

Recommendation no. 16

BPC Ad hoc Working Group on Human Exposure

Applicability of ConsExpo for water based disinfectants

(Agreed at the Human Health Working Group III-2019 on 23 May 2019)

1. Summary

At present, a number of water based H₂O₂ containing disinfectants are under assessment. It has been noticed that ConsExpo's evaporation model is used for exposure assessments, but this model seems to be unsuitable for some scenarios. Factually, the evaporation rate of H₂O₂ is largely determined by the evaporation of water, which is not considered by ConsExpo's evaporation model.

In some scenarios with water based products, disregarding the evaporation of water can result in a substantial underestimation of the exposure, while in other scenarios it may only make a minor difference. The differences are particularly considerable for application tasks where a significant change of the concentrations in the applied product is expected and when the substance in question has a (substantially) lower vapour pressure than water, as in the case of H₂O₂ products.

An acceptable approximation could be reached by simulating the evaporation of pure H₂O₂ by using the option 'product is substance in pure form' in ConsExpo's evaporation model. However, in some scenarios, e.g., for very short exposure durations, this approach can also result in an overestimation. Therefore, this approach should be considered as a Tier 1 option, which shall not exclude an assessment based on measured data or refined modelling considering risk mitigation measures in Tier 2.

Note: The Advanced REACH Tool (ART) was used for the assessment of some scenarios in the CAR for H₂O₂. If ART is the agreed model for assessing a particular scenario, it may still be used.

This document is intended to recommend a suitable mechanistic approach should ConsExpo be considered as the appropriate model for a particular scenario.

2. Background

Exposure from biocide uses which involve spreading a product onto a surface, e.g., painting or wiping activities, is often estimated using ConsExpo's evaporation model. This model simulates the evaporation of the substance in question from the product matrix based on physical properties (e.g. vapour pressure) and on scenario parameters such as concentration, application surface, duration and air exchange rate.

However, after looking closer into the mechanistic model implemented in ConsExpo, there are strong doubts in the applicability of ConsExpo for the assessment of water based disinfectants. The main concern is that the evaporation model in ConsExpo at present assumes that other components than the substance in question do not evaporate (see eq. 7a and 7b on p. 37 of the ConsExpo model documentation)¹. This is a good approximation for many scenarios, but it does not seem to reflect the behaviour of water based disinfectants properly, as will be shown below with the example of a disinfectant consisting of water and H₂O₂.

In the ConsExpo model, the evaporation of the substance in question (here: H₂O₂) in the liquid product is driven by the difference of the vapour pressure of this substance within the liquid (which according to Raoult's law depends on its molar fraction) and the vapour pressure of the substance in the air (p. 37)¹. As the matrix (here: water) is not allowed to evaporate in the model, the concentration of the substance in question in the liquid product decreases with ongoing evaporation of this substance, which also lowers its vapour pressure. Depending on the conditions, it is even possible that the vapour

¹ ConsExpo Web: Consumer Exposure models - model documentation, Update for ConsExpo Web 1.0.2, available at <https://www.rivm.nl/bibliotheek/rapporten/2017-0197.html>

pressure in the product reaches that of the vapour pressure in the air, which will stop any further evaporation in the simulation.

The vapour pressure of H₂O₂ at 20°C is 214 Pa, hence about one order of magnitude lower than the vapour pressure of water (2338 Pa), and its concentration in application solutions applied to surfaces is usually much lower than that of water. As a consequence, in reality the water will evaporate much faster than H₂O₂. This will result in increasing H₂O₂ concentrations in the liquid and, in turn, in faster evaporation of H₂O₂.

In order to calculate some examples, the equations given in the ConsExpo manual have been implemented in Excel using Visual Basic (VBA). In addition, to simulate a system with two components evaporating at the same time, the model has been extended by two additional equations (derived from equations 7a and 7b shown in the ConsExpo manual), which calculate the behaviour of the water².

The wiping and mopping task has been assumed with the parameters shown in Table 1.

Figure 1 shows the results of four simulations:

- I) one, in which water evaporates in parallel to H₂O₂ (red line)
- II) a second, in which water is not allowed to evaporate (blue line), and which corresponds to the ConsExpo assessment, and
- III) for comparison, a simulation of pure water, where the results have been multiplied with 0.25%, the assumed concentration of H₂O₂ in this scenario (green line), and
- IV) a simulation of pure H₂O₂ (purple line, proposed approximation for assessment).

Table 1: Parameters used for the wiping and mopping scenario (water based H₂O₂ solution). The shown symbols are those used in the equations below.

Parameter	Symbol	Value
Exposure duration [min]	-	120
Molecular weight matrix or solvent, respectively [g/mol] - water	$M_{\text{solv.}}$	18
Product amount [kg]	$m_{\text{prod.,tot}}$	0.8
Weight fraction H ₂ O ₂	w_f	0.25 %
Room volume [m ³]	V_{room}	80
Ventilation rate [/h]	Q	0.5
Vapour pressure H ₂ O ₂ [Pa], 20 °C	$p_{\text{vap, subst.}}$	214
Application temperature [°C]	T	20
Molecular weight [g/mol] H ₂ O ₂	$M_{\text{subst.}}$	34
Release area [m ²]	S	40
Mass transfer coefficient [m/h]	K	10
Application duration [min]	t_{app}	15
Does area increase?	-	yes
vapour pressure solvent [Pa] - water, 20 °C (only for 2-component-simulation)	$p_{\text{vap, solvent}}$	2338
Air humidity at start [%]		0

² For reference, the functional Excel spread sheet is included as an annex to this document.

