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PRIMET version 2.0, technical description and manual

A Decision Support System for assessing Pesticide Risks in the tropics to
Man, Environment and Trade

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Joost Vlaming
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Alterra-rapport 1648, ISSN 1566-7197



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Alterra-rapport 1648

Alterra, Wageningen, 2008

ABSTRACT

Peeters, F.M. ,P.J. van den Brink, J. Vlaming, J.G. Groenwold, W.H.J. Beltman and J.J.T.I Boesten, 2008. *PRIMET version 2.0, manual and technical description. A Decision Support System for assessing Pesticide RIks in the tropics to Man, Environment and Trade*. Wageningen, Alterra, Alterra-rapport 1648. 77 blz.; 29 figs.; 2 tables.; 22 refs.

Pesticide exposure via for instance spray drift or runoff to surface water, accumulation in the topsoil, and leaching to groundwater potentially affects organisms in water, in and around soil and on plants and might also pose risks to humans via dietary exposure, in case they consume contaminated products like groundwater, macrophytes and fish. To estimate these risks at the household level the PRIMET Decision Support System was developed. PRIMET runs with a minimum of input data and is developed to be used in developing countries. The risk assessment is expressed in Exposure Toxicity Ratio's which are calculated by dividing the predicted exposure by the safe concentration. This report provides a mathematical description of the processes incorporated into PRIMET and a user manual. PRIMET 2.0 is freely available at www.primet.wur.nl.

Keywords: Developing Countries, Human Health, Pesticides, Risk Assessment, Tropics, Vegetables

ISSN 1566-7197

This report is available in digital format at www.alterra.wur.nl.

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Summary

Within the last decade the agriculture sector in Southeast Asia and other regions has been intensifying at a rapid pace. A large increase in the use of external inputs, like pesticides, has taken place in many different agricultural sub-sectors such as horticulture. This increased productivity has been beneficial for human health in terms of food security. Pesticide exposure, however, may affect the environment and human health through different emission routes; for instance, via spray drift or runoff to surface water, accumulation in the topsoil, and leaching to groundwater. This potentially affects organisms in water, in and around soil and on plants and might also pose risks to humans via dietary exposure, in case they consume contaminated products like groundwater, macrophytes and fish. To estimate these risks the PRIMET Decision Support System was developed. PRIMET is the acronym for Pesticides RIks in the tropics to Man, Environment and Trade. This DSS is able to estimate the risks of pesticide application to 1) aquatic life, 2) terrestrial life (earthworms), 3) bees, 4) non target arthropods, 5) the use of groundwater as drinking water and 6) dietary exposure via the consumption of groundwater, vegetables, fish and macrophytes. The risks are assessed at the household level, i.e. actual pesticide application data at the farm level is needed as input parameters. The risk assessment is expressed as Exposure Toxicity Ratio's (ETR) which are calculated by dividing the exposure by the safe concentration. If the ETR is smaller than 1, i.e. the exposure lower than the "safe" concentration the risk is acceptable. If the ETR is larger than 1 but smaller than a certain value (in this report 100), a risk may present. If ETR's are very large (e.g. >100) risks are quite certain although the methods used are based on worst-case assumptions. The PRIMET 2.0 DSS is freely available on www.primet.wur.nl and incorporated in a Graphical User Interface. This report provides a mathematical description of the processes incorporated into PRIMET 2.0 and a user manual.

1 Introduction

Within the last decade the agriculture sector in Southeast Asia has been intensifying at a rapid pace. A large increase in the use of external inputs, like pesticides, has taken place in many different agricultural sub-sectors such as horticulture. This has led to an increase in productivity and income of the rural population. On the one hand this increased prosperity has been beneficial for human health in terms of food security, but on the other hand human health may be negatively affected by the consumption of pesticide residues. In addition to this, the negative impacts on ecosystems harm the biodiversity of agricultural ecosystems and can harm future productivity.

Pesticides may enter the environment through various emission routes, for instance, via spray drift or runoff to surface water, accumulation in the topsoil, and leaching to groundwater. This potentially affects organisms in water, in and around soil and on plants and might also pose risks to humans via dietary exposure, in case they consume contaminated products like groundwater, macrophytes and fish. To estimate these risks the PRIMET Decision Support System (DSS) was developed. Version 2.0 of this DSS is able to estimate the risks of pesticide application to 1) aquatic life, 2) terrestrial life (earthworms), 3) bees, 4) non target arthropods, 5) the use of groundwater as drinking water and 6) dietary exposure via the consumption of groundwater, vegetables, fish and macrophytes. The risks are assessed at the household level, i.e. actual pesticide application data at the farmer's level is needed as input parameters.

The risk assessment is expressed in Exposure Toxicity Ratio's which are calculated by dividing the estimated exposure concentrations by the safe concentration. The exposure concentrations are estimated using worst case scenarios for local conditions. The "safe" concentration is calculated from toxicity data and extrapolation factors. If the ETR is smaller than 1, i.e. the estimated exposure is lower than the "safe" concentration, the risk is acceptable. If the ETR is larger than 1 but smaller than a certain value (in this report 100), a risk may be present. Whether there is a real risk should be determined in a higher tier risk assessment by using more complex fate and effect models (e.g. PEARL, TOXSWA, PERPEST; see www.pesticidemodels.eu). If ETR's are very large (e.g. >100) risks are quite certain although the methods used are based on worst-case assumptions.

For the risk assessments physical-chemical as well as toxicity data and fate and behaviour data of the active ingredient have to be available. This includes data on toxicity, dissipation and sorption characteristics, solubility, etc. For some common active ingredients the required data are included in the PRIMET 2.0 database. For new active ingredients the required data have to be gathered from literature.

Further, the average pesticide application schemes practiced by farmers have to be defined in terms of dosage, number of applications and time interval between applications. This may involve a review of farmers' practices in the research area. In

some cases MonQi can be used to get the required information related to the application scheme. MonQi is a methodology for monitoring management of agricultural systems in the tropics with the aim to improve the quality of farm management, crop production, quality of produce, living standards and environment (www.monqi.org).

2 Incorporated processes and calculations

2.1 Introduction

As described in the introduction, PRIMET is able to assess the risks of pesticide application to 1) aquatic life, 2) terrestrial life (earthworms), 3) bees, 4) non target arthropods, 5) the use of groundwater as drinking water and 6) dietary exposure via the consumption of groundwater, vegetables, fish and macrophytes. The risks are calculated for (edge of) field situations, i.e. for the ecology of water courses adjacent to the treated field, for the terrestrial life within the treated soil, for invertebrates in and around plants (bees and non target arthropods), for the human consumption of the groundwater below the treated field and the human consumption of fish and macrophytes (aquatic water plants) present in the watercourse adjacent to the treated field as well as the cultivated crop itself.

For all risk assessments an exposure as well as an effect assessment is performed. The exposure assessment consists of estimating the concentrations in the watercourses, terrestrial soil, groundwater, fish and macrophytes. The effect assessment consists of determining safe concentrations for the different compartments and is based on laboratory toxicity data or international standards and the use of extrapolation factors. The risk assessment is then performed by dividing the predicted concentration by the predicted safe concentration. In each of the following sections one of the risk assessments is described. Each section is divided into subsections that describe the exposure, effect and risk assessments as well as a subsection describing the required input data and the calculated parameters.

2.2 Aquatic risk assessment

2.2.1 Aquatic exposure assessment

2.2.1.1 Limitations of approach

PRIMET is able to estimate the PECs (Predicted Exposure Concentrations) for watercourses adjacent to the field that is treated with a pesticide.

For the acute risk assessment of aquatic organisms an instantaneous PEC (peak concentration) will be calculated. For chronic risk assessment of aquatic organisms a time weighed average exposure concentration will be calculated. For compounds with K_{oc} larger than 30.000 L/kg PRIMET calculates an unrealistically high PEC because adsorption to sediment is ignored. To limit the number of input parameters, the concept for hydrology is very simple, e.g. residence time is used instead of flow. For a more refined calculation of the PEC the reader is referred to the TOXic substances in Surface WAters (TOXSWA) model (Adriaanse, 1996). The meta-model used by PRIMET is validated by TOXSWA.

2.2.1.2 Steps in calculating the aquatic exposure

To calculate the peak PECs and chronic TWAs five steps have to be done:

1. correct the temperature dependent pesticide parameters, for degradation and for volatilization to the temperature in the scenario;
2. calculate the overall dissipation rate coefficient for the processes degradation, volatilization and dilution;
3. calculate the PEC for a single application;
4. calculate the PEC for multiple applications;
5. calculate the TWA for chronic exposure.

In the following sections the four steps will be discussed.

2.2.1.3 Temperature dependent pesticide parameters

Degradation and volatilization rates of the pesticide from the watercourse are temperature dependent. In this section the methods for correcting the degradation rate, the saturated vapour pressure and the solubility (all needed for volatilization) to the values at the ambient temperature is described.

Degradation rate coefficient

With the Arrhenius equation the degradation rate coefficient at a given temperature T can be calculated from the degradation rate coefficient determined at a reference temperature T_{refkw} using Eq. (1):

$$k_w(T) = k_w(T_{refkw}) \exp \left[\frac{E}{R \cdot T_{refkw} \cdot T} (T - T_{refkw}) \right] \quad (1)$$

with,

- T = ambient temperature in scenario (K)
- T_{refkw} = reference temperature, at which $k_w(T_{refkw})$ or $DT50_{water}$ was determined (K), see Eq. (4)
- $k_w(T)$ = degradation rate coefficient at ambient temperature (1/d)
- $k_w(T_{ref})$ = degradation rate coefficient at reference temperature (1/d)
- E = molar Arrhenius activation energy (constant parameter = 54000 J/mol)
- R = universal gas constant (constant parameter ≈ 8.3144 J/mol*K)

The FOCUS Soil Modelling Workgroup (FOCUS, 1997) found an average value for the molar Arrhenius activation energy (E) of 54 kJ/mol (S.D. 15 kJ/mol). This was calculated from the results of about 50 experiments covering a range of pesticides and soils. The whole range covered 20 to 100 kJ/mol. Note that all evidence for the applicability of Eq. (1) and all values for E were determined for the soil compartment not for the aquatic compartment. In surface waters additional processes as photolysis may occur and in sediments anaerobic conditions may affect microbial degradation in an indirect way. Since $k_w(T)$ is determined in a water-sediment study that incorporates all degradation processes this does not lead to an underestimation of the loss processes.

