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Implementation report

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The TOXSWA model has been extended with the functionality to simulate pesticide volatilization from open water surfaces on the basis of a micro-meteorological framework. TOXSWA simulates the fate of pesticides in water bodies to calculate exposure concentrations for aquatic organisms or sediment-dwelling organisms as part of the aquatic risk assessment in the regulatory process of pesticides at EU level and in The Netherlands. Volatilization of pesticides from water to air has been described in the TOXSWA model based on the Liss and Slater method. This report describes the implementation in TOXSWA of an improved methodology to describe volatilization of pesticides from small water bodies. Hourly meteorological data on wind speed and air temperature are used to calculate the rate of volatilization of the pesticide from the water layer.

Keywords: volatilization, surface water, pesticide, TOXSWA model, Liss and Slater, water-air transport resistances

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Preface

Since June 1999 TOXSWA v1.2 has been applied in the Dutch registration procedure for plant protection products to calculate exposure concentrations in an edge-of-field ditch with constant flow rates. Since December 2003 FOCUS_TOXSWA has been applied in the EU registration procedure to calculate exposure concentrations in ponds, ditches and streams with transient flow conditions. The TOXSWA kernel has now been improved by the addition of an option to describe the volatilization using transport resistances to the exchange between the water layer and the air layer above the water surface. This report describes the implementation of the improved volatilization parametrization in the TOXSWA kernel.

We thank Cor Jacobs for his constructive comments and suggestions to this report.

Summary

The TOXSWA model has been extended with the functionality to simulate volatilization based on a micrometeorological framework. The volatilization is driven by the air-water concentration difference, and further controlled by two atmospheric resistances and one aqueous resistance against (pesticide) gas transport. The parameterization uses hourly meteorological data. TOXSWA simulates the fate of substances in small water bodies to calculate exposure concentrations for aquatic or sediment-dwelling organisms as part of the aquatic risk assessment of pesticides. Pesticide volatilization may be an important process determining the exposure concentration. In case of rapid volatilization a relatively large proportion of the mass in the water layer may end up in the atmosphere and exposure concentrations in water will rapidly lower. For water bodies with stagnant water or low flow velocities, slow volatilization in combination with slow degradation and repeated applications may lead to accumulation of pesticides in water and sediment. This may lead to high risks for the aquatic or sediment-dwelling organisms. In the new concept volatilization is simulated based upon hourly values of wind speed, and temperature in water and in the atmosphere.

In the new TOXSWA (kernel version 3.4), the user may select the (already existing) option to simulate volatilization from water using a parameterization of a coefficient for transfer between water and atmosphere developed by Liss and Slater (1974) for gas exchange over the oceans. The parameterisation of the transfer coefficient, however, can now also be done based upon the introduced micrometeorological framework which is probably more suitable for small water bodies. This framework has been described by Jacobs and Adriaanse (2012).

Tests with the new functionality of TOXSWA confirmed that the parameterization of Jacobs and Adriaanse is implemented correctly and that the numerical solutions are robust.

For simulations, we advise to use a reference height of 1.5 m for state variables, such as temperature and wind speed, both for the improved parameterization for volatilization and the extended temperature option in TOXSWA.

Now that TOXSWA is able to simulate the volatilization as function of environmental parameters, the simulated concentration profiles better reflect their variability in time and space in surface water. In this way TOXSWA provides a more robust picture of the environmental exposure concentrations used in the aquatic risk assessment of pesticides in the Netherlands and the European Union.

Samenvatting

Het TOXSWA model beschrijft het gedrag van gewasbeschermingsmiddelen in het water-sediment systeem in kleine oppervlaktewateren. Het berekent hier blootstellingsconcentraties voor water- en sedimentorganismen, die in de aquatische toelatingsprocedure in Nederland en de EU worden gebruikt. Het model is nu verbeterd door de toevoeging van een functionaliteit voor vervluchtiging op basis van een micro-meteorologische benadering. De vervluchtiging wordt bepaald door het concentratie verschil op het atmosfeer-water grensvlak en hangt verder af van twee atmosferische weerstanden en een aquatische weerstand tegen transport van het gewasbeschermingsmiddel in de gasfase. De parameterisatie gebruikt uurlijkse waarden voor windsnelheid en temperatuur in water en in atmosfeer. Vervluchtiging van gewasbeschermingsmiddel is een belangrijk proces voor de blootstellingsconcentratieberekening. Vooral in stilstaand oppervlaktewater of water met lage stroomsnelheden kan de combinatie van langzame vervluchtiging, lage omzetting en herhaald toepassen leiden tot accumulatie van het middel in water en/of sediment en mogelijk verhoogde risico’s voor de organismen.

In deze nieuwe versie van het TOXSWA model (rekenhart versie 3.4) kan de gebruiker nu kiezen uit twee parameterisaties voor de transportcoëfficiënt voor gasuitwisseling tussen water en atmosfeer; de (al bestaande) parameterisatie volgens Liss en Slater (1974) voor gas uitwisseling boven open water en de nieuwe parameterisatie op basis van een micrometereologische benadering (Jacobs en Adriaanse, 2012). De nieuwe parameterisatie is wellicht geschikter voor kleine waterlichamen.

In simulaties met TOXSWA waarin zowel de uitgebreide temperatuurmodule als de verbeterde parameterisatie voor vervluchtiging worden gebruikt, is voor beide processen de referentiehoogte voor toestandsvariabelen als bijvoorbeeld temperatuur en windsnelheid nodig. We adviseren om hiervoor een uniforme referentiehoogte van 1,5 m te gebruiken.

Testen met de nieuwe functionaliteit in TOXSWA wees uit dat de implementatie van de parameters voor vervluchtiging in het model correct is en dat de numerieke oplossingen robuust zijn.

Nu TOXSWA de vervluchtiging vanuit de waterlaag als functie van weersomstandigheden kan simuleren, geven de gesimuleerde concentratieprofielen een beter beeld van de variabiliteit in tijd en plaats in het oppervlaktewater. Op deze wijze geeft TOXSWA een robuuster beeld van de blootstellingsconcentraties in het milieu voor gebruik in de aquatische risicobeoordeling van gewasbeschermingsmiddelen in Nederland en op EU niveau.

1 Introduction

The TOXSWA model simulates the behaviour of pesticides in water bodies to calculate exposure concentrations for aquatic organisms or sediment-dwelling organisms as part of the aquatic risk assessment of pesticides. TOXSWA simulates the processes of convective and dispersive transport in water and sediment, diffusive transport in sediment, transformation, volatilization and sorption to suspended solids, macrophytes and sediment.

TOXSWA version 3.3 is the kernel of FOCUS_TOXSWA 5.5.3. (Beltman et al., 2018). This report concerns the new version 3.4. Hence, where in this report the TOXSWA model is mentioned, this refers to model kernel version 3.4, unless indicated otherwise.

Volatilization is the process of exchange of the pesticide between the water and the atmosphere. Volatilization affects exposure concentrations in surface water and in sediment. Especially for water bodies with stagnant water or low flow velocities, low volatilization in combination with low degradation and repeated applications may lead to accumulation of pesticides. As a result pesticide concentrations in water as well as in sediment may lead to increased acute and chronic risks for aquatic organisms (Westein *et al*., 1998). On the other hand, high volatilization may lead to lower exposure concentrations.

In the TOXSWA model (kernel versions up to 3.3), volatilization from water is simulated using a parameterization of a coefficient for transfer between water and atmosphere based on the method developed by Liss and Slater (1994). The parameterisation of the transfer coefficient, however, may also be based upon a micrometeorological framework, consisting of two atmospheric resistances and one aqueous resistance against gas transport (Jacobs and Adriaanse, 2012). Simulation of volatilization based on this parameterization is expected to improve the performance of TOXSWA as it accounts better for weather conditions related to specific pesticide properties. Jacobs and Adriaanse (2012) provided suggestions for how the parameterization could be implemented in TOXSWA. In this report we refer to this new parameterization as the improved parameterization.

Chapter 2 describes the implementation of the improved parameterization in TOXSWA. In Chapter 3 tests are described to check whether the parameterization has been implemented correctly in the source code and whether the model can handle the allowed range of input values. In Chapter 4 the input is described, and example simulations are given. In Chapter 5 some concluding remarks are given.

2 Implementation of an improved volatilization parameterization in TOXSWA

2.1 The TOXSWA model

The TOXSWA model describes the behaviour of pesticides in a water body at the edge-of-field scale, *i.e.* a ditch, pond or stream adjacent to a single, treated field (Adriaanse, 1996; Adriaanse *et al*., 2014; Ter Horst *et al*., 2016; Adriaanse *et al.*, 2017). The modelled system consists of two types of subsystem: the water layer containing suspended solids and macrophytes and the sediment. The properties of the sediment, *i.e.* porosity, organic matter content and bulk density, may vary with depth. In the water layer concentrations vary in the horizontal direction, whereas in the sediment concentrations vary in the horizontal and the vertical direction.