For simulation I), in which water evaporates in parallel to H₂O₂, humidity of room air and fresh air is a significant parameter. For the shown example, this parameter was set to 0% in order to display the worst case.

Comparison of the first two approaches I) and II) demonstrates that the H₂O₂ concentrations in air increase much faster and become much higher when evaporation of water is considered in the simulation. When only H₂O₂ is considered as volatile, the maximum of 3.0 mg/m³ is reached after 52 min (blue line). In contrast, when both, H₂O₂ and water, are calculated as volatiles, the maximum of 24.6 mg/m³ (red line) is already reached after 18 min, when the application has just finished. At that time, the 1-component model has just reached an air concentration of 2.1 mg/m³ (18 min, blue line). For the two approaches, the mean event concentrations for the simulated 120 min duration are 14.5 mg/m³ and 2.6 mg/m³, respectively.

Interestingly, the results of the 2-component model in I) (red line) show a very similar behaviour as the simulation of pure water in III) (adjusted to 0.25%, green line) as well as the simulation of pure H₂O₂ in IV) (purple line) which both could suggest a simple workaround for the present assessments. However, these approaches have neither been extensively tested, nor have they been validated.

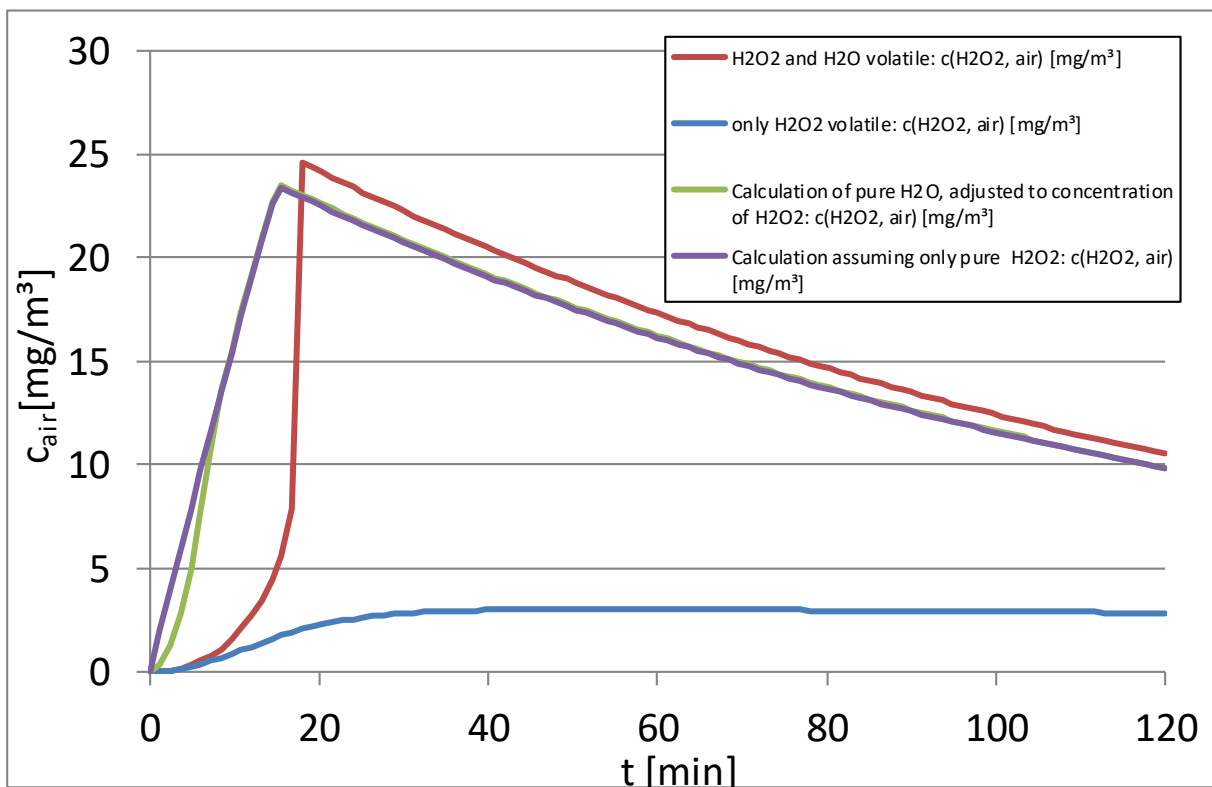


Figure 1: **Air Concentration of H₂O₂ in the room (in mg/m³)** resulting from four modelling approaches.