Saturated vapour pressure

The dependency of the saturated vapour pressure on the temperature is derived using the Van 't Hoff equation:

$$VP(T) = VP(T_{ref}) \exp \left[-\frac{\Delta H_p}{R} \left(\frac{1}{T} - \frac{1}{T_{refVP}} \right) \right] \quad (2)$$

(Van den Berg and Boesten, 1998) with,

- T = ambient temperature in scenario (K)
- T_{refVP} = reference temperature, at which VP was determined (K)
- $VP(T)$ = saturated vapour pressure of substance at ambient temperature (mPa)
- $VP(T_{ref})$ = saturated vapour pressure of substance at reference temperature (mPa)
- ΔH_p = enthalpy of vaporization (constant parameter = 95000 J/mol)
- R = universal gas constant (constant parameter ≈ 8.3144 J/mol*K)

The enthalpy of vaporization is substance dependent. Smit et al. (1997) estimated an average enthalpy of vaporization of 95 kJ/mol from available literature data on 16 pesticides (range: 58 to 146 kJ/mol). For most pesticides, the enthalpy of vaporization is not known, so 95 kJ/mol can then be used as the default value.

Solubility

The effect of the temperature difference on the water solubility is also accounted for using the Van 't Hoff equation:

$$SOL(T) = SOL(T_{ref}) \exp \left[-\frac{\Delta H_{sol}}{R} \left(\frac{1}{T} - \frac{1}{T_{refSOL}} \right) \right] \quad (3)$$

(Van den Berg and Boesten, 1998) with,

- T = ambient temperature in scenario (K)
- T_{refSOL} = reference temperature, at which SOL was determined (K)
- $SOL(T)$ = solubility of substance in water at ambient temperature (mg/L)
- $SOL(T_{ref})$ = solubility of substance in water at reference temperature (mg/L)
- ΔH_{sol} = enthalpy of dissolution (constant parameter = 27000 J/mol)
- R = universal gas constant (constant parameter ≈ 8.3144 J/mol*K)

The enthalpy of dissolution is also substance dependent and Bowman and Sans (1985) found a range of -17 to 156 kJ/mol, with an average of 27 kJ/mol. For most pesticides the enthalpy of dissolution is not known, so 27 kJ/mol can then be used as the default value.

2.2.1.4 Calculation of the overall dissipation rate coefficient

The overall dissipation rate of pesticides from the watercourse is the sum of the degradation rate coefficient, the volatilization rate coefficient and the dilution rate coefficient. This coefficient is needed to calculate the loss of pesticide between two

applications. When only one application is considered in the risk assessment this parameter is not needed and the exposure assessment is more simple (2.2.1.5)

Degradation rate

The $DT50_{\text{water}}$ is an input parameter for PRIMET, from which $k_w(T_{\text{ref}})$ can be calculated using Eq. (4):

$$k_w(T_{\text{ref}}) = \frac{\ln(2)}{DT50_{\text{water}}} \quad (4)$$

with,

$k_w(T_{\text{ref}})$ = degradation rate coefficient at reference temperature (1/d)
 $DT50_{\text{water}}$ = half-life for degradation in water (d)

The degradation rate can be adjusted to the ambient temperature using Eq. (1). Degradation in water includes all chemical and biochemical processes in the water layer because the degradation rate should be determined by a water-sediment study that may include a day-night light regime.

Volatilization rate

The volatilisation rate coefficient depends on the properties of the pesticide and ditch. It is calculated by:

$$k_v = \left(\frac{1}{k_l} + \frac{1}{k_g \cdot K_H} \right)^{-1} \cdot \left(\frac{O_x}{A} \right) \quad (5)$$

(Adriaanse et al., 1997) with,

k_v = volatilisation rate coefficient (1/d)
 k_l = exchange coefficient of the pesticide in water (m/d)
 k_g = exchange coefficient of the pesticide in air (m/d)
 K_H = dimensionless Henry coefficient (-)
 O_x = width of the water surface (m)
 A = cross section of water layer (m²)

The width of the water surface and cross section of the water surface can be calculated from the water depth, bottom width and side slope using Eq. (6) and (7):

$$O_x = b + 2 \cdot h \cdot s_1 \quad (6)$$

$$A = b \cdot h + h^2 \cdot s_1 \quad (7)$$

with,

- O_x = width of the water surface (m)
- b = water depth of water body (m)
- b = bottom width of water body (m)
- s_l = side slope, horizontal/vertical (-)
- A = cross section of water layer (m²)

According to Liss and Slater (1974), exchange coefficients of the pesticide in air (kg) and water (kl) can be derived, from

$$k_l = k_{l,CO_2} \cdot \frac{\sqrt{M_{CO_2}}}{\sqrt{M_{pesticide}}} \quad (8)$$

$$k_g = k_{g,H_2O} \cdot \frac{\sqrt{M_{H_2O}}}{\sqrt{M_{pesticide}}} \quad (9)$$

with,

- k_l = exchange coefficient of the pesticide in water (m/d)
- k_{l,CO_2} = exchange coefficient of CO₂ in the liquid phase (Liss and Slater, 1974 estimated a k_{l,CO_2} of 4.8 m/d = constant parameter);
- M_{CO_2} = molecular weight of CO₂ (constant parameter = 44 g/mol)
- $M_{pesticide}$ = molecular weight of the pesticide under investigation (g/mol)
- k_g = exchange coefficient of the pesticide in air (m/d)
- k_{g,H_2O} = exchange coefficient of H₂O in the vapour phase (Liss and Slater, 1974 estimated a k_{l,H_2O} of 720 m/d = constant parameter).
- M_{H_2O} = molecular weight of H₂O (constant parameter = 18 g/mol);

(Adriaanse, 1996; Beltman and Adriaanse, 1999).

The Henry coefficient can be calculated by:

$$K_H = \frac{VP(T) \cdot 0.001 \cdot M_{pesticide}}{R \cdot T \cdot SOL(T)} \quad (10)$$

(Adriaanse, 1996) with,

- K_H = dimensionless Henry coefficient (-)
- $VP(T)$ = saturated vapour pressure of substance at ambient temperature (mPa)
- $M_{pesticide}$ = molecular weight of the pesticide under investigation (g/mol)
- R = universal gas constant (constant parameter ≈ 8.3144 J/mol K)
- T = ambient temperature in scenario (K)
- $SOL(T)$ = solubility of substance in water at ambient temperature (mg/L)
- 0.001 = correction factor to convert from mPa to Pa

If the $SOL(T)$ is calculated using Eq. (3) and O_x and A by Eq. (6) and (7), the Henry coefficient by Eq. (10) and the exchange coefficients by Eq. (8) and (9), the volatilisation rate coefficient can be calculated using Eq. (5).

Dilution rate

The dilution of the pesticide due to water movement can be taken into account. It can be characterized via the residence time of the watercourse using Eq. (11):

$$\tau = \frac{L}{v} \quad (11)$$

with,

$$\begin{aligned} \tau &= \text{residence time (d)} \\ L &= \text{length of the water body (m)} \\ v &= \text{flow velocity (m/d)} \end{aligned}$$

From the residence time the dilution rate coefficient can be calculated using Eq. (12):

$$k_{\tau} = \frac{1}{\tau} \quad (12)$$

with,

$$\begin{aligned} k_{\tau} &= \text{dilution rate coefficient (1/d)} \\ \tau &= \text{residence time (d)} \end{aligned}$$

Total dissipation rate

The overall dissipation rate coefficient k^* can now be calculated using the rate coefficients calculated above by summing them according to Eq. (13):

$$k^* = k_w(T) + k_v + k_{\tau} \quad (13)$$

with,

$$\begin{aligned} k^* &= \text{overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)} \\ k_w(T) &= \text{degradation rate coefficient at ambient temperature (1/d)} \\ k_v &= \text{volatilization rate coefficient (1/d)} \\ k_{\tau} &= \text{dilution rate coefficient (1/d)} \end{aligned}$$

Where the overall half-life DT50* then becomes:

$$DT50^* = \frac{\ln(2)}{k^*} \quad (14)$$

with,

$$\begin{aligned} k^* &= \text{overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)} \\ DT50^* &= \text{overall half-life accounting for degradation, volatilization and dilution (d)} \end{aligned}$$

2.2.1.5 Calculation of peak PEC^1_{water} for one application

The momentary concentration is the concentration in water after the redistribution of the pesticide between water and suspended solids. Firstly, the nominal concentration in the watercourse can be calculated using Eq. (15):

$$c^* = \frac{M \cdot \frac{\%drift - ditch}{100} \cdot 0.1}{V_1} \quad (15)$$

with,

c^* = total mass concentration in water layer ($\text{mg}/\text{m}^3 = \mu\text{g}/\text{L}$)
 M = individual dose applied ($\text{g a.i.}/\text{ha}$)
 $\%drift - ditch$ = percentage of spray drift (default value = 2.77%)
100 = correction factor to convert from percentage to fraction
0.1 = correction factor to convert from g/ha to mg/m^2
 V_1 = ratio between volume of watercourse and surface (m)

The default value for drift is based on the drift value used for non target arthropods (see 2.5.1). The value of 2.77% is applicable if the distance to the ditch is 1 meter.