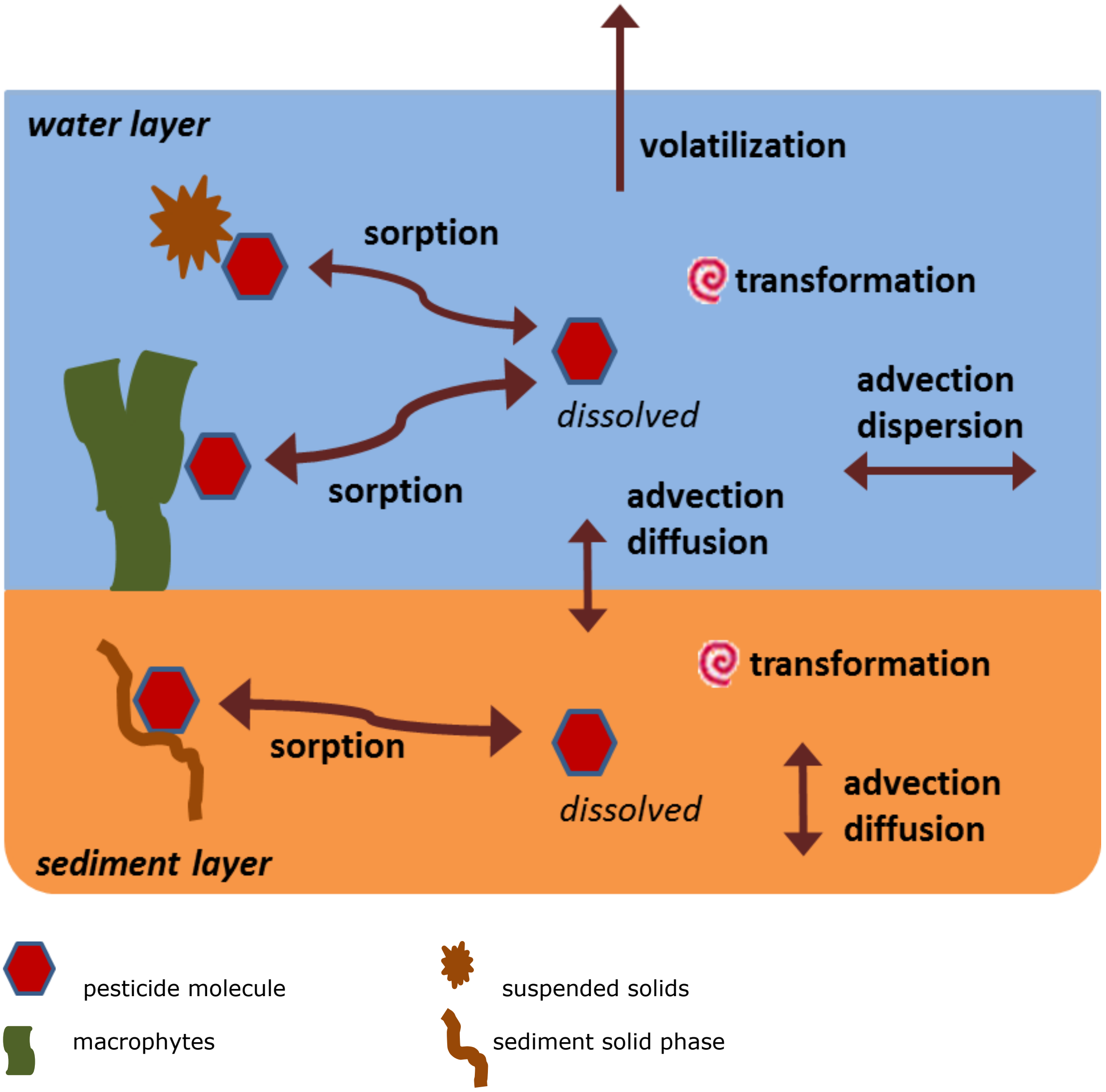

Figure 1 *Processes in TOXSWA.*

TOXSWA considers four processes for the parent substance and its metabolites: (i) transport, (ii) transformation, (iii) sorption and (iv) volatilization (see Figure 1). In the water layer substances are transported by advection and dispersion, dissolved in the water phase or sorbed to suspended solids. In the sediment substances are transported by advection, dispersion and by diffusion in the liquid phase. Exchanges across the water-sediment interface are facilitated by advection (upward seepage or downward infiltration) and by diffusion. Transformation is simulated in the water layer as well as in the sediment. Up to version 3.3 included, the transformation rate covers the combined effects of hydrolysis, photolysis and biodegradation. The transformation rates are assumed to be temperature-dependent, using the Arrhenius equation to describe the temperature dependence of the rate coefficient of transformation. Sorption to suspended solids and to sediment is described by the Freundlich isotherm. Sorption to macrophytes is described by a linear sorption isotherm.

2.2 Volatilization

The mass flux density of volatilization is determined by the transfer coefficient $k_{t,l}$ (in Eq (61) in Ter Horst *et al.*, 2016):

$$J_a = -k_{t,l,L+S}\left(c_w - \frac{c_a}{K_H}\right) \tag{1}$$

With:

J_a = aeric mass flux of substance across the water-air interface ($kg.m^{-2}.s^{-1}$) [the flux is negative in upward direction]

$k_{t,l,L+S}$ = transfer coefficient of substance between liquid and gas phase based on Liss and Slater (1974) ($m\ s^{-1}$)

K_H = Henry coefficient (-)

c_w = mass concentration of substance dissolved in the water layer ($kg.m^{-3}$)

c_a = mass concentration of substance in the air ($kg.m^{-3}$)

Henry's coefficient is calculated form the ratio of saturated concentration in air and the solubility of the substance in water (see p.43 in Ter Horst et al, 2016). The saturated vapour pressure and the solubility both are temperature dependent.

The Liss and Slater parameterisation is based on a two film model and has been applied in TOXSWA, using air resistance and aqueous resistance, the transfer coefficient is calculated with[1]:

$$\frac{1}{k_{t,l,L+S}} = \frac{1}{k_l} + \frac{1}{K_H.k_g} \tag{2}$$

With:

k_l = exchange coefficient of substance in the liquid phase ($m\ s^{-1}$)

k_g = exchange coefficient of substance in the gas phase ($m\ s^{-1}$)

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[1] Liss and Slater (1974) state that $1/k_{t,l,L+S}$ may be expressed as r_l, resistance of liquid phase, and $1/K_H k_g$ as r_g, resistance of gas phase.

In a micrometeorological framework, the volatilization flux density J_a is given by:

$$J_a = -\frac{K_H c_w - c_a}{r_a + r_b + K_H r_w} \tag{3}$$

With:

r_a = air resistance ($s.m^{-1}$)

r_b = boundary layer resistance ($s.m^{-1}$)

r_w = aqueous resistance ($s.m^{-1}$)

Hence for the improved parameterization the transfer coefficient based on the micrometeorological framework is calculated with:

$$k_{t,l,micromet} = \frac{1}{(r_a + r_b)/K_H + r_w} \tag{4}$$

With:

$k_{t,l,micromet}$ = transfer coefficient of substance between liquid and gas phase based on micrometeorological framework (m s^{-1}).

It may be assumed that the concentration difference of the modelled compound between the water and the air, approximated by $K_H c_w$ - c_a, is known from the dynamic mass balance calculations in TOXSWA at each time step (concentration in air is assumed to be zero). This leaves the resistances to be further parameterized.

The dimensionless Henry coefficient K_H and therefore the aqueous resistance $K_H r_w$ varies over many more orders of magnitude than the atmospheric resistance $r_a + r_b$. This feature allows a useful distinction of two physical regimes (see Figure 4 and Table 1 in Jacobs and Adriaanse (2012): the air-controlled regime where $r_a + r_b >> K_H r_w$ and the water controlled regime where $r_a + r_b << K_H r_w$. In the first regime, gas exchange is only sensitive to the parameterization of atmospheric turbulence and therefore of $r_a + r_b$. Obviously, the two regimes are not strictly separated. In an 'intermediate regime' the effects of both the atmospheric resistances and the water resistance are noticeable, since $r_a + r_b$ and $K_H r_w$ are of a similar order of magnitude.

Most pesticides (~80-90%) belong to the first, atmospherically controlled regime. In this regime, at very low values of K_H (< 10^{-7}) the volatilization rate is so slow - with volatilization half-life times of tens to hundreds of years - that pesticide loss from water bodies will be dominated by processes other than volatilization, such as biological or chemical degradation. If K_H becomes larger than 10^{-2} the volatilization become quite fast - with volatilization half-life times in the order of one to a few hours -, but only a small minority of pesticides belongs to this group.

The distribution of K_H-values among pesticides implies that for the problem of volatilization of pesticides from water bodies a simple but reasonable description of r_w would give acceptable results in most cases. Also, it would be justifiable to put more effort in improving $r_a + r_b$ than in improving r_w.

For the much smaller group of pesticides with $K_H > 10^{-2}$ the reverse is true. An improved parameterization of volatilization will be most effective for pesticides with K_H -values between 10^{-6} and 10^{-3}. Pesticides with K_H-values in this range are either in the intermediate regime where atmospheric resistance and water resistance are of a similar order of magnitude ($\sim 10^{-4} < K_H < \sim 10^{-2}$) or in the atmospherically controlled regime but with still relatively fast volatilization rates (up to tens of days, for $\sim 10^{-6} < K_H < \sim 10^{-4}$).

For calculating the aquatic resistance a method based upon the so-called Schmidt number similarity (see Eq. (15) in Jacobs and Adriaanse, 2012) is selected. From the available parameterizations with wind velocity U, based on a review of gas exchange observations at relatively small water bodies, Eq. (3) was selected (see Jacobs and Adriaanse (2012)).

2.3 Implementation into the TOXSWA model

The mass conservation equation for the water layer, solved by TOXSWA version 3.4 is given in Ter Horst et al. (2016). In a micrometeorological framework, the volatilization flux density is given by Eq (2): The difference in concentration of the modelled substance between the water and the air, approximated by $K_H c_w - c_a$, is known from the dynamic mass balance calculations in TOXSWA at each time step. The parameterization of the resistances is described in this section.

Aerodynamic resistance r_a

The aerodynamic resistance, r_a, is computed using:

$$r_a = \frac{\left(\ln\frac{z_r}{z_0}\right)^2}{\kappa^2 U_r} \qquad (5)$$

U at the reference height z_r and for the roughness length z_0.

z_0 = roughness length (m) = 0.03 m
z_r = reference height (m)
U_r = wind speed at reference height z_r (m s^{-1})
K = Von Kármán constant (-) = 0.4

The value of 0.03 m is the roughness length representative for grass, applied in TOXSWA as default value. It represents the local conditions for measurement stations and is valid for neutral atmospheric conditions. For areas with agricultural crops and ditches z_0 is higher (for details, see Jacobs and Adriaanse, 2012).

The reference height, z_r, is an entity that must be chosen. Generally speaking selecting the same reference height when combining several variables is most straightforward. However, this is not always possible due to conventions with respect to measurement heights in experiments. We advise to here use a 1.5 m reference height. This height is used for temperature measurements by the Dutch KNMI institute, while the WMO states heights of 1.25-2 m, so the same range. Consequently the aerodynamic resistance r_a as well as wind speeds measured at 10 m height should be converted to 1.5 m. Eq (5) and (6) can do so. Note that these type of flux-profile relations take care that the state variables (temperature, wind, moisture content, etc.) and the curve of their profile are consistent. This is correct as long as the assumption of a constant flux is realistic (usually within 10% up to tens of meters distance to the soil surface). So, e.g. a reference height z_r of 1.5 m to convert wind speeds at 10 m fulfils the assumption. When z_r is chosen at a lower value, the wind velocity U (state variable) also becomes lower and u^* (representing the impulse flux) remains constant (personal communication C. Jacobs, May 2022).

The wind speed U_r at any reference height is calculated with:

$$U_r = \frac{\ln\frac{z_r}{z_0}}{\ln\frac{z_{obs}}{z_0}} U_{obs} \qquad (6)$$

With:
z_{obs} = height of observation of wind speed (m)
U_{obs} = wind speed observed at z_{obs} (m s^{-1})

Using Eq. (6) with z_0 = 0.03 m gives a wind speed at a height of 1.5 m that is 0.67 times the one obtained at 10 m (or conversely, the wind speed at a height of 10 m is 1.48 times the one at 1.5 m).

The minimum value for wind speed is set to 0.1 m s^{-1}.

