window and save multiple assessments in one file.
- A feature frequently encountered in other exposure assessment tools is the possibility to include toxicological data. This data could then be compared to the exposure assessment and be used to calculate a margin of safety.

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