The ratio between volume and water surface in 1 m length of watercourse is calculated with:

$$V_1 = \frac{b(b + b \cdot s_1) \cdot 1}{(b + 2 \cdot b \cdot s_1) \cdot 1} \quad (16)$$

with:

V_1 = ratio between volume and surface of watercourse (m)
 b = water depth of water body (m)
 b = bottom width of water body (m)
 s_1 = side slope, horizontal/vertical (-)
1 = length of watercourse

Then the momentary concentration of a single application, PEC^d_{water} , of a single application is calculated via:

$$PEC^1_{water} = \frac{c^*}{1 + ss \cdot m_{om,ss} \cdot K_{om}} \quad (17)$$

(Adriaanse, 1996) with,

PEC^d_{water} = momentary water concentration from a single application ($\mu\text{g}/\text{L}$)
 c^* = total mass concentration in water layer ($\mu\text{g}/\text{L}$)
 ss = mass concentration of suspended solids in water (kg/L)
 $m_{om,ss}$ = mass fraction organic matter in suspended solids (g/g)
 K_{om} = sorption coefficient on organic matter (L/kg)

If K_{om} is not available it can be calculated from the more available K_{oc} using Eq. (18):

$$K_{om} = \frac{K_{oc}}{1.724} \quad (18)$$

(FOCUS, 2001) with,

K_{om} = sorption coefficient on organic matter basis (L/kg)
 K_{oc} = sorption coefficient on organic carbon basis (L/kg)

2.2.1.6 Calculation of peak PEC_{water}^n for multiple applications

The PEC from a series of applications with fixed time interval between applications is calculated via:

$$PEC_{water}^n = PEC_{water}^1 \frac{1 - e^{-n \cdot k^* \cdot \Delta t}}{1 - e^{-k^* \cdot \Delta t}} \quad (19)$$

with,

PEC_{water}^1 = momentary water concentration from a single application ($\mu\text{g/L}$)

PEC_{water}^n = momentary water concentration from n applications ($\mu\text{g/L}$)

n = number of applications (-)

k^* = overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)

Δt = time interval between applications (d)

2.2.1.7 Calculation of TWA for chronic exposure

To assess the risks of chronic exposure of aquatic organisms to pesticides the PRIMET tool includes the calculation of Time Weighted Average concentrations. The calculation of exposure concentrations in the assessment of aquatic risk in PRIMET is based on a water body system of a water layer only, linear equilibrium sorption to suspended solids and to aquatic macrophytes, and a total dissipation rate constant accounting for degradation, volatilization and dilution, which is corrected for temperature (see 2.2.1.4).

2.2.1.7.1 TWA concentration of a single application

A pesticide application at $t = 0$, results after instantaneous linear equilibrium sorption to suspended solids and aquatic macrophytes in a Predicted Exposure Concentration PEC_{water}^1 (2.2.1.5). The concentration after the application as a function of time is given by Eq (20):

$$c(t) = PEC_{water}^1 \exp(-k^* t) \quad (20)$$

with:

c = concentration of pesticide dissolved in water ($\mu\text{g/L}$)

t = time (d)

PEC_{water}^1 = momentary water concentration from a single application ($\mu\text{g/L}$)

k^* = overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)

How PEC_{water}^1 and k^* are derived is described in Sections 2.2.1.4 and 2.2.1.5.

The TWA concentration results from integration over $t = 0$ to $t = t_{TWA}$, and division by the length of the TWA period t_{TWA} , giving Eq (21):

$$TWA_t = \frac{PEC_{water}^1}{k^* t_{TWA}} \left[1 - \exp(-k^* t_{TWA}) \right] \quad (21)$$

with:

- TWA_t = Time Weighted Average concentration for period with length t_{TWA} ($\mu\text{g/L}$)
- PEC_{water}^1 = momentary water concentration from a single application ($\mu\text{g/L}$)
- t_{TWA} = length of period for TWA (d)
- k^* = overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)

2.2.1.7.2 TWA concentration of repeated applications

Analytical solutions have been derived using equation (21) for the TWA of a single application and equation (19) for calculation of PEC_{water}^n , the peak concentration after n applications. The parameters that determine the TWA concentration are: the number of applications, the time interval between loadings and the number of applications within the TWA period. Four different situations determining the TWA are discriminated, called Case 1 to Case 4 (see Eq. (22 – 25)). Which case applies should be determined, going from Case 1 tot Case 4.

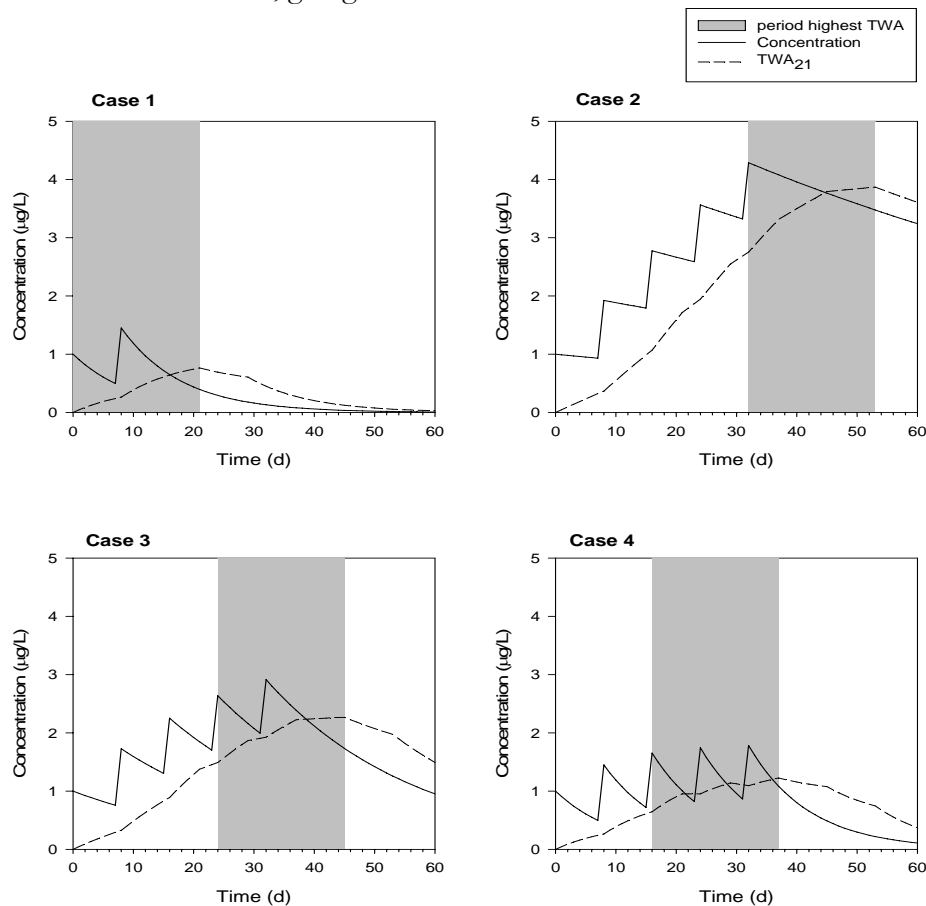


Figure 1 Illustration of case 1 to 4. Concentration and TWA concentration as a function of time for cases as indicated in the graphs. The grey area shows the period over which the maximum TWA concentration was calculated.

Case 1

The period in which the applications occur is shorter than the TWA period
hence $n \cdot \Delta t < t_{TWA}$.

$$TWA_t = \frac{PEC_{water}^1}{k^* t_{TWA}} \left[n - \left(\frac{1 - \exp(nk^* \Delta t)}{1 - \exp(k^* \Delta t)} \right) \exp(-nk^* \Delta t) + \left(\frac{1 - \exp(-nk^* \Delta t)}{1 - \exp(-k^* \Delta t)} \right) \exp(-k^* \Delta t) (1 - \exp(-k^* (t_{TWA} - n\Delta t))) \right] \quad (22)$$

with:

- TWA_t = Time Weighted Average concentration for period with length t_{TWA} (µg/L)
- PEC_{water}^1 = momentary water concentration from a single application (µg/L)
- t_{TWA} = length of period for TWA (d)
- k^* = overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)
- n = number of applications (-)
- Δt = time interval between applications (d)

Case 2

Concentrations in the Δt interval after the final application are all higher than in the period before the final application; $c(t_n + \Delta t) > PEC^{n-1}$. Hence, the condition for use of the Case 2 solution is:

$$(1 - \exp(-nk^* \Delta t)) \exp(-k^* \Delta t) + \exp(-(n-1)k^* \Delta t) > 1 \quad (23)$$

The solution for Case 2 is given by:

$$TWA_t = \frac{PEC_{water}^1}{k^* t_{TWA}} \left[\left(\frac{1 - \exp(-nk^* \Delta t)}{1 - \exp(-k^* \Delta t)} \right) (1 - \exp(-k^* t_{TWA})) \right] \quad (24)$$

Case 3

Concentrations of the final m applications determine the highest TWA;

$c(t = t_{n-m} + \Delta t) < c(t = t_n + \Delta t + t_{rest})$. Hence, the condition for use of the Case 3 solution is:

$$(1 - \exp(-nk^* \Delta t)) \exp(-k^* t_{rest}) + \exp(-(n-m)k^* \Delta t) > 1 \quad (25)$$

The solution for Case 3 is given by:

$$TWA_t = \frac{PEC_{water}^1}{k^* t_{TWA}} \left[m - \left(\frac{1 - \exp(mk^* \Delta t)}{1 - \exp(k^* \Delta t)} \right) \exp(-nk^* \Delta t) + \right. \\ \left. + \left(\frac{1 - \exp(-nk^* \Delta t)}{1 - \exp(-k^* \Delta t)} \right) \exp(-k^* \Delta t) (1 - \exp(-k^* t_{rest})) \right] \quad (26)$$

m = whole number of application intervals within TWA period (-)
 t_{rest} = time remaining from TWA period ($= t_{TWA} - m \cdot \Delta t$) (d)

Case 4

Concentrations of the final $m+1$ applications determine the highest TWA; $PEC^{n-m-1} > c(t = t_n + t_{rest})$. Hence, the condition for use of the Case 4 solution is:

$$(1 - \exp(-nk^* \Delta t)) \exp(-k^* t_{rest}) + \exp(-(n-m)k^* \Delta t) < 1 \quad (27)$$

The solution for Case 4 is given by:

$$TWA_t = \frac{PEC_{water}^1}{k^* t_{TWA}} \left[m - \left(\frac{1 - \exp(mk^* \Delta t)}{1 - \exp(k^* \Delta t)} \right) \exp(-(n-1)k^* \Delta t) + \right. \\ \left. + \left(\frac{1 - \exp(-nk^* \Delta t)}{1 - \exp(-k^* \Delta t)} \right) (1 - \exp(-k^* t_{rest})) \right] \quad (28)$$

2.2.2 Aquatic effect assessment

For the effect assessment a “safe” concentration is calculated from toxicity values for some standard test species and an extrapolation factor. The toxicity values are gathered for a limited number of “standard” species, viz., an alga, *Daphnia* and fish. These species have been chosen because of their ease of handling and rearing in the laboratory. Their test procedures are highly protocolised and well described in, for instance, OECD guidelines (Organisation for Economic Co-operation and Development; OECD, 1993). The standard test species are regarded as convenient surrogates for sensitive indigenous species of aquatic ecosystems, despite a general awareness of the uncertainty associated with the extrapolation from one species to another. To protect sensitive indigenous aquatic populations, the NEC is usually calculated by multiplying the toxicity value of the most sensitive standard test species by an extrapolation factor (e.g. EU, 1997).