Boundary layer resistance r_b

The boundary layer resistance r_b is computed using Deacon (1977).

$$r_b = 15.2 \frac{Sc_a^{0.61}}{u_*} \tag{7}$$

With:

Sc_a = Schmidt number in air (-)

The Schmidt number in air is calculated with:

$$Sc_a = \frac{\nu_a}{D_a} \tag{8}$$

With:

ν_a = kinematic viscosity of the air ($m^2 s^{-1}$) = $1.5 \cdot 10^{-5}$ $m^2 s^{-1}$

D_a = molecular diffusion coefficient of substance in air at a temperature, T_a ($m^2 s^{-1}$)

The diffusion coefficient in air at temperature T_a is calculated with:

$$D_a = \frac{T_a}{T_{dif,ref}^{1.75}} D_{a,ref} \tag{9}$$

(Tucker and Nelken, 1982)

With:

$D_{a,ref}$ = molecular diffusion coefficient of substance in air at reference temperature $T_{dif,ref}$ ($m^2 s^{-1}$)

$T_{dif,ref}$ = temperature for which the molecular diffusion coefficient in air is given (K)

For the diffusion coefficient in air we suggest to use a default value of 0.43 $m^2 d^{-1}$ (FOCUS, 2021).

The friction velocity u_* [$m s^{-1}$] is obtained from the logarithmic wind profile, again assuming neutral atmospheric stability:

$$u_* = \frac{\kappa U_r}{\ln \frac{z_r}{z_0}} \tag{10}$$

Aqueous resistance r_w

The aqueous resistance r_w is computed using[2]

$$\frac{1}{r_w} = k_w = k_{600} \left(\frac{600}{Sc_w}\right)^{0.5} \tag{11}$$

With:

k_{600} = reference value at resistance Sc_w = 600 ($m s^{-1}$)

k_w = transport coefficient in water ($m s^{-1}$)

Sc_w = Schmidt number in water (-)

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[2] Eq. (11) is based upon the so-called Schmidt number similarity: $\frac{k_{w,1}}{k_{w,2}} = \left(\frac{Sc_{w,1}}{Sc_{w,2}}\right)^{0.5}$
The rationale for this choice is given in Jacobs and Adriaanse (2012). In the scaling represented by the Schmidt number similarity the power 0.5 is used to take into account the impact of turbulence on the laminar layer in the water. Note that the Liss & Slater parameterization applied in Eq. (11) is consistent with power 1, which applies to the stagnant film model.

The actual r_w at Sc_w is converted from the reference value of r_{600} at $Sc_w = 600$, because most parameterizations of k_w are given for a $Sc_w = 600$ for (small) inland water bodies (Cole and Caraco, 1998):

$$k_{600} = \frac{1}{r_{600}} = 0.215\ U^{1.7} + 2.07 \tag{12}$$

Seems appropriate. Note that in Eq. (12) U should be given at a height of 10 m. If the wind speed is available for another height, that wind speed can be converted to yield U at 10 m (Eq. (6)).

Eq. (11) belongs to the family of parameterizations that assume turbulence in the water to be directly or indirectly related to wind speed U.

The Schmidt number in water is:

$$Sc_w = \frac{\nu_w}{D_w} \tag{13}$$

With:
ν_w = kinematic viscosity of water at water temperature T_w ($m^2\ s^{-1}$)
D_w = molecular diffusion coefficient ($m^2\ s^{-1}$) of substance in water at reference temperature T_w

The kinematic viscosity of water ν_w is a function of temperature. Jacobs and Adriaanse (2012) fitted a polynomic function from tabled data of viscosity of water as a function of temperature (Lide, 2003):

$$\nu_w = -1.388 \cdot 10^{-9}\ T_w^3 + 1.3114 \cdot 10^{-9}\ T_w^2 +\ 5.986 \cdot 10^{-8}\ T_w +\ 1.7887 \cdot 10^{-6} \tag{14}$$

Note that the temperature of water T_w in this equation has dimension °C. In TOXSWA for $T_w < 0$°C, $T_w = 0$°C is used, and for $T_w > 40$°C, $T_w = 40$°C is used.

The calculation of the molecular diffusion coefficient as a function of water temperature in TOXSWA has been described in Annex 2 of Beltman et al. (2017).

2.4 Value for reference height, z_r

Here we summarize how we opted for the reference height of measurement: one model simulation of TOXSWA should make use of variables that are all brought back to the same reference level. Here we have selected the reference height of 1.5 m, because this is the height used by the Dutch meteorological institute KNMI for temperature measurements and it also falls within the recommended range of the WMO of 1.25 to 2 m. As temperature measurements are less easy to correct than wind speed measurements (personal communication C. Jacobs, May 2022), we opted for this reference height used for temperature measurements and next, converted the wind speed measurements at 10 m height to corresponding wind speeds at 1.5 m height. Accordingly, also the aerodynamic resistance has been calculated for a reference height of 1.5 m.

3 Verification of the improved parameterization for volatilization in TOXSWA

3.1 Introduction

To verify the implementation of the improved parameterization TOXSWA simulation results were compared to an analytical solution of the mass balance equation for the water layer. Also, the robustness of TOXSWA was tested for important volatilization-related input parameter values. So, two tests were performed:

- Implementation of volatilization in the source code by testing TOXSWA against an analytical solution for concentration in water as a function of time in an ideally-mixed reservoir due to volatilization only.
- The robustness of the model was tested for some minimum and maximum values of substance parameters and watercourse parameters that directly affect the volatilization rate from water.

3.2 Test against an analytical solution

3.2.1 Set up of the test

The aim of the test is to verify that the improved parameterization is implemented correctly in TOXSWA. Concentrations (dissolved) in the water layer as a function of time resulting from a TOXSWA simulation considering volatilization as the only dissipation process in the system are compared with concentrations (dissolved) in the water layer as a function of time resulting from a calculation with an analytical solution.

The analytical solution used is (see Annex 4):

$$c_w = c_{w,0} e^{-k_v t} \tag{15}$$

With:

$c_{w,0}$ = initial mass concentration of substance in the water phase (kg m^{-3})
c_w = mass concentration of substance in the water phase, *i.e.* at time t (kg m^{-3})
t = time (s)
k_v = volatilization rate coefficient (s^{-1})

Two calculations were performed: 1) volatility high: substance with a high Henry coefficient and a low wind speed, and 2) volatility moderate: substance with a low Henry coefficient and a high wind speed. An overview of these parameters is given in Table 1, including the Henry coefficient calculated (no input for TOXSWA). The calculation of the analytical solution for the two volatilization rates is given in Annex 4.

Table 1 *Substance properties and wind speed used in two simulations.*

Simulation	*Volatility conditions*	Solubility at 20°C (mg L^{-1})	Saturated vapour pressure at 20°C (d)	Henry coefficient at 20°C (-) *calculated*	Wind speed at 10 m (m s^{-1})	Transfer coefficient at 20°C and wind speed given (m d^{-1})
1	high	1.231	0.1	0.01	1	1.503
2	moderate	0.1231	0.00001	0.00001	10	0.01503

We simulated a stagnant water-sediment system (ditch without inflow and outflow) with a length of 100 m, a rectangular cross section with a width of 1 m and a water depth of 0.3 m. For the suspended solids in the water layer the mass ratio of organic matter in suspended solids was set to zero; hence no sorption to suspended solids can occur. Macrophytes were not simulated, *i.e.* the dry mass of macrophyte biomass was set to zero. The water layer of the ditch consisted of one segment (100 m) for the numerical solution of the mass conservation equation. Time steps used in the model simulations varied. The option to optimise the time step (`OptTimStp = Calc`) was used.

All parameter values for the ditch and also the substance properties of the example run are given in Annex 1.

The meteorological input file (DeBilt.meth) is adapted to set those conditions that are relevant for volatilization to a constant value, to make a comparison with the analytical solution possible. Hence, the temperature in air was set to 20°C for the whole month, and the wind speed was set to 1 m s^{-1} for simulation 1 and set to 10 m s^{-1}, for the whole month.

TOXSWA calculates the temperature of water from the input of the meteorological file and the initial temperature set in the txw file. To apply a constant temperature in water in the whole month, an intermediate temperature file with temperature 20°C for the whole month was made. In the txw file the option `OptTem` was set to `OffLine`; then TOXSWA runs with the intermediate file, and the water temperature is 20°C for the whole month.

For the test sediment processes were excluded by minimizing diffusion from water to pore water in sediment; the pore fraction in sediment was set to its minimal value of 0.001.

The substance enters the water layer as a spray drift even at 9 a.m. in TOXSWA resulting in an initial concentration of 3.33 µg L^{-1}. This initial concentration was applied for the analytical solution.

TOXSWA simulations were done with version 3.4 (version date 23 March 2021). The analytical calculation was done in an Excel spreadsheet.

3.2.2 Results

The results of the simulations with TOXSWA and the analytical solution are shown for both substances in Figure 2.

For the highly volatile substance at the end of May 1st (15 hours after application, 5% remaining) the concentration calculated with TOXSWA is 0.1783 µg L^{-1} and the concentration calculated with the analytical solution of Eq. (15) at the same time is 0.1792 µg L^{-1}. The comparison of the concentrations as a function of time is shown in Fig. (2) up to 2 May (left-hand panel). As well the quantitative concentrations as the visual correspondence of the concentration profiles indicate that the test is satisfactory (the difference is less than 1%, i.e. 0.0009/0.1783=0.5%).

For the moderate volatile substance at the end of 31 May (30 days after application, 5% remaining) the concentration calculated with TOXSWA is 0.7184 µg L^{-1} and the concentration calculated with the analytical solution of Eq. (15) at the same time is 0.7200 µg L^{-1}. The comparison of the concentrations as a function of time is shown in Fig. (2) below right-hand panel) for the whole simulation period 1 - 31 May. As well the quantitative concentrations as the visual correspondence of the concentration profiles indicate that the test is satisfactory (the difference is less than 1%, i.e. 0.0016/0.1784=0.9%).