- red line:** result of the 2-component model in which both, H₂O₂ and water, are treated as volatile (complex calculation)
- blue line:** result of the 1-component model which considers only H₂O₂ as volatile (corresponds to the ConsExpo assessment)
- green line:** result of a simulation of pure water, which was then multiplied by 0.25%, the assumed concentration of H₂O₂ in this scenario
- purple line:** result of a simulation of pure substance (correct amount, i.e. 0.25% x 800 g = 2 g) (**proposed approximation for assessment**)

3. Proposed conclusion

- For water-based disinfectants where the substance in question has a (substantially) lower vapour pressure than water and where the concentrations in the applied products change during the application, it is proposed to use the model option 'product is substance in pure form' when ConsExpo's evaporation model is used for assessment taking into account the correct substance amount as 'product amount'. However, for scenarios with a short exposure duration, this approach can overestimate exposure, because the delayed evaporation that can occur in the beginning of the application (see red line in Figure 1) is not considered. If risks are identified, an assessment based on measured data, or a refined modelling including risk mitigation measures in Tier 2 may be considered.
- It is acknowledged that this is a simple workaround and that the modelling approaches discussed here share some limitations which are briefly described in the Appendix.
- This approach might not be suitable for calculation of airing durations required for safe re-entry of contaminated areas as it may lead to underestimation.

Appendix: Details and limitations of the 2-component calculations

A) Calculations

The calculations used to demonstrate the assumed behaviour of the 2-component system (substance in question and solvent) are based on the equations shown in the ConsExpo Manual for the evaporation model. In detail, the system of the two differential equations 7a and 7b on p. 37 of the manual has been extended by two additional ones, which simulate the behaviour of the solvent:

$$\text{Eq 1: } \frac{dm_{\text{air,solv.}}}{dt} = K \cdot S \cdot \frac{M_{\text{solv.}}}{RT} \cdot (p_{\text{eq,solv.}} - p_{\text{air,solv.}}) - Q \cdot V_{\text{room}} \cdot c_{\text{air,solv.}} + Q \cdot V_{\text{room}} \cdot c_{\text{fresh air,solv.}}$$

with

$m_{\text{air, solv.}}$ = amount (mass) of solvent in the air [kg]

t = time [s]

R = ideal gas constant = 8.314 J/mol/K

$p_{\text{eq, solv.}}$ = equilibrium vapour pressure of solvent in the liquid product mixture [Pa]

$p_{\text{air, solv.}}$ = vapour pressure of solvent in the air [Pa]

$c_{\text{fresh air, solv.}}$ = humidity of the fresh air exchanging the air in the room [kg/m³]

$$\text{Eq 2: } \frac{dm_{\text{prod,solv.}}}{dt} = -K \cdot S \cdot \frac{M_{\text{solv.}}}{RT} \cdot (p_{\text{eq,solv.}} - p_{\text{air,solv.}}) + \frac{m_{\text{prod,tot}}}{t_{\text{app}}} \cdot (1 - w_f)$$

with

$m_{\text{prod,solv.}}$ = amount (mass) of solvent in the air [kg]

The substance in question and the solvent are “interacting” in this model through their molar fractions ($x_{\text{subst.}}$ and $x_{\text{solv.}}$), which are then used for the calculation of the equilibrium vapour pressure $p_{\text{eq, solv.}}$:

$$\text{Eq. 3a: } x_{\text{subst.}} = \frac{\frac{m_{\text{prod,subst.}}}{M_{\text{subst.}}}}{\frac{m_{\text{prod,subst.}}}{M_{\text{subst.}}} + \frac{m_{\text{prod,solv.}}}{M_{\text{solv.}}}} \quad \text{Eq. 3b: } x_{\text{solv.}} = \frac{\frac{m_{\text{prod,solv.}}}{M_{\text{solv.}}}}{\frac{m_{\text{prod,subst.}}}{M_{\text{subst.}}} + \frac{m_{\text{prod,solv.}}}{M_{\text{solv.}}}}$$

and

$$\text{Eq 4a: } p_{\text{eq,subst.}} = p_{\text{vap,subst.}} \cdot x_{\text{subst.}} \quad \text{Eq 4b: } p_{\text{eq,solv.}} = p_{\text{vap,solv.}} \cdot x_{\text{solv.}}$$

B) Limitations

This approach provides a very basic way to simulate a product consisting of water and a second volatile substance. However, it should be underlined that there are still major limitations in this approach. Most importantly, this model assumes (as ConsExpo does) that the treated area keeps increasing during the entire application duration. However, the simulated water based product is applied as a very thin layer, which will evaporate rather quickly. In reality, the area of the wetted surface will therefore decrease again from the side at which the application has started. In the calculations, the surface area will therefore become larger than in reality, which will result in too fast evaporation towards the end of the application duration. In addition, the concentrations are assumed to be the same throughout the entire liquid layer (though changing over time). Activity coefficients of H₂O₂ and H₂O are likewise not considered.

Nevertheless, the shown approach is considered sufficient to demonstrate the principle effect of the evaporating solvent in these products.

C) Model used for calculation of the examples shown in Figure 1

For reference, the functional Excel spread sheet is included as an Annex.