To establish the size of the extrapolation factor, a number of uncertainties must be addressed to extrapolate from single-species laboratory data to a multi-species ecosystem. These uncertainties include:

- extrapolation from 50% effect to no effect;
- intra- and inter- species variation (biological variance);
- laboratory data to field impact extrapolations.

2.2.2.1 Effect assessment acute exposure

The acute No Effect Concentration is calculated using:

$$NEC_{water-acute} = \text{lowest value of:} \\ EF_{water, acute-fish} * (\text{lowest value of: LC50 or EC50 fish}) * 1000 \\ EF_{water, acute-Daphnia} * (\text{lowest value of: LC50 or EC50 } Daphnia) * 1000 \quad (29) \\ EF_{water, acute-algae} * (EC50 algae) * 1000$$

with,

$NEC_{water-acute}$ = Acute No Effect Concentration for the water compartment ($\mu\text{g/L}$)

LC50 fish = concentration that kills 50% of the test organisms, fish (mg/L)

LC50 *Daphnia* = concentration that kills 50% of the test organisms, *Daphnia* (mg/L)

EC50 fish = concentration that affects 50% of the test organisms, fish (immobilisation in mg/L)

EC50 *Daphnia* = concentration that affects 50% of the test organisms, *Daphnia* (immobilisation in mg/L)

EC50 algae = concentration that affects 50% of the test organisms, algae (growth inhibition in mg/L)

$EF_{water, acute-fish}$ = extrapolation factor for acute effect assessment of fish (default value = 0.01)

$EF_{water, acute-Daphnia}$ = extrapolation factor for acute effect assessment of *Daphnia* (default value = 0.01)

$EF_{water, acute-algae}$ = extrapolation factor for acute effect assessment of algae (default value = 0.1)

1000 = factor to correct from mg/L to $\mu\text{g/L}$

The extrapolation factors are corresponding with the Plant Protection Products Directive (91/414/EEC). See also the Guidance Document on Aquatic Ecotoxicology in the context of Directive 91/414/EEC. Sanco/3268/2001 rev.

2.2.2.2 Effect assessment chronic exposure

The chronic No Effect Concentration for fish and daphnia is calculated using:

$$NEC_{water-chronic-fish} = EF_{water, chronic-fish} * NOEC_{fish} * 1000 \quad (30a)$$

$$NEC_{water-chronic-Daphnia} = EF_{water, chronic-Daphnia} * NOEC_{Daphnia} * 1000 \quad (30b)$$

with,

$NEC_{water-chronic-fish}$ = Chronic No Effect Concentration for the fish (µg/L)

$NEC_{water-chronic-Daphnia}$ = Chronic No Effect Concentration for *Daphnia* (µg/L)

$NOEC_{fish}$ = No Observed Effect Concentration of fish (mg/L)

$NOEC_{Daphnia}$ = No Observed Effect Concentration of *Daphnia* (mg/L)

$EF_{water, chronic-fish}$ = extrapolation factor for chronic effect assessment of fish (default value = 0.1)

$EF_{water, chronic-Daphnia}$ = extrapolation factor for chronic effect assessment of *Daphnia* (default value = 0.1)

1000 = factor to correct from mg/L to µg/L

The extrapolation factors are corresponding with the Plant Protection Products Directive (91/414/EEC). See also the Guidance Document on Aquatic Ecotoxicology in the context of Directive 91/414/EEC. Sanco/3268/2001 rev.

2.2.3 Aquatic risk assessment

2.2.3.1 Acute aquatic risk assessment

The risk, expressed in Exposure Toxicity Ratio ($ETR^n_{water-acute}$) as a result of n applications is:

$$ETR^n_{water-acute} = PEC^n_{water} / NEC_{water-acute} \quad (31)$$

$ETR^n_{water-acute}$ = Acute Exposure Toxicity Ratio due to n applications (-)

PEC^n_{water} = momentary peak water concentration from n applications (µg/L)

$NEC_{water-acute}$ = No Acute Effect Concentration for the water compartment (µg/L)

If:	$ETR^n_{water-acute} < 1$	No Risk	(indicated by a green colour)
	$1 \leq ETR^n_{water-acute} \leq 100$	Possible risk	(indicated by a orange colour)
	$ETR^n_{water-acute} > 100$	Risk	(indicated by a red colour)

2.2.3.2 Chronic aquatic risk assessment

The risk, expressed in Exposure Toxicity Ratio ($ETR^n_{\text{water-chronic}}$) as a result of n applications is:

$$ETR^n_{\text{water-chronic}} = \text{lowest value of:}$$

$$\begin{aligned} ETR^n_{\text{water-chronic-fish}} &= TW A_{\text{fish}} / NEC_{\text{water-chronic-fish}} & (32 \text{ a}) \\ ETR^n_{\text{water-chronic-Daphnia}} &= WA_{\text{Daphnia}} / NEC_{\text{water-chronic-Daphnia}} & (32 \text{ b}) \end{aligned}$$

$ETR^n_{\text{water-chronic}}$	= Chronic Exposure Toxicity Ratio due to n applications (-)
$ETR^n_{\text{water-chronic-fish}}$	= Chronic Exposure Toxicity Ratio for fish due to n applications (-)
$ETR^n_{\text{water-chronic-Daphnia}}$	= Chronic Exposure Toxicity Ratio for <i>Daphnia</i> due to n applications (-)
$TW A_{\text{fish}}$	= Time Weighted Average concentration for fish (default period of length = 28 days (µg/L))
$TW A_{\text{Daphnia}}$	= Time Weighted Average concentration for <i>Daphnia</i> (default period of length = 21 days (µg/L))
$NEC_{\text{water-chronic-fish}}$	= Chronic No Effect Concentration for fish (µg/L)
$NEC_{\text{water-chronic-Daphnia}}$	= Chronic No Effect Concentration for <i>Daphnia</i> (µg/L)
If: $ETR^n_{\text{water-chronic}} < 1$	No Risk (indicated by a green colour)
$1 \leq ETR^n_{\text{water-chronic}} \leq 100$	Possible risk (indicated by a orange colour)
$ETR^n_{\text{water-chronic}} > 100$	Risk (indicated by a red colour)

2.2.4 List of parameters needed for the aquatic risk assessment

2.2.4.1 Input scenario parameters

T	= ambient temperature in scenario (K)
L	= length of the water body (m)
v	= flow velocity (m/d)
h	= water depth of water body (m)
b	= bottom width of water body (m)
s_1	= side slope, horizontal/vertical (-)
ss	= mass concentration of suspended solids in water (kg/L)
$m_{\text{om,ss}}$	= mass fraction organic matter in suspended solids (g/g)
$EF_{\text{water, acute-fish}}$	= extrapolation factor for acute effect assessment of fish (default value = 0.01)
$EF_{\text{water, acute-Daphnia}}$	= extrapolation factor for acute effect assessment of <i>Daphnia</i> (default value = 0.01)
$EF_{\text{water, acute-algae}}$	= extrapolation factor for acute effect assessment of algae (default value = 0.1)
$EF_{\text{water, chronic-fish}}$	= extrapolation factor for chronic effect assessment of fish (default value = 0.1)

$EF_{\text{water, chronic-Daphnia}}$ = extrapolation factor for chronic effect assessment of *Daphnia* (default value = 0.1)

2.2.4.2 Input pesticide parameters

T_{refkw}	= reference temperature, at which $K_w(T_{ref})$ or $DT50_{\text{water}}$ was determined (K)
T_{refVP}	= reference temperature, at which VP was determined (K)
T_{refSOL}	= reference temperature, at which SOL was determined (K)
$VP(T_{ref})$	= saturated vapour pressure of substance at reference temperature (Pa)
$SOL(T_{ref})$	= solubility of substance in water at reference temperature (g/m^3)
$DT50_{\text{water}}$	= half-life for degradation in water (d)
$M_{\text{pesticide}}$	= molecular weight of the pesticide under investigation (g/mol)
K_{om}	= sorption coefficient organic matter (L/kg). Not needed if K_{oc} is available
K_{oc}	= sorption coefficient on organic carbon (L/kg). Not needed if K_{om} is available
LC50 fish	= concentration that kills 50% of the test organisms, fish (mg/L)
LC50 <i>Daphnia</i>	= concentration that kills 50% of the test organisms, <i>Daphnia</i> (mg/L)
EC50 fish	= concentration that affects 50% of the test organisms, fish (immobilisation in mg/L)
EC50 <i>Daphnia</i>	= concentration that affects 50% of the test organisms, <i>Daphnia</i> (immobilisation in mg/L)
EC50 algae	= concentration that affects 50% of the test organisms, algae (growth inhibition in mg/L)
NOEC fish	= No Observed Effect Concentration of fish (mg/L)
NOEC <i>Daphnia</i>	= No Observed Effect Concentration of <i>Daphnia</i> (mg/L)

2.2.4.3 Input pesticide application parameters

M	= individual dose applied ($\text{g a.i.}/\text{ha}$)
$\%drift - ditch$	= percentage of spray drift (%)
n	= number of applications (-)
Δt	= time interval between applications (d)

2.2.4.4 Constant parameters

E	= molar Arrhenius activation energy (= 54000 J/mol)
R	= universal gas constant ($\approx 8.3144 \text{ J}/\text{mol}\cdot\text{K}$)
ΔH_p	= enthalpy of vaporization (= 95000 J/mol)
ΔH_{sol}	= enthalpy of dissolution (= 27000 J/mol)
k_{i,CO_2}	= exchange coefficient of CO_2 in the liquid phase (= 4.8 m/d);

M_{CO_2}	= molecular weight of CO ₂ (= 44 g/mol)
k_{g,H_2O}	= exchange coefficient of H ₂ O in the vapour phase (= 720 m/d).
M_{H_2O}	= molecular weight of H ₂ O (= 18 g/mol);