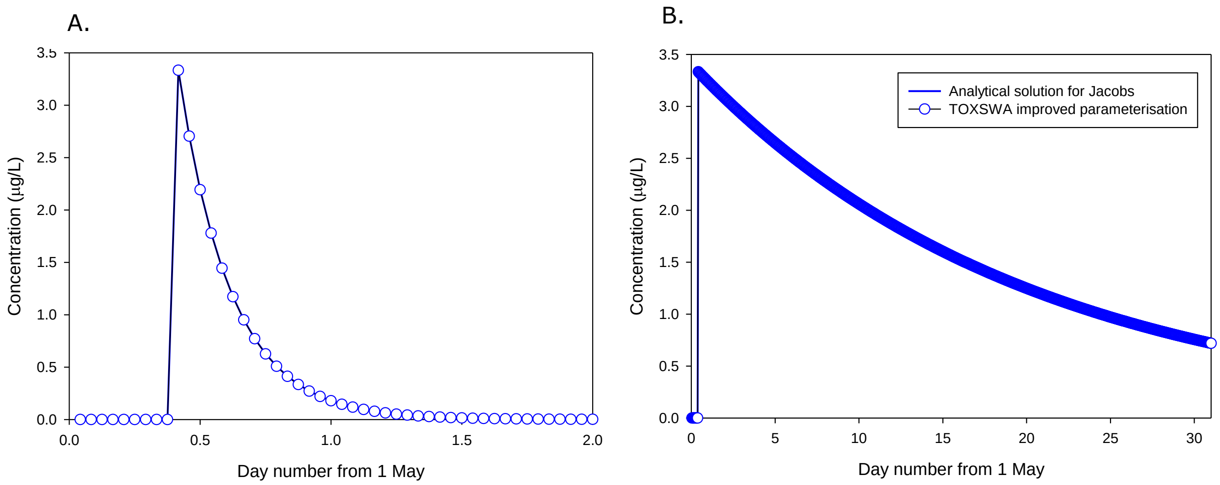

Figure 2 *Substance concentration in the water layer as function of time for volatilization using the improved parameterization with TOXSWA and with an analytical solution since a spray drift event on May 1st. A. highly volatile substance (Henry coefficient 0.01) and wind speed of 1 m s-1, and B. moderate volatile substance (Henry coefficient 0.00001) and wind speed of 10 m s-1. Blue circles are from TOXSWA simulation and the black lines calculated by Eq. (15).*

As the difference between TOXSWA simulations and the analytical solution is less than 1% of the remaining 5% mass in the water layer, we conclude that the improved parameterization has been correctly implemented in the TOXSWA model.

3.3 Robustness for the implemented parameterization

3.3.1 Set up of the test

The aim of the test is to check if the kernel 3.4 of the TOXSWA model is numerically robust for the implemented parameterization. The parameters that affect the volatilization were tested using the outer values of the parameter ranges or combinations of parameters setting extreme conditions, i.e. by using a Henry coefficient = 1 (very volatile). This is not an extensive test, but a focussed test on some key parameters based on our experience with TOXSWA. It was tested whether, when using these outer values, TOXSWA did not stop or report numerical errors, and that resulting Time Weighted Average (TWA)[3] concentrations are plausible. The TWA is calculated for a 7-day window starting from the time of application.

For volatilization we used the scenario and substance properties specified in Annex 1. In the simulation only volatilization from the water phase is considered. Other processes that may decrease the concentration are not considered, *i.e.* transformation, sorption to suspended solids or macrophytes have been set to zero and transport to sediment is minimized by setting the porosity of sediment to its minimal value of 0.001. The changed parameter values for the two cases are given in Table 2.

---

[3] It is not sensible to evaluate maximum concentrations because these occur at the time of the spray drift event and are not affected by volatilization. By viewing TWA concentrations the effect of volatilization on the concentrations can be evaluated.

Table 2 *Combinations of parameter values used for testing the robustness, that differ from the values used in the example simulation in Annex 1.*

Test nr	description	Substance parameters	Other parameters
1	High wind speed	Solubility 1.25 mg L^{-1} Saturated vapour pressure 1 Pa	Wind speed[1] 100 m s^{-1}
2	Low water depth	Solubility 1.25 mg L^{-1} Saturated vapour pressure 1 Pa	Water depth 0.02 m[4]

[1] In the Netherlands the highest wind speed measured was in 1921 and mounted to 45 m s^{-1} (KNMI). Therefore, we applied a wind speed of 100 m s^{-1} for the test. The wind speed in the meteorological file was changed to 100 m s^{-1} for the whole simulation period.

3.3.2 Results

The results of the simulations are summarized in Table 3. TOXSWA finalized all runs without stopping and without reporting numerical problems or errors in the mass balance. The PECs are shown in the table and are considered plausible for the case simulated.

Table 3 *Results of the robustness test of TOXSWA for some selected cases.*

Test nr	description	Stop, reporting of numerical errors of error in mass balance	TWA 7 days* (μg L^{-1})
1	Low Henry coefficient and high wind speed	no	< 1e-6
2	Low Henry coefficient and low water depth	no	0.000213

* time window starts at time of application.

3.4 Conclusions

Example calculations and calculations done for comparison with an analytical solution using the improved parameterisation showed that both for highly and for moderately volatile substances the concentration profiles of TOXSWA and the analytical solution agreed very well. Moreover, extreme input parameter values for volatilization resulted in plausible concentrations, thus demonstrating that the implementation of the new concept is robust.

So, the conclusions of the tests with TOXSWA kernel version 3.4 described in sections 3.2 – 3.3 are:
- The improved parameterisation is implemented correctly in TOXSWA.
- The calculation of volatilization with the improved parametrisation with the TOXSWA model is robust.

---

[4] 0.02 m is the lowest acceptable values for the water depth for the temperature module, and therefore this value has been selected.

4 Input, output and example calculations

4.1 Introduction

TOXSWA requires minimally two input files: (1) the txw file, with parameter values for the scenario, the substance and the entries of the substance, and (2) a meteo or temperature file. The meteo file gives a time series of hourly or daily weather data. The temperature file gives daily or monthly air temperatures. Additional input files are needed when drainage or runoff entries occur (Beltman *et al.*, 2018). TOXSWA reports a summary of the results in the sum output file.

New input parameters are needed to simulate volatilization using the improved parameterization. In this chapter the required input and how to use the options for the improved parameterisation for the transfer coefficient are discussed, as well as how to do a simulation.

4.2 Input and output

In this section changes in the txw file and in the summary output file are discussed. The txw file consists of 10 sections, of which section 7 'Substance properties' needs to be adapted to use the improved parameterization. The parameterization selected for the calculation of the transfer coefficient, can be either Liss (= Liss and Slater, 1974) or "Improved" (= Jacobs and Adriaanse, 2012). If the latter parameterization is selected the diffusion coefficient of the substance in air needs to be entered as well. FOCUS (2021) advised to use a default value of 0.43 m^2 d^{-1} (p. 33). We propose to use this value as a default for the simulation of volatilization as well.

```
*---------------------------------------------------------------------------------------
* Section 7b: Substance properties for parent 'EXSW2'
* (note extension of parameter name is substance code)
*---------------------------------------------------------------------------------------


Liss       OptVol   ! Volatilization simulation method [Liss,Improved]

    * If OptVol is 'Improved' then specify
    0.43       CofDifAirRef_SubA (m2.d-1)  ! Reference diffusion coefficient in air [0|200]
```

Figure 3 *Excerpt from Substance properties section of the txw file.*

Figure 4 shows an excerpt from the summary output file (runID.sum). The user is informed on the volatilization option chosen.

```
* --------------------------------------------------------------------------------
* TOXSWA REPORT: Substance properties and substance loadings
*
* Summary for the following substances
*
* Substance  1:  EXSW_2

* Volatilization transfer coefficient parameterization: Improved
```

Figure 4 *Excerpt from substance properties and loadings section in the summary output file.*

4.3 Example calculation

In this section examples of TOXSWA simulations with a parameterization of the transfer coefficient with the Liss and Slater (1974) method and with the Jacobs and Adriaanse (2012) method are presented.

We simulated the stagnant water-sediment system of Section 3.2 (ditch without inflow and outflow) with a length of 100 m, a rectangular cross section with a width of 1 m and a water depth of 0.3 m, without sorption to suspended solids or macrophytes, and spatial and temporal discretizations (see p. 19). The substance used in the example is moderate volatile.

All parameter values for the ditch and also the substance properties of the example run are given in Annex 1. The saturated vapour pressure is 0.00001 Pa at 20°C and solubility 1.23 mg/L at 20°C, giving a Henry coefficient of 0.00001 at 20°C. The TOXSWA input file (txw file) of the run with the improved parameterization is given in Annex 2.

Three simulations were done; (i) with the Liss and Slater parameterisation, (ii) with the improved parameterisation, and (iii) with the improved parameterisation and three times as high values for values of hourly wind speed. The simulation started at the day of the spray drift event and 30 days were simulated. Simulations were done using a spray drift deposition of 1 mg/m^2 (equivalent of 1% of 1 kg/ha) entering the water layer over the entire length of the ditch (x = 0 to x = 100 m).

Hourly meteorological data of 1 – 31 May 1986 of De Bilt in the Netherlands were used (first part of the file is shown in Annex 3). The temperature in water is calculated from the hourly meteorological data, modelled in TOXSWA as described in Beltman et al. (2017). The water temperature is relevant for both parameterizations, because the solubility and the saturated vapour pressure of the substance are temperature-dependent (see Ter Horst et al., 2016). With the improved parameterization the diffusion coefficients in water and in air are corrected for temperature. Furthermore the wind speed strongly affects the transfer rate. The water temperature calculated by TOXSWA ranged from 6.1 to 21.9°C. The air temperature in May 2016 ranged from 1.6 to 24.8°C, and the wind speed from 0 to 8.7 m s^{-1}. For the simulation with the improved parameterisation and three times as high values for wind speed, the wind speed ranged from 0 to 26.1 m s^{-1}.

The effect of the transfer coefficient parameterisation (including wind speed) for the improved parameterization is illustrated by the decline of the substance concentration in the water layer (Figure 5). The figure shows the concentration in the water layer (3.33 µg/L) for a spray drift event as a function of time for the two parameterizations. With the Liss and Slater parameterization 91% of the substance is still present at the end of the month (3.02 µg/L), with the improved parameterization 74% (2.46 µg/L), and with the improved parameterization and three times as high values for wind speed 40% (1.33 µg/L). For the simulation using the Liss and Slater method the decrease in concentration is almost constant, whereas using the improved parameterisation there are some fluctuations. These fluctuations are due to the effect of wind. For example 2 May is a day with the highest wind speed of the month (8.7 m/s), and this wind results in somewhat faster decrease of concentration on this day. The conclusion is that for the example substance, a moderate volatile compound with Henry coefficient of 0.00001, applying the improved parameterization results in a significantly increased volatilization to the air and reflects more realistically the effect of wind speed on volatilization.