2.2.4.5 Calculated parameters

$k_w(T_{ref})$	= degradation rate coefficient at reference temperature (1/d)
$VP(T)$	= saturated vapour pressure of substance at ambient temperature (Pa)
$k_w(T)$	= degradation rate coefficient at ambient temperature (1/d)
$SOL(T)$	= solubility of substance in water at ambient temperature (g/m ³)
k_v	= volatilisation rate coefficient (1/d)
O_x	= width of the water surface (m)
A	= cross section of water layer (m ²)
k_l	= exchange coefficient of the pesticide in water (m/d)
k_g	= exchange coefficient of the pesticide in air (m/d)
K_H	= dimensionless Henry coefficient (-)
τ	= residence time (d)
k_τ	= dilution rate coefficient (1/d)
k^*	= overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)
$DT50^*$	= overall half-life accounting for degradation, volatilization and dilution (d)
c^*	= total mass concentration in water layer (mg/m ³ = µg/L)
c	= concentration of pesticide dissolved in water (µg/L)
V_l	= ratio between volume and surface of watercourse (m)
K_{om}	= sorption coefficient on organic matter (L/kg). Only when K_{oc} is available
PEC^1_{water}	= momentary peak water concentration from a single application (µg/L)
PEC^n_{water}	= momentary water concentration from n applications (µg/L)
TWA_t	= Time Weighted Average concentration for period with length t_{TWA} (µg/L)
TWA_{fish}	= Time Weighted Average concentration for fish (default period of length = 28 days (µg/L)
$TWA_{Daphnia}$	= Time Weighted Average concentration for <i>Daphnia</i> (default period of length = 21 days (µg/L)
t_{TWA}	= length of period for TWA (d)
m	= whole number of application intervals within TWA period (-)
t_{rest}	= time remaining from TWA period (= $t_{TWA} - m \cdot \Delta t$) (d)
$NEC_{water-acute}$	= Acute No Effect Concentration for the water compartment (µg/L)
$NEC_{water-chronic-fish}$	= Chronic No Effect Concentration for fish (µg/L)
$NEC_{water-chronic-daphnia}$	= Chronic No Effect Concentration for <i>Daphnia</i> (µg/L)
$ETR^n_{water-acute}$	= Acute Exposure Toxicity Ratio due to n applications (-)

$ETR_{water-chronib}^n$	= Chronic Exposure Toxicity Ratio due to n applications (-)
$ETR_{water-chronic-fish}^n$	= Chronic Exposure Toxicity Ratio for fish due to n applications (-)
$ETR_{water-chronic-daphnia}^n$	= Chronic Exposure Toxicity Ratio for <i>Daphnia</i> due to n applications (-)

2.3 Terrestrial risk assessment for earthworms

2.3.1 Terrestrial exposure assessment for earthworms

The concentration for the within field soil compartment is calculated from the dose of the pesticide divided by the amount of soil (kg) in the upper part of the soil (default depth of upper part of the soil = 0.05 m).

$$C_{soil} = \frac{0.1 \cdot M}{DEPTH} \quad (33)$$

with,

C_{soil}	= concentration in the upper part of the soil (default depth of upper part of the soil = 0.05 m, in mg pesticide/m ³ soil)
0.1	= correction factor to convert from g/ha to mg/m ²
M	= individual dose applied (g a.i./ha)
DEPTH	= depth of the field (default value = 0.05 m)

The Predicted Environmental Concentration (PEC_{soil}^1) for the soil compartment after one application is:

$$PEC_{soil}^1 = \frac{C_{soil}}{\rho_b \cdot 1000} \quad (34)$$

with,

PEC_{soil}^1	= concentration in the upper part of the soil from one application (default depth of upper part of the soil = 0.05 m, in mg pesticide/kg soil)
C_{soil}	= concentration in the upper part of the soil (default depth of upper part of the soil = 0.05 m, in mg pesticide/m ³ soil)
ρ_b	= dry bulk density soil (default value = 1.0 kg/dm ³)
1000	= factor to convert from kg/dm ³ to kg/m ³

The realistic worst case bulk dry density for an average soil is 1.0 kg/ dm³. This value can be used as a default value, but is not applicable for peat soils (bulk dry density for peat soil = 0.25 kg / dm³). If measured values for bulk dry densities are available these values can be used to calculate the PEC_{soil}^1 .

The PEC from a series of n applications with fixed time interval between applications is calculated using (FOCUS Soil Modeling Workgroup,1997):

$$PEC_{soil}^n = PEC_{soil}^1 \frac{1 - e^{-n \cdot k_d \cdot \Delta t}}{1 - e^{-k_d \cdot \Delta t}} \quad (35)$$

with,

PEC_{soil}^n = concentration in the upper part of the soil from n applications (default depth of upper part of the soil = 0.05 m, in mg pesticide/kg soil)

n = number of applications (-)

k_s = degradation rate coefficient in soil (1/d), where $k_s = \ln(2)/DT50_{soil}$

Δt = time interval between applications (d)

2.3.2 Terrestrial effect assessment for earthworms

For the effect assessment a “safe” concentration is calculated from toxicity values and, in case of earthworms, an extrapolation factor (EU, 1997). To establish the size of the extrapolation factor, a number of uncertainties must be addressed to extrapolate from single-species laboratory data to a multi-species ecosystem. These uncertainties include:

- intra- and inter- laboratory variation of toxicity data;
- intra- and inter- species variation (biological variance);
- laboratory data to field impact extrapolations.

2.3.2.1 Effect assessment acute exposure

The acute No Effect Concentration is calculated using:

$$NEC_{soil-acute} = EF_{soil-acute} * LC50_{earthworms} \quad (36)$$

with,

$NEC_{soil-acute}$ = No Acute Effect Concentration for the soil compartment (mg/kg)

$LC50_{earthworms}$ = concentration that kills 50% of the test organisms, earthworms (mg/kg)

$EF_{soil-acute}$ = extrapolation factor for acute effect assessment of earthworms (default value = 0.1)

The extrapolation factor is corresponding with the Plant Protection Products Directive (91/414/EEC). For more information see also the Guidance Document on Terrestrial Ecotoxicology under Council Directive 91/414/EEC (SANCO/10329/2002 rev. 2 final - noted by the SCFA on 18 October 2002).

2.3.2.2 Effect assessment chronic exposure

The chronic No Effect Concentration is calculated using:

$$NEC_{soil-chronic} = EF_{soil-chronic} * NOEC_{earthworms} \quad (37)$$

with,

$NEC_{soil-chronic}$ = No Chronic Effect Concentration for the soil compartment (mg/kg)

NOEC_{earthworms} = No observed effect concentration of earthworms (mg/kg)
 EF_{soil-chronic} = extrapolation factor for chronic effect assessment of earthworms
 (default value = 0.2)

The extrapolation factor is corresponding with the Plant Protection Products Directive (91/414/EEC). For more information see also the Guidance Document on Terrestrial Ecotoxicology under Council Directive 91/414/EEC (SANCO/10329/2002 rev. 2 final - noted by the SCFA on 18 October 2002).

2.3.3 Terrestrial risk assessment for earthworms

2.3.3.1 Acute terrestrial risk assessment to earthworms

The risk, expressed in Exposure Toxicity Ratio (ETR_{soil-acute}) as a result of all stacked applications is:

$$ETR_{soil-acute} = PEC_{soil}^n / NEC_{soil-acute} \quad (38)$$

with,

ETR_{soil-acute} = Acute Exposure Toxicity Ratio due to *n* applications (-)

PEC_{soil}ⁿ = concentration in the upper part of the soil from *n* applications
 (default depth of upper part of the soil = 0.05 m, in mg pesticide/kg soil)

NEC_{soil-acute} = No Acute Effect Concentration for the soil compartment (mg/kg)

If:	$ETR_{soil-acute} < 1$	No Risk	(indicated by a green colour)
	$1 \leq ETR_{soil-acute} \leq 100$	Possible risk	(indicated by a orange colour)
	$ETR_{soil-acute} > 100$	Risk	(indicated by a red colour)

2.3.3.2 Chronic terrestrial risk assessment to earthworms

The risk, expressed in Exposure Toxicity Ratio (ETR_{soil-chronic}) as a result of all stacked applications is:

$$ETR_{soil-chronic} = PEC_{soil}^n / NEC_{soil-chronic} \quad (39)$$

with,

ETR_{soil-chronic} = Chronic Exposure Toxicity Ratio due to *n* applications (-)

PEC_{soil}ⁿ = concentration in the upper part of the soil from *n* applications
 (default depth of upper part of the soil = 0.05 m, in mg pesticide/kg soil)

NEC_{soil-chronic} = No Chronic Effect Concentration for the soil compartment
 (mg/kg)

If:	$ETR_{soil-chronic} < 1$	No Risk	(indicated by a green colour)
	$1 \leq ETR_{soil-chronic} \leq 100$	Possible risk	(indicated by a orange colour)

$$ETR_{\text{soil-chronic}} > 100 \quad \text{Risk} \quad (\text{indicated by a red colour})$$

Since the chronic toxicity tests for earthworms are static tests the acute PEC_{soil}^n will be used to calculate the chronic risk to earthworms.

2.3.4 List of parameters needed for the terrestrial risk assessment

2.3.4.1 Input scenario parameters

ρ_b	= dry bulk density soil (kg soil/dm ³ soil)
DEPTH	= depth of the field (default value = 0.05 m)
$EF_{\text{soil-acute}}$	= extrapolation factor for acute effect assessment of earthworms (default value = 0.1)
$EF_{\text{soil-chronic}}$	= extrapolation factor for chronic effect assessment of earthworms (default value = 0.2)

2.3.4.2 Input pesticide parameters

$LC50_{\text{earthworms}}$	= concentration that kills 50% of earthworms (mg/kg)
$NOEC_{\text{earthworms}}$	= No observed effect concentration of earthworms (mg/kg)
$DT50_{\text{soil}}$	= half life for degradation in soil (d)

2.3.4.3 Input pesticide application parameters

M	= individual dose applied (g a.i. /ha)
n	= number of applications (-)
Δt	= time interval between applications (d)

2.3.4.4 Constant parameters

0.1	= correction factor to convert from g/ha to mg/m ² .
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2.3.4.5 Calculated parameters

C_{soil}	= concentration in the upper part of the soil (default depth of the upper part of the soil = 0.05 m, in mg pesticide/m ³ soil)
k_s	= degradation rate coefficient in soil (1/d), where $k_s = \ln(2)/DT50_{\text{soil}}$
PEC_{soil}^1	= concentration in the upper part of the soil from one application (default depth of upper part of the soil = 0.05 m, in mg pesticide/kg soil)
PEC_{soil}^n	= concentration in the upper part of the soil from n applications (default depth of upper part of the soil = 0.05 m, in mg pesticide/kg soil)

$NEC_{soil-acute}$	= No Acute Effect Concentration for the soil compartment (mg/kg)
$NEC_{soil-chronic}$	= No Chronic Effect Concentration for the soil compartment (mg/kg)
$ETR_{soil-acute}$	= Acute Exposure Toxicity Ratio due to n applications (-)
$ETR_{soil-chronic}$	= Chronic Exposure Toxicity Ratio due to n applications (-)

2.4 Risk assessment for bees

2.4.1 Exposure assessment for bees

For products applied as sprays, exposure should be established as the maximum single application rate expressed as gram active ingredient per hectare (g a.i./ha).

$$PEC_{bee} = M \quad (40)$$

PEC_{bee}	= exposure concentration to bees
M	= individual dose applied (g a.i./ha)

2.4.2 Effect assessment for bees

For the effect assessment a “safe” concentration is calculated from toxicity values and, in case of bees, an assessment correction factor (to convert from µg/bee to g/ha).

The No Effect Concentration for bees is calculated using:

$$NEC_{bee} = EF_{bee} * LD50_{bee} \quad (41)$$

with,	
NEC_{bee}	= No effect concentration for bees (g/ha)
$LD50_{bee}$	= concentration (oral or contact) that kills 50% of bees (µg/bee), the most sensitive endpoint of oral LD50 and contact LD50.
EF_{bee}	= extrapolation correction factor for effect assessment of bees, to convert from µg/bee to g/ha (default value = 50).

The extrapolation correction factor is corresponding with the Plant Protection Products Directive (91/414/EEC). For more information see also the Guidance Document on Terrestrial Ecotoxicology under Council Directive 91/414/EEC and EPPO 2002b: Environmental risk assessment scheme for plant protection products, Chapter 11. Honeybees. In EPPO 2002b the extrapolation correction factor of 50 was validated against incidents.

2.4.3 Risk assessment for bees

The risk, expressed in Exposure Toxicity Ratio (ETR_{bee}) as a result of applications is:

$$ETR_{bee} = PEC_{bee} / NEC_{bee} \quad (42)$$

with,

ETR_{bee} = Exposure Toxicity Ratio due to application (-)

PEC_{bee} = exposure concentration to bees = individual dose applied (g/ha).

NEC_{bee} = No Effect Concentration for bees (g/ha)

If: $ETR_{bee} < 1$	No Risk	(indicated by a green colour)
$1 \leq ETR_{bee} \leq 100$	Possible risk	(indicated by a orange colour)
$ETR_{bee} > 100$	Risk	(indicated by a red colour)

2.4.4 List of parameters needed for the risk assessment for bees

2.4.4.1 Input scenario parameters

EF_{bee} = extrapolation correction factor for effect assessment of bees, to convert from $\mu\text{g}/\text{bee}$ to g/ha (default value = 50).

2.4.4.2 Input pesticide parameters

$LD50_{bee}$ = concentration that kills 50% of bees ($\mu\text{g}/\text{bee}$), the most sensitive endpoint of oral LD50 and contact LD50.

2.4.4.3 Input pesticide application parameters

M = individual dose applied (g a.i. /ha)

2.4.4.4 Constant parameters

No data.

2.4.4.5 Calculated parameters

PEC_{bee} = exposure concentration to bees = individual dose applied (g a.i./ha)

ETR_{bee} = Exposure Toxicity Ratio due to application (-)

NEC_{bee} = No Effect Concentration for bees (g/ha)

2.5 Risk assessment for non target arthropods

In this version of PRIMET the risk assessment for non target arthropods will be performed for the EU standard species. These standard species include two sensitive indicator species, the cereal aphid parasitoid *Aphidius rhopalosiphi* and the predatory mite *Typhlodromus pyri*. The selection of these indicator species was based on a sensitivity analyses of available test species and associated laboratory test methods performed by Beneficial Arthropod Regulatory Testing Group (Candolfi et al. 1999) and International Organisation for Biological and Integrated Control of Noxious Animals and Plants (IOBC, Vogt 2000). The standard species are only suitable for risk assessment of formulations that are sprayed on the fields.

2.5.1 Exposure assessment for non target arthropods

The following equations are used to describe the exposure in-field and off-field. For both exposures, the key input is the nominal field application rate:

$$PEC(in-field) = M * MAF. \quad (43)$$

$$PEC(off-field) = M * MAF * (\%drift / 100 / veg) \quad (44)$$

with,

$PEC(in-field)$ = exposure in-field (g a.i./ha)

$PEC(off-field)$ = exposure off-field (g a.i./ha)

M = individual dose applied (g a.i./ha)

MAF = Multiple Application Factor (-)

% drift = percentage of drift spray (default value = 2.77%)

100 = factor to convert from % drift to drift factor

veg = vegetation distribution factor (default value = 10)

The MAF depends on the number of application (n) and is provided in Table 1:

Table 1: MAF after n applications (default values for leaf dwelling arthropods)

n applications	1	2	3	4	5	6	7	8	> 8
MAF after n applications	1.0	1.7	2.3	2.7	3.0	3.2	3.4	3.5	3.5

The Multiple Application Factor, the drift factor and the vegetation distribution factor are corresponding with the values used in EU (SANCO/10329/2002) and mentioned in SETAC (ESCORT 2 workshop) the drift factor is based on the tables published by Rautmann et al (2001). The standard assessment could be conducted for 1 meter distance with a default value of 0.0277.

2.5.2 Effect assessment for non target arthropods

For the effect assessment a “safe” concentration is calculated from toxicity values and an extrapolation factor. In case of non target arthropods the Acceptable Effect

Concentration will be used in stead of the No Effect Concentration. This is because some effects are considered acceptable in accordance SANCO/10329/2002. The Acceptable Effect Concentration is calculated using:

$$AEC_{NTA} = EF_{NTA} * LR50_{NTA} \quad (45)$$

with,

AEC_{NTA} = Acceptable effect concentration for Non Target Arthropods (g a.i./ha)

$LR50_{NTA}$ = Rate that kills 50% of *Typhlodromus pyri* or *Aphidius rhopalosiphi*, the most sensitive endpoint of the two organisms will be taken.

EF_{NTA} = extrapolation factor for effect assessment of Non Target Arthropods

The extrapolation factor is based on available (semi) field data where lethal, sub lethal and reproduction endpoints have been measured for a considerable number of types of substances and species. This means that this risk assessment (in which the extrapolation factor of 2 is applied) also covers sub lethal and reproduction effects and it is not necessary to separately consider sub lethal and reproduction endpoints in the risk assessment.

2.5.3 Risk assessment for non target arthropods

Version 2.0 of PRIMET makes a distinction between the risk assessment of non target arthropods in the field and out of the field (in-field and off-field). For both risk assessment (in-field and off-field) the same criteria are used.

In EU legislation different criteria will be used in higher tier risk assessment. The criterion for potential recovery or recolonisation for 'in-field' is that this must be the case before the following spraying season. The period for 'off-field' is shorter, for the time being without a specific definition. SANCO/10329/2002 mentions an ecologically relevant period. Higher tier risk assessment of NTA is not taken into account in Version 2.0 of PRIMET.

2.5.3.1 Risk assessment for non target arthropods, in-field

The risk, expressed in Exposure Toxicity Ratio ($ETR(in-field)$) as a result of applications is:

$$ETR_{NTA}(in-field) = PEC_{infield} / AEC_{NTA} \quad (46)$$

with,

$ETR(in-field)$ = Exposure Toxicity Ratio in-field due to application (-)

$PEC(in-field)$ = exposure in-field (g a.i./ha)

AEC_{NTA} = Acceptable Effect Concentration to *Typhlodromus pyri* and *Aphidius rhopalosiphi* (g/ha)

If:	$ETR_{NTAI}(in-field) < 1$	No Risk	(indicated by a green colour)
	$1 \leq ETR_{NTAI}(in-field) \leq 100$	Possible risk	(indicated by a orange colour)
	$ETR_{NTAI}(in-field) > 100$	Risk	(indicated by a red colour)

2.5.3.2 Risk assessment for non target arthropods, off-field

The risk, expressed in Exposure Toxicity Ratio ($ETR(off-field)$) as a result of applications is:

$$ETR_{NTAI}(off-field) = PEC_{off-field} / AEC_{NTAI} \quad (47)$$

with,

$ETR(off-field)$ = Exposure Toxicity Ratio off-field due to application (-)

$PEC(off-field)$ = exposure off-field (g a.i./ha)

AEC_{NTAI} = Acceptable Effect Concentration to *Typhlodromus pyri* and *Aphidius rhopalosiphii* (g/ha)

If:	$ETR_{NTAI}(off-field) < 1$	No Risk	(indicated by a green colour)
	$1 \leq ETR_{NTAI}(off-field) \leq 100$	Possible risk	(indicated by a orange colour)
	$ETR_{NTAI}(off-field) > 100$	Risk	(indicated by a red colour)

2.5.4 List of parameters needed for the risk assessment for non target arthropods

2.5.4.1 Input scenario parameters

veg = vegetation distribution factor (default value = 10)

EF_{NTAI} = extrapolation factor for effect assessment of non target arthropods (default value = 2)

2.5.4.2 Input pesticide parameters

$LR50_{NTAI}$ = Rate that kills 50% of *Typhlodromus pyri* or *Aphidius rhopalosiphii*, the most sensitive endpoint of the two organisms will be taken.

2.5.4.3 Input pesticide application parameters

M = individual dose applied (g a.i./ha)

drift factor = drift factor = (% drift / 100) (default value = 0.0277)

n = number of applications (-)

2.5.4.4 Constant parameters

MAF = Multiple Application Factor (-) (see table 1)

2.5.4.5 Calculated parameters

$PEC(in-field)$ = exposure in-field (g a.i./ha)
 $PEC(off-field)$ = exposure off-field (g a.i./ha)
 AEC_{NTA} = Acceptable effect concentration for *Typhlodromus pyri* and *Aphidius rhopalosiphii* (g a.i./ha)
 $ETR_{NTA}(in-field)$ = Exposure Toxicity Ratio in-field due to application (-)
 $ETR_{NTA}(off-field)$ = Exposure Toxicity Ratio off-field due to application (-)

2.6 Groundwater risk assessment

2.6.1 Groundwater exposure assessment

To estimate the leaching of pesticides to the groundwater a meta-model of the spatially distributed European pesticide leaching model EuroPEARL is incorporated into version 2.0 of PRIMET. EuroPEARL consists of a link between the one-dimensional, multi-layer, mechanistic pesticide leaching model PEARL and a Geographical Information System. EuroPEARL considers transient flow and solute transport and assumes Freundlich adsorption, first-order degradation and passive plant uptake of pesticides. Physical parameters are depth dependent while (bio)-chemical parameters are depth, temperature, and moisture dependent. The meta-model (Tiktak et al. 2006) is based on an analytical expression that describes the mass fraction of pesticide leached. The meta-model ignores vertical parameter variations and assumes steady state flow. The meta-model is based on simulations in which the pesticide is applied each year.