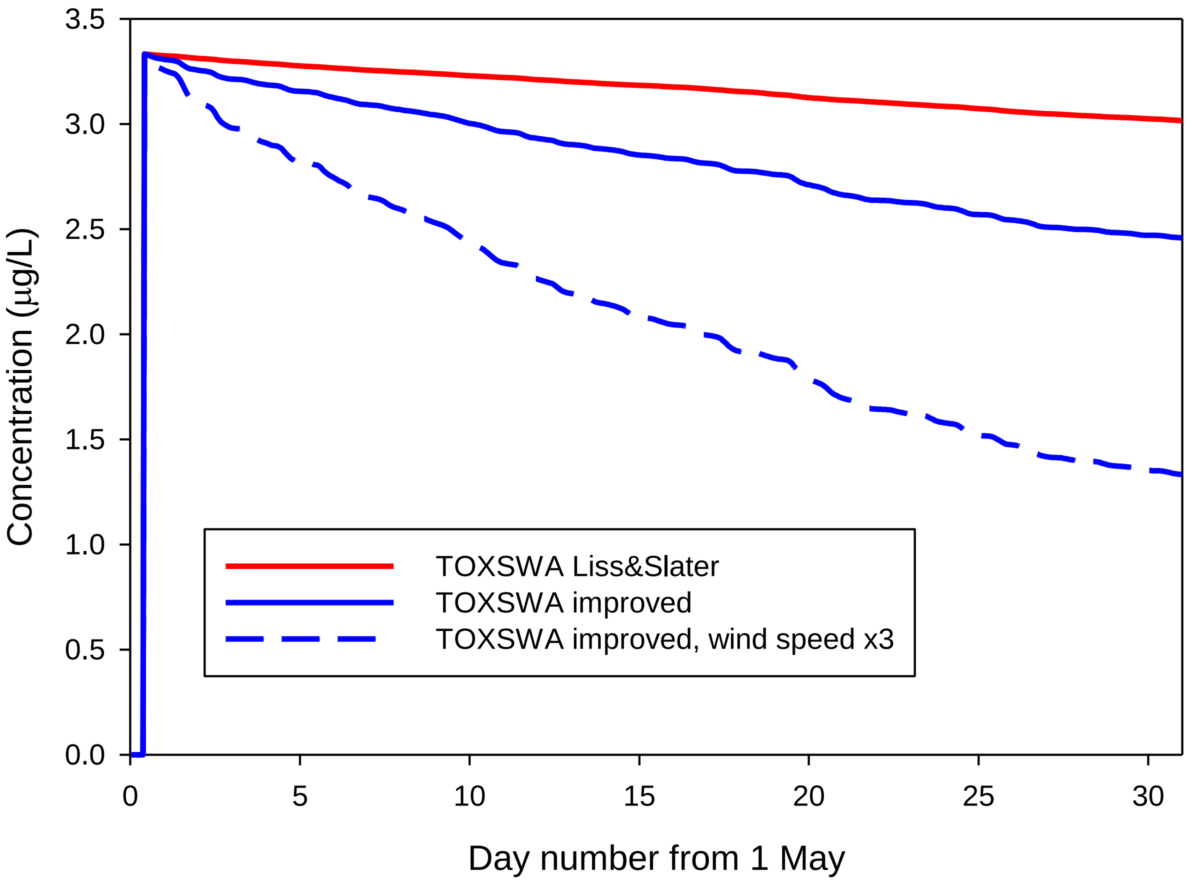

Figure 5 *Substance concentration in the water layer as function of time since a spray drift event simulated with Liss and Slater parameterization (red curve), with the improved parameterization (blue curve) and with the improved parameterization and wind speed values three times as high (dashed blue curve).*

5 Concluding remarks

The TOXSWA model has been extended with the functionality to simulate volatilization using an improved parameterisation, based on a micro-meteorological framework and selecting an air-water transfer coefficient that better reflects gaseous transport at surfaces of inland water bodies. The parameterisation uses hourly variable air and water temperatures and wind speed. The rationale of this improved parameterisation has been described in Jacobs and Adriaanse (2012). This report summarizes the parameterization and describes technical tests to verify the correct implementation in TOXSWA.

For simulations with TOXSWA, we advise to use a reference height of 1.5 m for state variables, such as temperature and wind speed, both for the improved parameterization for volatilization and the extended temperature option in TOXSWA.

Example calculations and calculations done for comparison with an analytical solution using the improved parameterisation (Jacobs and Adriaanse, 2012) showed that for highly and for moderately volatile conditions the dissipation of the substance from water to the air was higher than simulated using the current Liss and Slater (1974) parameterisation. The simulations also showed that volatilization to the air increases with increasing wind speed.

Tests with TOXSWA confirmed that the improved parameterization is implemented correctly. It was also shown for some selected cases that calculation of volatilization using the improved parameterisation is robust in the TOXSWA model.

By having implemented the improved parameterization for use of volatilization calculation TOXSWA is now able to account better for changes in weather conditions. In this way simulated concentration profiles may reflect reality better.

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Annex 1 Scenario and substance properties used to illustrate the effect of the improved parameterization for volatilization

In Table A1 the values of the scenario and substance properties as used for the example calculations in section 3.3 are given for TOXSWA. In this simulation only volatilization from the water phase is considered. Other processes that may decrease the concentration are not considered, *i.e.* transformation, sorption to suspended solids or macrophytes (ConSus = 0, CofSorMph = 0) have been set to zero and transport to sediment minimized (ThetaSat set to minimal value of 0.001). Input parameters in TOXSWA that are not relevant for the calculations are not specified in Table A1.

Table A1 *Values of scenario and substance properties used in the TOXSWA example calculation to illustrate the effect of two parameterizations of the transfer coefficient for volatilization.*

Property	**TOXSWA**
Flow velocity	VelWatFlwBas (m/d) =0
Seepage	FlwWatSpg (mm/d) = 0
Water body dimensions	
Water depth	DepWat (m) = 0.3
Width of the bottom	WidWatSys (m) = 1.0
Side slope	SloSidWatSys (-) = 0
Depth defining perimeter	DepWatDefPer (m) = 0
Length of the water body	Len (m) = 100
Number of segments	NumSeg (-) = 1
	OptWaterSystemType: pond
Sediment dimensions and properties[5]	
Thickness of the sediment	ThiHor (m) = 0.1
Number of segments	NumLay (-) = 14 (FOCUS segmentation)
Dry bulk density	Rho (kg.m^{-3}) = 800
Organic matte mass content	CntOM (kg.kg-1) = 0.09
Porosity	ThetaSat (-) = 0.001
Relative diffusion coefficient (tortuosity)	CofDifRel (-) = 0.001
Loading on water body	
Mass loading cross section	no input
Drift deposition	01-May-1986-09h00 Drift 1.0 (mg/m^2)
	OptLoa: DriftOnly
SUBSTANCE	
Molar mass	MolMas (g.mol^{-1}) = 300
Saturated vapour pressure	PreVapRef (Pa) = 0.00001
Reference temperature for saturated vapour pressure	TemRefVap (C) = 20
Molar enthalpy of the vaporization process	MolEntVap (kJ/mol) = 95
Solubility in water	SlbWatRef (mg/L) = 1.23
Reference temperature for water solubility	TemRefSlb (C) = 20
Molar enthalpy of dissolution	MolEntSlb (kJ/mol) = 27

---

[5] Note that substance properties relating to transformation and sorption processes in the sediment are not relevant (negligible) for the calculations because the porosity (ThetaSat) is set to its lowest value of 0.001.

Property	**TOXSWA**
Diffusion	
Diffusion coefficient	CofDifWatRef = $4.3.10^{-5}$ (m^2.d^{-1})
Reference temperature for diffusion	TemRefDif = 20 (C)
Transformation in water	
Half-life	DT50Wat (d) = 100000.
Temperature at which half-life in water was measured	TemRefTraWat (C) = 20
Molar activation enthalpy of transformation in water	MolEntTraWat (kJ/mol) = 65.4
	OptTraWatLumped = Yes OptTraWatHdr = No OptTraWatPho = No OptTraWatBio = No
Transformation in sediment[6]	
Half-life transformation in sediment	DT50SedRef (d) = 10000.
Temperature at which half-life in sediment was measured	TemRefTraSed (C) = 20
Molar activation enthalpy of transformation in sediment	MolEntTraSed (kJ/mol) = 65.4
Sorption to sediment[2]	
Coefficient for equilibrium sorption in sediment	KomSed (L/kg) = 0.
Reference concentration in liquid phase in sediment	ConLiqRefSed (mg/L) = 1.
Freundlich exponent in sediment	ExpFreSed (-) = 1.
Sorption to suspended solids	
Concentration suspended solids	ConSus (g/m^3) = 0.
Coefficient for equilibrium sorption of suspended solids	KomSusSol (L/kg) = 0.
Mass ratio of organic matter in suspended solids	CntOmSusSol (kg/kg) = 0.0
Reference concentration	ConLiqRefSusSol (mg/L) = 1.
Freundlich exponent	ExpFreSusSol (-) = 1.
Sorption to macrophytes	
Coefficient for linear sorption on macrophytes	CofSorMph (L/kg) = 0
Dry mass of macrophyte biomass per m^2 bottom	AmaMphWatLay (g/m^2) = 0

---

[6] Note that substance properties relatied to transformation and sorption processes in the sediment are not relevant (negligible) for the calculations because the porosity (ThetaSat) is set to its lowest value of 0.001.