The 80th percentile of the leaching concentration at 1-m depth, the predicted environmental concentration (PEC) can be derived using equation (52). The meta-model estimates the predicted environmental concentration (PEC) for an standard application of 1 kg a.i./ha and is not calibrated to estimate the PEC at other depths than 1-m.

$$\ln PEC_{gw(1\text{ kg/ha})} = (\alpha_0 - \alpha_1 X_1 - \alpha_2 X_2) \quad (48)$$

(Tiktak et al., 2006) with,

$PEC_{gw(1\text{ kg/ha})}$ = Predicted Environmental Concentration, annual average concentration leaching from the soil profile at 1 m depth ($\mu\text{g/L}$)
 α_0, α_1 and α_2 = regression coefficients which can be derived from table 2
 X_1 and X_2 = independent regression variables (-)

X1 is defined as follows:

$$X1 = k_s \Theta D_{gw} / q \quad (49)$$

with,

$$\begin{aligned} k_s &= \text{degradation rate coefficient in soil (1/d)} \\ \Theta &= \text{volume fraction of water (default value} = 0.25 \text{ m}^3/\text{m}^3) \\ D_{gw} &= \text{depth ground water (default value} = 1 \text{ m)} \\ q &= \text{volume flux of water (m/d)} \end{aligned}$$

where:

$$k_s = \ln(2) / DT50_{soil} \quad (50)$$

with,

$$\begin{aligned} k_s &= \text{degradation rate coefficient in soil (1/d)} \\ DT50_{soil} &= \text{half-life in soil (d) due to degradation} \end{aligned}$$

where:

$$q = (-0.2849 / 365) + (0.8634 \text{ Pr} / 365) \quad (51)$$

with,

$$\begin{aligned} q &= \text{volume flux of water (m/d)} \\ \text{Pr} &= \text{mean annual precipitation (m/yr)} \end{aligned}$$

X2 is defined as follows:

$$X2 = k_s \rho_b f_{om} K_{om} D_{gw} / q \quad (52)$$

with,

$$\begin{aligned} k_s &= \text{degradation rate coefficient in soil (1/d), where } k_s = \ln(2)/DT50_{soil} \\ \rho_b &= \text{dry bulk density soil (kg/dm}^3) \\ f_{om} &= \text{organic matter content (kg/kg)} \\ K_{om} &= \text{coefficient for distribution over organic matter and water (dm}^3/\text{kg)} \\ D_{gw} &= \text{depth (default value} = 1 \text{ m)} \\ q &= \text{volume flux of water (m/d)} \end{aligned}$$

Where k_s is analogous to equation (50) and q is analogous to equation (51). If K_{om} is not available it can be calculated from the more available K_{oc} analogous to equation (18). Values for α_0 , α_1 and α_2 can be picked from table 2.

Table 2. Regression coefficients resulting from calibration of the meta-model.

Leaching set	Region	α_0	α_1	α_2
Autumn	TD	5.30	0.16	0.46
	TW	4.95	0.16	0.60
	WD	5.20	0.07	0.37
	WW	5.02	0.23	0.57
Spring	TD	5.09	0.44	0.46
	TW	4.72	0.39	0.58
	WD	5.07	0.28	0.30
	WW	4.81	0.58	0.46

Regions:

- TD = temperate and dry: mean annual rainfall < 0.8 m/yr, mean annual temperature < 12.5 °C;
 TW = temperate and wet: mean annual rainfall > 0.8 m/yr, mean annual temperature < 12.5 °C;
 WD = warm and dry: mean annual rainfall < 0.8 m/yr, mean annual temperature > 12.5 °C;
 WW = warm and wet: mean annual rainfall > 0.8 m/yr, mean annual temperature > 12.5 °C,

The metamodel estimates the predicted environmental concentration (PEC) for a standard application of 1 kg a.i./ha. To estimate the PEC for a chosen situation all applications in one year in kg a.i./ha have to be added. The PEC will be calculated using:

$$PEC_{gw} = PEC_{gw (1 \text{ kg/ha})} * M_{stacked} * 0.001 \quad (53)$$

with,

$PEC_{gw (1 \text{ kg/ha})}$ = Predicted Environmental Concentration of an application of 1 kg a.i./ha, annual average concentration leaching from the soil profile at 1 m depth (ug/L)

PEC_{gw} = Predicted Environmental Concentration of the sum of all applications within one year, annual average concentration leaching from the soil profile at 1 m depth (ug/L),

$M_{stacked}$ = dose applied stacked over a growing season (g a.i./ha)

0.001 = factor to convert from g a.i./ha to kg a.i./ha

2.6.2 Groundwater effect assessment

The methodology that the World Health Organisation (WHO) uses to calculate drinking water standards is included in PRIMET to calculate a threshold value for the use of groundwater as drinking water. The standard is based on the Acceptable Daily Intake (ADI) which is set by the FAO (JMPR, 2003) or calculated from toxicity studies performed with e.g. rats:

$$ADI = \frac{\text{NOAEL mammals}}{\text{EF mammals}} \quad (54)$$

with,

ADI = Acceptable Daily Intake (mg/kg*d)

NOAEL = No Observed Adverse Effect Level for mammals (mg/kg*d)

$\text{EF}_{\text{mammals}}$ = extrapolation factor to account for interspecies and intraspecies extrapolation, adequacy of study, nature and severity of effect (default value = 100)

The ADI is converted to a Drinking Water Standard using (WHO, 1996):

$$DWS = \frac{ADI \cdot bw \cdot P}{\text{ConsWater}} \quad (55)$$

with,

DWS = Drinking Water Standard (mg/L)

ADI = Acceptable Daily Intake (mg/kg*d)

bw = course weight (60 kg for adults)

P = fraction of the ADI allocated to drinking-water (default value = 0.1)

$\text{Cons}_{\text{Water}}$ = daily drinking-water consumption (default value = 2 litres for adults, L/d).

2.6.3 Groundwater risk assessment

The risk, expressed in Exposure Toxicity Ratio (ETR_{gw}) for using the groundwater as drinking water as a result of all stacked applications is:

$$\text{ETR}_{\text{gw}} = \frac{\text{PEC}_{\text{gw}}}{DWS \cdot 1000} \quad (56)$$

ETR_{gw} = Exposure Toxicity Ratio due to application (-)

PEC_{gw} = annual average concentration leaching from the soil profile at 1 m depth ($\mu\text{g/L}$)

1000 = factor to correct from $\mu\text{g/L}$ to mg/L

DWS = Drinking Water Standard (mg/L)

If:	$\text{ETR}_{\text{gw}} < 1$	No Risk	(indicated by a green colour)
	$1 \leq \text{ETR}_{\text{gw}} \leq 100$	Possible risk	(indicated by a orange colour)
	$\text{ETR}_{\text{gw}} > 100$	Risk	(indicated by a red colour)

2.6.4 Parameters groundwater risk assessment

2.6.4.1 Input scenario parameters

D_{gw}	= depth ground water (default value = 1 m)
Pr	= mean annual precipitation (m/yr)
ρ_b	= dry bulk density of the soil (default value = 1.0 kg/dm ³)
f_{om}	= organic matter content (default value = 0.02 kg/kg)
α_0, α_1 and α_2	= regression coefficients (see table 2)
bw	= course weight (default value = 60 kg for adults)
$ConsWater$	= daily drinking-water consumption (default value = 2 litres for adults, L/d).
Θ	= volume fraction of water (default value = 0.25 m ³ /m)
P	= fraction of the ADI allocated to drinking-water (default value = 0.1)
$EF_{mammals}$	= assessment factor to account for interspecies and intraspecies extrapolation, adequacy of study, nature and severity of effect (default value = 100)

2.6.4.2 Input pesticide parameters

ADI	= Acceptable daily intake (mg/ kg*d)
$DT_{50 \text{ soil}}$	= overall half-life in soil (d)
K_{om}	= coefficient for distribution over organic matter and water (dm ³ /kg)
K_{oc}	= coefficient for distribution over organic carbon and water (dm ³ /kg)
$NOAEL_{mammals}$	= No Observed Adverse Effect Level for mammals (mg/kg*d)

2.6.4.3 Input pesticide application parameters

$M_{stacked}$	= dosages applied stacked over a growing season (g a.i./ha).
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2.6.4.4 Constant parameters

No data available.

2.6.4.5 Calculated parameters

$PEC_{gw (1 \text{ kg/ha})}$	= Predicted Environmental Concentration of an application of 1 kg a.i./ha, annual average concentration leaching from the soil profile at 1 m depth (ug/L)
k_d	= degradation rate coefficient in soil (1/d)
PEC_{gw}	= Predicted Environmental Concentration of the sum of all applications within one year, annual average concentration leaching from the soil profile at 1 m depth (ug/L),.

q	= volume flux of water (m/d)
ADI	= Acceptable Daily Intake (mg/kg*d)
DWS	= Drinking Water Standard (mg/L)
ETR_{gw}	= Exposure Toxicity Ratio due to application (-)
$X1$	= independent regression variables (-)
$X2$	= independent regression variables (-)

2.7 Dietary risk assessment

2.7.1 Dietary exposure assessment

2.7.1.1 Considered food items and diet

The food items considered by PRIMET for the dietary exposure assessment are drinking water, fish, macrophytes and crops. Different diets can be used, but a few regional food diets are set by the WHO (2003), which can be used as best estimates of the daily intakes of the different commodities. For the far east the WHO estimates an average daily intake of 451 g cereals, 109 g roots and tubers, 15 g pulses, 50 g sugars, 50 g nuts and oilseeds, 14 g vegetable oils and fats, 2 g stimulants, 3 g spices, 179 g vegetables, 32 g fish and seafood, 13 g eggs, 85 g fruits, 33 g of milk products, 47 g of meat and 2 g of animal oils and fats (WHO, 2003). For each of the four food items an Estimated Daily Intake (EDI) is calculated which are summed to a total EDI. In the following paragraphs the calculation of the individual EDIs is described.