Annex 2 TOXSWA input file

The TOXSWA input file (*.txw) is given for the example presented in Section 3.2, with the improved parameterization selected for calculation of volatilization.

```
*-----------------------------------------------------------------------------------------------
* INPUT FILE for TOXSWA
*
*-----------------------------------------------------------------------------------------------
* This file is intended to be used by expert users.
*
* E-mail: toxswa@pesticidemodels.nl
*
* (c) Wageningen University & Research
*-----------------------------------------------------------------------------------------------

* Section 0: Run identification
* Section 1: Control
* Section 2: Waterbody
* Section 3: Hydrology
* Section 4: Sediment
* Section 5: Weather
* Section 6: Temperature
* Section 7: Substance
* Section 8: Loadings
* Section 9: Initial and boundary conditions for mass balance equations
* Section 10: Output control

* This input file considers the current scenario. Input that is not needed for
* this scenario is omitted. For a descrEXGE1tion of the full input file, see the
* user manual for the FOCUS & ascii version or in your TOXSWA download package.

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 0: Run identification
*-----------------------------------------------------------------------------------------------

Example       Location          ! Name of the location [1|25 characters]
Testpond      WaterbodyID       ! ID of the water body [1|25 characters]
FOCUS         SedimentTypeID    ! Name of sediment type [1|25 characters]
no_crop       CropName          ! Name of the crop [1|25 characters]
A_test        SubstanceName     ! Name of parent substance [1|15 characters]
scheme01      ApplicationScheme ! Name of the applicaton scheme [1|25 characters]

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 1: Control
*
*-----------------------------------------------------------------------------------------------

FOCUS       CallingProgram        ! Release type of scenario [NL98, NL, GEM, FOCUS, CHINA]
0.0.0       CallingProgramVersion ! Version numbers for model, interface and database,
                                  ! respectively

01-May-1986 TimStart   ! Starting time of simulation [01-Jan-1900|31-Dec-9999]
31-May-1986 TimEnd     ! End time of simulation [01-Jan-1900|31-Dec-9999]

Hourly      OptInp     ! Option for hourly or daily input data of lateral entries [Hourly, Daily]

* OptHyd: options for hydrology simulation
* Only      Simulate only hydrology
* OnLine    Simulate hydrology and substance
* OffLine   Assumption hydrology has been simulated, runID.hyd file must be present
* Automatic TOXSWA checks if hydrology file (runID.hyd) exists; so, hydrology
*           simulation is skipped
* ExtModel  Hydrology file present, simulated by external model
OnLine      OptHyd     ! Option selected for hydrology simulation
                       ! [Only, OnLine, OffLine, Automatic]

   * If CallingProgram is 'FOCUS',then specify path and file name for intermediate data files
   C:\UserData\dirdata          DirData ! Directory for data files
   1_volat       HydFile ! Name of .hyd file with hydrology of waterbody
   May86var      TemFile ! Name of .tem file with temperature of waterbody

* If CallingProgram is 'FOCUS', 'GEM' or 'China' then specify time step for hydrology
900         TimStpHyd (s)    ! Calculation time step for hydrology [0.001|3600]

* OptTem: options for temperature simulation
* Only      Simulate only temperature
* OnLine    Simulate temperature and substance
* OffLine   Assumption temperature has been simulated, runID.tem file must be present
* Automatic TOXSWA checks if the temperature file (runID.tem) exists; so, temperature
*           simulation is skipped
Automatic             OptTem          ! [Only, OnLine, OffLine, Automatic, ExtModel]

Calc        OptTimStp  ! Option for time step in mass balance calculation [Input, Calc]
Yes         OptCalcStabilityWater    ! Option for check of stability of the numerical solution for
                                     ! the water layer
Yes         OptCalcStabilitySediment ! Option for check of stability of the numerical solution for
                                     ! the sediment [Yes, No]
                                     ! Yes = Full check on stability
                                     ! No = Check on positivity

* If OptTimStp is 'Calc' then specify
60        MaxTimStpWat (s) ! Maximum calculation time step in water layer [0.001|3600]
60        MaxTimStpSed (s) ! Maximum calculation time step in sediment [0.001|3600]
```

```
* OptDif: option to simulate diffusion affected by temperature ('No' can be used for
* released scenarios for which diffusion was considered independent op tempeature)
Yes        OptDif          ! Diffusion in water temperature dependent [Yes, No]
                           ! Default is 'No'

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 2: Waterbody
*
*-----------------------------------------------------------------------------------------------

* WaterBody table: descrEXGE1tion of waterbody
* Len           Length [0.05||]
* NumSeg        Number of segments [1||]
* WidWatSys     Width of the bottom of water system [0.05|100]
* SloSidWatSys  Side slope  of the water system [0|10]
* DepWatDefPer  Water depth defining perimeter for exchange between water layer
*               and sediment [0|lowest water depth]
table WaterBody
Len   NumSeg   WidWatSys   SloSidWatSys DepWatDefPer
(m)    (-)       (m)            (-)          (m)
100       1          1          0           0
end_table

0          ConSus (g.m-3)       ! Concentration of suspended solids [0|100000]
0          CntOmSusSol (g.g-1)  ! Mass ratio of organic matter in suspended solids [0|1]
0          AmaMphWatLay (g.m-2) ! Dry mass of macrophyte biomass per m2 bottom [0|1000]

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 3: Hydrology:
*   Section 3a: General
*-----------------------------------------------------------------------------------------------

Constant  OptFloWat   ! Water flow type [Constant, SimpleDitch, Transient, InfiltrationPond]

* If OptFloWat is 'Transient' or 'SimpleDitch' then specify
Pond        OptWaterSystemType    ! Water system type [Pond, WaterCourse]

* If OptWaterSystemType is 'WaterCourse' then specify
Fischer     OptDis                ! Dispersion calculation method [Input, Fischer]

*-----------------------------------------------------------------------------------------------
* Section 3b: Constant water flow
*
* If OptFloWat is 'Constant'
*-----------------------------------------------------------------------------------------------

0.3                DepWat (m)           ! Water depth
0.0                VelWatFlwBas (m.d-1) ! Constant flow velocity

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 4: Sediment
*-----------------------------------------------------------------------------------------------

* SedimentProfile table: thickness and number of layers in horizon
* ThiHor  Thickness of horizon [0.0001|-]
* NumLay  Number of layers in horizon [1|500]
table SedimentProfile
ThiHor NumLay
(m)
0.004    4
0.006    3
0.01     2
0.03     3
0.02     1
0.03     1
end_table

Input      OptSedProperties   ! Sediment properties for ThetaSat and CofDifRel [Input, Calc]

* SedimentProperties table: properties for each horizon:
* Nr        Number horizon [1|500]
* Rho       Bulk density [10|3000]
* CntOm     Organic matter mass content [0|1]
* If OptSedProperties 'Input' then specify ThetaSat and CofDifRel
* ThetaSat  Saturated water content [0.001|0.999]
* CofDifRel Relative diffusion coefficient [0|1]
table  horizon SedimentProperties
Nr     Rho        CntOm     ThetaSat   CofDifRel
       (kg.m-3)   (kg.kg-1)  (m3.m-3)   (-)
1      800        0.09       0.001       0.001
2      800        0.09       0.001       0.001
3      800        0.09      0.001       0.001
4      800        0.09       0.001       0.001
5      800        0.09       0.001       0.001
6      800        0.09       0.001       0.001
end_table

0.      FlwWatSpg (m3.m-2.d-1) ! Percolation rate through the sediment [-0.01|0.01]

*-----------------------------------------------------------------------------------------------
```

```
*-----------------------------------------------------------------------------------------------
* Section 5: Weather
*-----------------------------------------------------------------------------------------------

DeBiltMay86  MeteoStation      ! Name of file with meteo data (*.met or *.meth file)
Hourly       OptMetInp         ! Input data [Hourly, Monthly]

* If OptMetInp is 'Hourly' or OptTraWatPho is 'Yes' then specify time zone
1        TimZone (-)        ! Time zone [0|23]

* if: OptMetInp = Hourly
52.00    LocMetLat (Degrees)   ! Latitude of meteostation [-180|180]
-4.00    LocMetLong (Degrees)  ! Longitude of meteostation [-180|180]
1.50     MetLvlRef (m)      ! Reference level meteo measurements [0|]
10.00    MetLvlObs (m)      ! Height of meteo measurements [0|]

* if: missing values <shortwave radiation> in meteo file
1041     FacAtmWavLenShort1 (W.m-2) ! Atmospheric attenuation shortwave radiation
                                    ! factor a1 [??|??]
-69      FacAtmWavLenShort2 (W.m-2) ! Atmospheric attenuation shortwave radiation
                                    ! factor a2 [??|??]
-0.75    FacCldB1 (-)       ! Cloud contribution factor b1 [??|??]
3.4      FacCldB2 (-)       ! Cloud contribution factor b2 [??|??]

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 6: Temperature
* If OptMetInp is 'Hourly'
*-----------------------------------------------------------------------------------------------

20.0      TemWatIni (C)     ! Initial temperature in water layer [0|35]
4.25      CofSorPAR (m-1)   ! Absorption coefficient for PAR in water [0|??]
1000      CofSorNIR (m-1)   ! Absorption coefficient for NIR in water [0|??]

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 7: Substance
*   Section 7a: general
*-----------------------------------------------------------------------------------------------
* Compounds table: first entry is parent, next entries are metabolites [1|15 characters]
table compounds
A_test
end_table

* FraPrtDauWat table: parent-daughter relationshEXGE1s transformation in water
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauWat (mol.mol-1)
end_table

* FraPrtDauSed table: parent-daughter relationshEXGE1s transformation in sediment
* Column 1: fraction formed from parent into daughter [0|]
* Column 2: name of parent
* Column 3: name of daughter
table FraPrtDauSed (mol.mol-1)
end_table

Jacobs    OptVol   ! Volatilization simulation method [Liss, Jacobs]

*-----------------------------------------------------------------------------------------------
* Section 7b: Substance properties for parent 'A_test'
* (note extension of parameter name is substance code)
*-----------------------------------------------------------------------------------------------

300        MolMas_A_test (g.mol-1) ! Molar mass of parent substance [10.0 - 10000]

    * If OptVol is 'Jacobs' then specify
    0.43   CofDifAirRef_A_test (m2.d-1)  ! Reference diffusion coefficient in air [0|200]

* Volatilization from water layer
0.00001    PreVapRef_A_test (Pa)         ! Saturated vapour pressure of substance [0|2e5]
20         TemRefVap_A_test (C)          ! Reference temperature for saturated vapour pressure
                                       ! [0|40]
95         MolEntVap_A_test (kJ.mol-1)   ! Molar enthalpy of vaporization [-200|200]
0.1230896  SlbWatRef_A_test (mg.L-1)     ! Water solubility of substance [0.001|1e6]
20         TemRefSlb_A_test (C)          ! Reference temperature for water solubility [0|40]
27         MolEntSlb_A_test (kJ.mol-1)   ! Molar enthalpy of dissolution  [-200|200]

* Diffusion in liquid and gas phases
4.3e-05    CofDifWatRef_A_test (m2.d-1)  ! Reference diffusion coefficient in water [0|2E-3]
20         TemRefDif_A_test (C)          ! Reference temperature for diffusion [0|35]

* Sorption
0          KomSed_A_test (L.kg-1)       ! Freundlich coefficient of  equilibrium sorption for
                                        ! sediment [0|1e7]
1          ConLiqRefSed_A_test (mg.L-1) ! Reference concentration in liquid phase for
                                        ! Freundlich coefficient for sediment [0.001|100]
1          ExpFreSed_A_test (-)         ! Freundlich exponent  in sediment [0.1|1.5]
0          KomSusSol_A_test (L.kg-1)    ! Freundlich coefficient of  equilibrium sorption
                                        ! for suspended solids [0|1e7]
1          ConLiqRefSusSol_A_test (mg.L-1) ! Reference concentration in liquid phase
                                        ! for Freundlich sorption coefficient for
                                        ! suspended solids [0.001|100]
1          ExpFreSusSol_A_test (-)      ! Freundlich exponent suspended solids [0.1|1.5]
0          CofSorMph_A_test (L.kg-1)    ! Coefficient for linear sorption on
                                        ! macrophytes [0|1e7]
```

```
* Transformation in water

* Options are lumped or specified: hydrolysis, photolysis, biotic transformation.
* Using option lumped excludes use of the specified options.

* Selection of transformation processes in water layer, lumped or specified; hydrolysis, photolysis,
* biotic transformation. Using option lumped excludes use of the specified options.
* Using option photolysis, hourly meteo data are needed; for option OptMetInp select 'Hourly'
Yes       OptTraWatLumped_A_test       ! Option for lumped transformation in water [Yes, No]
No        OptTraWatHdr_A_test          ! Option for hydrolysis in water [Yes, No]
No        OptTraWatPho_A_test          ! Option for photolysis in water [Yes, No]
No        OptTraWatBio_A_test          ! Option for biotic transformation in water [Yes, No]

    * If OptTraWatLumped is 'Yes' specify
    10000       DT50WatRef_A_test (d)        ! Half-life transformation in water at reference
                                           ! temperature [0.1|1e5]
    20         TemRefTraWat_A_test (C)       ! Reference temperature for half-life measured in water
                                           ! [5|30]
    75         MolEntTraWat_A_test (kJ.mol-1) ! Molar activation enthalpy of transformation in water
                                           ! [0|200]
* Transformation in sediment
1000       DT50SedRef_A_test (d)          ! Half-life transformation in sediment at reference
                                          ! temperature [0.1|1e3]
20         TemRefTraSed_A_test (C)        ! Reference temperature for half-life in sediment [5|30]
65.4       MolEntTraSed_A_test (kJ.mol-1) ! Molar activation enthalpy of transformation in sedment
                                          ! [0|200]
    * Transformation parameters entered for soil models MACRO/PRZM (not used by TOXSWA)
    100.         DT50SoilRef_A_test (d)      ! Half-life transformation in soil at reference
                                             ! temperature [0.1|1e5]
    20.          TemRefTraSoil_A_test (C)    ! Reference temperature for half-life in soil [0.1|1.5]

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 8: Loadings
*-----------------------------------------------------------------------------------------------

* OptLoa options for loading type
* DriftOnly  spray drift only entry route
* PEARL      drainage calculated by PEARL
* MACRO      drainage calculated by MACRO
* PRZM       runoff and erosion calculated by PRZM
* GEM        greenhouse discharge calculated by GEM
DriftOnly       OptLoa   ! Loading option [DriftOnly, PEARL, MACRO, PRZM, GEM]

* Loadings table: details loading
* Column 1  Date and time of application
* Column 2  Application type []
* Column 3  Mass of loading [kg.ha-1) [0|]
* Column 4  Crop interception [%) [0|100]
* Column 5  Drift deposition (mg.m-2) [0|]
* Note that the info in columns 2 - 4 is not used in the calculation
table Loadings
01-May-1986-09h00       ground_spray   1    0    1.0
end_table

* Stretch for all loading types
Yes     OptLoaStr   ! Loading to full stretch of water body [Yes|No]

0.01        ThiLayTgt1 (m)   ! Depth defining the thickness of the target sediment layer 1
                             ! for output of (averaged) content [1e-5|1]

No          OptOutputThiLayTgt2  ! Output of contents in 2nd target layer of sediment [Yes|No]

* Specify warming-up period
0           InitYears (-)    ! Length of warming-up period in years [0|]

* Target percentile in time
0           TargetPercentile (%) ! Target percentile resulting in selected year [0|100]

* Target percentile in time,and target period for selection
01-May    StaTimPrdTgt         ! Start date of target period for selection of
                               ! year with target percentile [01-Jan|31-Dec]
31-May    EndTimPrdTgt         ! End date of target period for selection of
                               ! year with target percentile [01-Jan|31-Dec]

*-----------------------------------------------------------------------------------------------
*-----------------------------------------------------------------------------------------------
* Section 9: Initial and boundary conditions for mass balance equations
*-----------------------------------------------------------------------------------------------

* Initial conditions

0          ConSysWatIni (g.m-3)  ! Initial total concentration in water layer [0|-]

* CntSysSedIni table: initial total substance content in sediment
* If metabolites are included then initail contents for these substances are set tot zero
* Column 1  Depth in sediment (m) [0|-]
* Column 2  Substance content (mg.kg-1) [0|-]
table interpolate CntSysSedIni (mg.kg-1)
end_table

* Boundary conditions
0          ConAir (g.m-3)        ! Concentration  in air [0|-]
0          ConWatSpg (g.m-3)     ! Concentration in incoming seepage water [0|-]

*-----------------------------------------------------------------------------------------------
```

```
*-----------------------------------------------------------------------------------------------
* Section 10: Output control
*   Section 10a: General
*-----------------------------------------------------------------------------------------------

No        OptDelOutFiles   ! Remove *.out file after simulation [Yes|No]

* DateFormat: options for format of date and time in the output file
* DaysFromSta   Print number of days since start of simulation
* DaysFrom1900  Print number of days since 1900
* Years         Print years
DaysFromSta  DateFormat [DaysFromSta, DaysFrom1900, Years]

* RealFormat: format of the ordinary output - use FORTRAN notation:
* e is scientific notation, g  is general notation,
* then the number of positions, then the number of digits
e14.6     RealFormat       ! Format of ordinary output

* OptDelTimPrn: options for output time step
* Hour,Day,Decade,Month,Year  Time step for output
* Automatic                   Length of simulation period
* Other                       User defined
Hour      OptDelTimPrn     ! Output time step [Hour|Day|Decade|Month|Year|
                           ! Automatic|Other]

No        PrintMasStrTgt   ! Print additional mass balance of specified stretch in
                                             ! watercourse [Yes, No]

All     OptOutputDistances ! Options for distances of water layer grid points at which
                           ! output can be obtained[None, All, table]

* If OptOutputDistances is 'table' then specify output distances in waterbody
* OutputDistances-table: output distances in waterbody, i.e. water layer and sediment
* subsystem
* Column 1  Distance (m) [0|-]
table OutputDistances (m)
end_table

table        OptOutputDepths  ! Options for depths of sediment grid poinst at which
                              ! output can be obtained [None, All, table]

* If OptOutputDepths is 'table' then specify
* OutputDepths-table: depths of sediment nodes at which output can be obtained
* Column 1   Depth (m) [0|-]
table OutputDepths (m)
end_table

* Specify dates for output of additional profiles; options set via OptOutputDistances and
* OptOutputDepths are used
* HorVertProfiles table: profiles in horizontal direction for water layer and in vertical
* direction for sediment are given; values given are:
* Water layer: output distance, water depth, total and dissolved concentration,
* Sediment: output node water layer, output depth, pore volume, total and dissolved
* concentration.
table HorVertProfiles
end_table

* Specify type of summary report
FOCUS     OptReport        ! [DutchRegistration|FOCUS]
Yes       ExposureReport   ! Exposure report [Yes|No]

*  ! Print column oriented output files (csv format)
Yes        ConcentrationsTgt  ! Concentration in water FOCUS target segment and contents in
                              ! FOCUS target sediment layers
No         MassBalWaterLayer  ! Mass balance of substance in water layer
No         MassBalSediment    ! Mass balance of substance in sediment
No         Distribution       ! Distribution of substance in water body
No         Hydrology          ! Water depth and discharge
No         LateralFluxes      ! Lateral water flows and substance fluxes from drainage
                              ! runoff and erosion

*-----------------------------------------------------------------------------------------------
* Section 10b: Print variables in *.out file
* State variables, fluxes and rates given as momentary values.
* Volume,energy and mass changes given as cumulative values.
*-----------------------------------------------------------------------------------------------

* Specify for all print variables whether output is wanted [Yes, No]
* When print variable is not in file; TOXSWA assumes 'No'

* PrintCumulatives: options for printing cumulatives of volume, energy and mass fluxes
* Yes   : cumulative terms have been summed up from start of simulation and have been
*         allocated to the last moment of the period considered
* No    : cumulative terms have been summed up from start of user defined output time step
*         OptDelTimPrn and have been allocated to the last moment of the period
*         considered
Yes       PrintCumulatives      ! [Yes, No]

* If PrintCumulatives is 'Yes' and OptReport is 'DutchRegistration'
No        PrintCumulativesSta    ! Accumulate from start of simulation [Yes] or
                                    ! skip warming up period  [No] (only for mass fluxes)


* Concentrations and contents in water layer segments as specified by
* OptOutputDistances
Yes       print_ConLiqWatLay     ! Concentration dissolved in water (g.m-3)

* Mass balance for entire water layer
Yes       print_MasWatLay       ! Mass in water layer (g)

*-----------------------------------------------------------------------------------------------
* End of TOXSWA input file
*-----------------------------------------------------------------------------------------------
```

Annex 3 Meteorological file

This annex shows the first part of De Bilt meteorological file used for the example simulation presented in Section 3.2. The description of the header of the file is given in Table A2.

Table A2 *Description of header of the meteorological file (see also Table 2 in Beltman et al., 2017).*

Parameter in “meth” file	**Unit**	**Description**
MSTAT	-	name of meteo station
YYYY	-	year
MM	-	month
DD	-	day
HH	hours	time
RAD	kJ/m^2	shortwave radiation, sum in hour
T	°C	temperature at reference level
HUM	-	relative atmospheric humidity at reference level (relative to 1(=100%))
CLD	octants	cloud cover, (and 9=sky invisible)
WIND	m/s	hourly mean wind speed at observation level
PA	kPa	air pressure reduced to mean sea level
RAIN	mm	hourly precipitation amount (-1 for <0.05 mm)
ETref	mm	evapotranspiration reference (ETref = -99.9 is a dummy value)

```
*  MSTAT  YYYY  MM  DD  HH     RAD      T    HUM    CLD   WIND     PA   RAIN  ETref
*                          kJ.m-2      C      -      -  m.s-1    kPa     mm     mm
**********************************************************************************
'DeBilt'  1986   5   1   1       0    4.4   0.94   0.12    0.5 102.86    0.0  -99.9
'DeBilt'  1986   5   1   2       0    3.7   0.97   0.25    1.0 102.85    0.0  -99.9
'DeBilt'  1986   5   1   3       0    3.6   0.97   0.12    0.5 102.81    0.0  -99.9
'DeBilt'  1986   5   1   4      40    3.9   0.99   0.38    0.5 102.81    0.0  -99.9
'DeBilt'  1986   5   1   5     370    8.5   0.73   0.25    0.5 102.81    0.0  -99.9
'DeBilt'  1986   5   1   6     960   11.2   0.60   0.12    1.5 102.78    0.0  -99.9
'DeBilt'  1986   5   1   7    1540   13.3   0.58   0.12    1.5 102.75    0.0  -99.9
'DeBilt'  1986   5   1   8    2100   14.8   0.47   0.12    3.6 102.72    0.0  -99.9
'DeBilt'  1986   5   1   9    2510   16.1   0.41   0.25    4.1 102.64    0.0  -99.9
'DeBilt'  1986   5   1  10    2830   16.9   0.30   0.38    4.1 102.56    0.0  -99.9
'DeBilt'  1986   5   1  11    2980   18.1   0.33   0.38    4.1 102.48    0.0  -99.9
'DeBilt'  1986   5   1  12    2880   18.4   0.34   0.38    3.6 102.39    0.0  -99.9
'DeBilt'  1986   5   1  13    2570   19.2   0.38   0.25    4.1 102.31    0.0  -99.9
'DeBilt'  1986   5   1  14    2180   19.6   0.38   0.25    4.1 102.21    0.0  -99.9
'DeBilt'  1986   5   1  15    1710   19.5   0.39   0.25    4.1 102.15    0.0  -99.9
'DeBilt'  1986   5   1  16    1050   19.1   0.42   0.38    4.6 102.07    0.0  -99.9
'DeBilt'  1986   5   1  17     510   17.6   0.44   0.38    4.1 102.01    0.0  -99.9
'DeBilt'  1986   5   1  18     110   16.6   0.43   0.38    3.6 101.98    0.0  -99.9
'DeBilt'  1986   5   1  19      10   14.9   0.50   0.25    2.6 101.94    0.0  -99.9
'DeBilt'  1986   5   1  20       0   14.5   0.55   0.25    2.6 101.88    0.0  -99.9
'DeBilt'  1986   5   1  21       0   14.3   0.59   0.12    3.6 101.83    0.0  -99.9
'DeBilt'  1986   5   1  22       0   13.4   0.64   0.12    4.1 101.78    0.0  -99.9
'DeBilt'  1986   5   1  23       0   12.7   0.68   0.00    3.1 101.72    0.0  -99.9
'DeBilt'  1986   5   1  24       0   12.3   0.72   0.12    3.1 101.68    0.0  -99.9
'DeBilt'  1986   5   2   1       0   11.8   0.75   0.12    2.6 101.65    0.0  -99.9
'DeBilt'  1986   5   2   2       0   11.7   0.76   0.12    2.6 101.58    0.0  -99.9
'DeBilt'  1986   5   2   3       0   11.8   0.75   0.12    2.6 101.52    0.0  -99.9
'DeBilt'  1986   5   2   4      30   12.0   0.75   0.00    3.1 101.48    0.0  -99.9
'DeBilt'  1986   5   2   5     320   13.2   0.72   0.00    3.1 101.46    0.0  -99.9
'DeBilt'  1986   5   2   6     780   16.1   0.64   0.00    4.6 101.40    0.0  -99.9
'DeBilt'  1986   5   2   7    1340   17.4   0.56   0.00    6.2 101.36    0.0  -99.9
'DeBilt'  1986   5   2   8    1870   18.9   0.54   0.00    6.2 101.31    0.0  -99.9
'DeBilt'  1986   5   2   9    2290   20.4   0.53   0.00    6.7 101.26    0.0  -99.9
'DeBilt'  1986   5   2  10    2590   22.2   0.45   0.00    6.7 101.17    0.0  -99.9
'DeBilt'  1986   5   2  11    2710   23.3   0.42   0.00    8.7 101.10    0.0  -99.9
'DeBilt'  1986   5   2  12    2660   23.9   0.38   0.00    8.2 101.05    0.0  -99.9
'DeBilt'  1986   5   2  13    2370   24.3   0.37   0.00    8.2 100.98    0.0  -99.9
'DeBilt'  1986   5   2  14    1960   24.2   0.39   0.00    6.7 100.93    0.0  -99.9
'DeBilt'  1986   5   2  15    1460   24.0   0.40   0.00    6.2 100.88    0.0  -99.9
'DeBilt'  1986   5   2  16     930   23.8   0.41   0.00    6.2 100.84    0.0  -99.9
'DeBilt'  1986   5   2  17     440   23.1   0.42   0.00    4.1 100.82    0.0  -99.9
'DeBilt'  1986   5   2  18     150   21.0   0.49   0.25    3.1 100.85    0.0  -99.9
'DeBilt'  1986   5   2  19      10   19.5   0.55   0.38    2.1 100.89    0.0  -99.9
'DeBilt'  1986   5   2  20       0   18.8   0.55   0.12    1.5 100.87    0.0  -99.9
'DeBilt'  1986   5   2  21       0   17.4   0.59   0.12    2.1 100.87    0.0  -99.9
'DeBilt'  1986   5   2  22       0   18.8   0.54   0.12    3.1 100.87    0.0  -99.9
'DeBilt'  1986   5   2  23       0   18.3   0.55   0.12    3.1 100.85    0.0  -99.9
'DeBilt'  1986   5   2  24       0   17.0   0.62   0.25    2.6 100.83    0.0  -99.9
.
.
```

Reference

Beltman, W.H.J., Adriaanse, P.I., Jacobs, C.M.J., Mulder, H.M. (2017). Temperature in water and sediment in the pesticide model TOXSWA. Implementation report. Wageningen, Wageningen Environmental Research, Report 2794.

Annex 4 Analytical solution for calculation of volatilization

An analytical solution for volatilization from the water layer to the air is given (see Jacobs and Adriaanse, 2012). Assuming the concentration in air is zero and volatilization is the only sink term in a well-mixed water body, the analytical solution is given by

$$c_w = c_{w,0} \, exp[-k_v t] \tag{A1}$$

With:

c_w	= concentration in water at time t (kg m^{-3})
$c_{w,0}$	= concentration in water at time 0 (kg m^{-3})
t	= time (s)
k_v	= volatilization rate coefficient (s^{-1})

For the improved parameterization the volatilization rate at the temperature of water is given by:

$$k_v = \left(\frac{K_h}{r_a + r_b + K_H r_w}\right)\left(\frac{O_x}{A}\right) \tag{A2}$$

With:

K_H	= Henry coefficient (-)
r_a	= air resistance (s.m^{-1})
r_b	= boundary layer resistance (s.m^{-1})
r_w	= aqueous resistance (s.m^{-1})
O_x	= width of the water surface (m)
A	= cross section of water layer (m^2)

Note that the water depth h in Jacobs and Adriaanse (2012) is replaced by the division of O_x by A, representing the average depth of the waterbody.

The equations for calculation of Henry's coefficient and correction for temperature of water, saturated vapour pressure and solubility are given in Ter Horst et al. (2016).

The input used for the calculations and intermediate calculation results are given in Table A3.

References

Jacobs, C.M.J. and Adriaanse, P.I., 2012. Pesticide volatilization from small surface waters: rationale of a new parameterization for TOXSWA. Wageningen, Alterra, Alterra Report 2316. 44p.

Ter Horst, M.M.S., Beltman, W.H.J., Van den Berg, F. 2016. The TOXSWA model version 3.3 for pesticide behaviour in small surface waters: description of processes. Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu), WOt-technical report 84. 72p.

Table A3 *Input and results of calculations with analytical solution for volatilization.*

Parameter	Symbol	TOXSWA variable	Units	Value	Value
Substance					
molar mass	M_m	MolMas	g mol^{-1}	300	300
universal gas constant	R	Rgas	J K^{-1} mol^{-1}	8.31432	8.31432
saturated vapour pressure at reference temperature	$P_{sat,ref}$	PreVapRef	Pa	0.1	0.1
molar enthalpy of vaporization	ΔH_v	MolEntVap	J mol^{-1}	95000	95000
reference temperature for saturated vapour pressure	$T_{v,r}$	TemRefVap	C	20	20
water solubility of substance at reference temperature	$c_{slb,r}$	SlbWatRef	g m^{-3}	1.230896	1.230896
molar enthalpy of dissolution	ΔH_d	MolEntSlb	J mol^{-1}	27000	27000
reference temperature for water solubility	$T_{d,r}$	TemRefSlb	C	20	20
molecular diffusion coefficient of substance in air at $T_{dif,ref}$	$D_{a,r}$	CofDifAirRef	m^2 s^{-1}	4.9769.10^{-6}	4.9769.10^{-6}
molecular diffusion coefficient of substance in water at Tw,ref	$D_{w,r}$	CofDifWatRef	m^2 s^{-1}	4.9769.10^{-10}	4.9769.10^{-10}
temperature for which the molecular diffusion coefficient in air is given	$T_{dif,r}$	TemRefDif	°C	20	20
Meteo					
reference level	z_r	MetLvlRef	m	1.5	1.5
height of observation of wind speed	z_{obs}	MetLvlObs	m	10	10
roughness length	z_0	CofRghAer	-	0.03	0.03
Von Karman constant	κ	VonKarmanConst	-	0.4	0.4
kinematic viscosity of the air	v_a	VisKinAirCal	m^2 s^{-1}	0.000015	0.000015
air temperature	T_a	TemAir	K	293.15	293.15
water temperature	T_w	TemWat	K	293.15	293.15
wind speed observed at z_{obs}	U_{obs}	VelWndObs	m^2 s^{-1}	1	10
Calculations					
saturated vapour pressure of substance	P_{sat}	PreVap	Pa	0.1	0.00001
water solubility of substance	c_{slb}	SlbWat	g m^{-3}	1.230896	0.12309
Henry coefficient	K_H	CofHenry	-	0.01000	0.00001
wind speed at reference level z_r	U	VelWndRef	m s^{-1}	0.67342515	6.734252
friction velocity	$u*$	FrcVel	m s^{-1}	0.06885697	0.68857
kinematic viscosity of water at T_w	v_w	VisKinWat	m^2 s^{-1}	1.005.10^{-6}	1.01.10^{-6}
molecular diffusion coefficient of substance in air at T_a	D_a	CofDifAir	m^2 s^{-1}	4.9769.10^{-6}	4.98.10^{-6}
molecular diffusion coefficient of substance in water at T_w	D_w	CofDifWat	m^2 s^{-1}	4.9769.10^{-10}	4.98.10^{-10}
Schmidt number in air	Sc_a	SchNumAir	-	3.01395349	3.013953
Schmidt number in water	Sc_w	SchNumWat	-	2019.38902	2019.389
transfer rate at Sc_w = 600	k_{600}	K600	m s^{-1}	2.285	12.84553
transfer rate	k_w	Kw	m s^{-1}	1.24552324	7.001926
air resistance	r_a	RstAirLay	m s^{-1}	142.034381	14.20344
boundary layer resistance	r_b	RstBouLay	m s^{-1}	432.682127	43.26821
aqueous resistance	r_w	RstWatLay	m s^{-1}	0.80287543	0.142818
volatilization rate coefficient	k_v	CofTrfLiq	s^{-1}	1.7399.10^{-5}	1.74.10^{-7}
volatilization rate coefficient in d^{-1}		-	d^{-1}	1.5032	0.01503

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