2.7.1.2 Consumption via drinking water

It is assumed that people drink groundwater pumped up from 1 m depth. The annual average concentration leaching from the soil profile at 1 m depth (PEC_{gw} in $\mu\text{g/L}$), as calculated within the groundwater risk assessment, is used as a representative pesticide concentration for drinking water. The Estimated Daily Intake due to drinking of water is estimated by:

$$EDI_{dw} = \frac{PEC_{gw} \cdot Cons_{water}}{bw \cdot 1000} \quad (58)$$

with,

EDI_{dw}	= Estimated Daily Intake due to drinking of water (mg/kg*d)
PEC_{gw}	= annual average concentration leaching from the soil profile at 1 m depth ($\mu\text{g/L}$)
$Cons_{water}$	= daily drinking-water consumption (default value = 2 litres for adults, L/d)
bw	= course weight (default value = 60 kg for adults)
1000	= factor to correct from $\mu\text{g/L}$ to mg/L

2.7.1.3 Consumption via fish

The amount of pesticide consumed via eating of fish is calculated by multiplying the amount of fish eaten per day with the concentration of the pesticide in the fish. The concentration of the pesticide in the fish is calculated using the PEC^1_{water} or, in case of multiple applications, the PEC^n_{water} as calculated in the surface water risk assessment, and bioconcentration factors (BCF) values for the different pesticides:

$$PEC_{fish} = \frac{PEC^n_{water} \cdot BCF}{1000} \quad (59)$$

with,

- PEC_{fish} = concentration in the fish (mg pesticide/kg fish)
- PEC^n_{water} = momentary water concentration from n applications ($\mu\text{g/L}$)
- 1000 = factor to correct from $\mu\text{g/L}$ to mg/L
- BCF = Bioconcentration factor (L/kg)

The BCF can be calculated from the more available K_{ow} using the following relation as determined by Veith et al. (1979):

$$BCF = 10^{(0.85 \cdot \text{Log}(K_{ow}) - 0.70)} \quad (60)$$

with,

- BCF = Bioconcentration factor (L/kg)
- K_{ow} = Octanol-water partitioning coefficient (L/kg)

The EDI for fish can now be calculated using:

$$EDI_{fish} = \frac{PEC_{fish} \cdot Cons_{fish}}{bw} \quad (61)$$

with,

- EDI_{fish} = Estimated Daily Intake due to eating of fish ($\text{mg/kg} \cdot \text{d}$)
- PEC_{fish} = concentration in the fish (mg pesticide/kg fish)
- $Cons_{fish}$ = daily fish consumption (kg/d).
- bw = course weight (default value = 60 kg for adults)

2.7.2 Consumption via macrophytes

The amount of pesticide consumed via eating of macrophytes is calculated analogous as done for fish, i.e. by multiplying the amount of macrophytes eaten per day with the concentration of the pesticide in the macrophytes. The concentration of the pesticide in the macrophytes was calculated using the PEC^1_{water} or, in case of multiple applications the PEC^n_{water} as calculated in the surface water risk assessment, and sorption coefficient values (K_d) for the different pesticides:

$$PEC_{mf} = \frac{PEC_{water}^n \cdot K_d}{1000} \quad (62)$$

with,

- PEC_{mf} = concentration in the macrophytes (mg pesticide/kg macrophytes)
- PEC_{water}^n = momentary water concentration from n applications ($\mu\text{g/L}$)
- 1000 = factor to correct from $\mu\text{g/L}$ to mg/L
- K_d = sorption coefficient for macrophytes (L/kg)

The K_d can be calculated from the more available solubility SOL (T) using the following relation as determined by Crum et al. (1999):

$$K_d = 3.20 - 0.65 \cdot \log[SOL(T)] \quad (63)$$

with,

- K_d = sorption coefficient for macrophytes (L/kg)
- $SOL(T)$ = solubility of substance in water at ambient temperature (g/m^3)

SOL (T) is calculated using Eq. (3). The EDI for fish can now be calculated using:

$$EDI_{mf} = \frac{PEC_{mf} \cdot Cons_{mf}}{bw} \quad (64)$$

with,

- EDI_{mf} = Estimated Daily Intake due to eating of macrophytes ($\text{mg/kg} \cdot \text{d}$)
- PEC_{mf} = concentration in the macrophytes (mg pesticide/kg macrophytes)
- $Cons_{mf}$ = daily macrophytes consumption (kg/d).
- bw = course weight (default value = 60 kg for adults)

2.7.2.1 Consumption via vegetables

Since no good model exists that predicts the concentration of the pesticide on the vegetables ($PEC_{vegetem}$) this is an input variable for the PRIMET decision support system.

The EDI for a vegetable item can now be calculated using:

$$EDI_{veg} = \frac{PEC_{veg} \cdot Cons_{veg}}{bw} \quad (65)$$

with,

- EDI_{veg} = Estimated Daily Intake due to eating of a defined vegetable item ($\text{mg/kg} \cdot \text{d}$)
- PEC_{veg} = concentration in the defined vegetable item (mg pesticide/kg macrophytes)
- $Cons_{veg}$ = daily consumption of the vegetable item (kg/d).

2.7.2.2 Calculation of Estimated Daily Intake

The EDI for the overall consumption can now be calculated by summing all individual items:

$$EDI = EDI_{dw} + EDI_{fish} + EDI_{mf} + EDI_{veg} \quad (66)$$

with,

- EDI = Estimated Daily Intake (mg/kg*d)
- EDI_{dw} = Estimated Daily Intake due to drinking of water (mg/kg*d)
- EDI_{fish} = Estimated Daily Intake due to eating of fish (mg/kg*d)
- EDI_{veg} = Estimated Daily Intake due to eating of a vegetables (mg/kg*d)
- EDI_{mf} = Estimated Daily Intake due to eating of macrophytes (mg/kg*d)

2.7.3 Dietary effect assessment

The effect standard is based on the Acceptable Daily Intake (ADI) which is set by the FAO (JMPR, 2003) or which is calculated from toxicity studies performed using Eq. (54). Like ADI, the ADI is an estimate of the amount of a substance, expressed on a body weight basis that can be ingested daily over a lifetime without appreciable health risk.

2.7.4 Dietary risk assessment

The risk, expressed in Exposure Toxicity Ratio (ETR) for eating different food items is:

$$ETR_{diet} = \frac{EDI}{ADI} \quad (67)$$

ETR_{diet} = Exposure Toxicity Ratio due to application (-)

EDI = Estimated Daily Intake (mg/kg*d)

ADI = Acceptable Daily Intake (mg/kg*d)

If: $ETR_{diet} < 1$ No Risk (indicated by a green colour)
 $1 \leq ETR_{diet} \leq 100$ Possible risk (indicated by a orange colour)
 $ETR_{diet} > 100$ Risk (indicated by a red colour)

2.7.5 Parameters dietary risk assessment

2.7.5.1 Input diet scenario parameters

PEC_{gw} = annual average concentration leaching from the soil profile at 1 m depth (µg/L)

PEC_{water}^n = momentary water concentration from n applications (µg/L)

PEC_{veg}	= concentration in the defined vegetable item (mg pesticide/kg macrophyte)
$Cons_{fish}$	= daily fish consumption (kg/d).
$Cons_{mf}$	= daily macrophyte consumption (kg/d).
$Cons_{veg}$	= daily consumption of the vegetable item (kg/d).
$Cons_{Water}$	= daily drinking-water consumption (default value = 2 litres for adults, L/d).
bw	= course weight (default value = 60 kg for adults)
$EF_{mammals}$	= assessment factor to account for interspecies and intraspecies extrapolation, adequacy of study, nature and severity of effect (default value = 100)

2.7.5.2 Input pesticide parameters

K_{ow}	= Octanol-water partitioning coefficient (L/kg)
$SOL(T)$	= solubility of substance in water at ambient temperature (g/m ³)
ADI	= Acceptable Daily Intake (mg/kg*d)
$NOAEL_{mammals}$	= No Observed Adverse Effect Level for mammals (mg/kg*d)

2.7.5.3 Input pesticide application parameters

None, is captured in PEC_{gw} and PEC_{water}

2.7.5.4 Constant parameters

No parameters

2.7.5.5 Calculated parameters

EDI_{dw}	= Estimated Daily Intake due to drinking of water (mg/kg*d)
PEC_{fish}	= concentration in the fish (mg pesticide/kg fish)
BCF	= Bio concentration factor (L/kg)
EDI_{fish}	= Estimated Daily Intake due to eating of fish (mg/kg*d)
PEC_{mf}	= concentration in the macrophytes (mg pesticide/kg macrophytes)
K_d	= sorption coefficient for macrophytes (L/kg)
EDI_{mf}	= Estimated Daily Intake due to eating of macrophytes (mg/kg*d)
EDI_{veg}	= Estimated Daily Intake due to eating of a defined vegetable item (mg/kg*d)
EDI_{veg}	= Estimated Daily Intake due to eating of a vegetables (mg/kg*d)
EDI	= Estimated Daily Intake (mg/kg*d)
ETR_{diet}	= Exposure Toxicity Ratio due to application (-)

3 User manual

3.1 What's new in PRIMET 2.0

The main new features in PRIMET 2.0 are:

- Risk assessment with MonQI application scenario's, see section 3.5.10.
- Two new PRA's (Pesticide Risk Assessment) added: Bees and non target arthropods.
- Possibility added to estimate the chronic risk to aquatic organisms and earthworms.

3.2 Getting Started

3.3 Installation

Before you can use the PRIMET application, you have to download the PRIMET 2.0 package from the website (www.primet.wur.nl). Save the package at a special folder on your computer and unzip the application and the databases.

3.3.1 Resolution

The minimum screen resolution for optimal use of PRIMET is 1024*768 pixels or higher.

3.3.2 Menu's in the menu bar

The menu bar at the top of the screen contains the menus: 'File', 'Tools', 'View', and 'Help'.

3.3.2.1 File

The 'File' menu includes two menu commands: 'select PRIMET database' and 'exit'. The 'select database' option is described in more detail in section 3.3.1. A click on the 'exit' command will close PRIMET.

3.3.2.2 Tools

The commands in the menu 'Tools' are all, except for 'Customize toolbar', described in more detail in section 3.6 Options. Clicking on the command 'Customize toolbar' will show Figure 2.

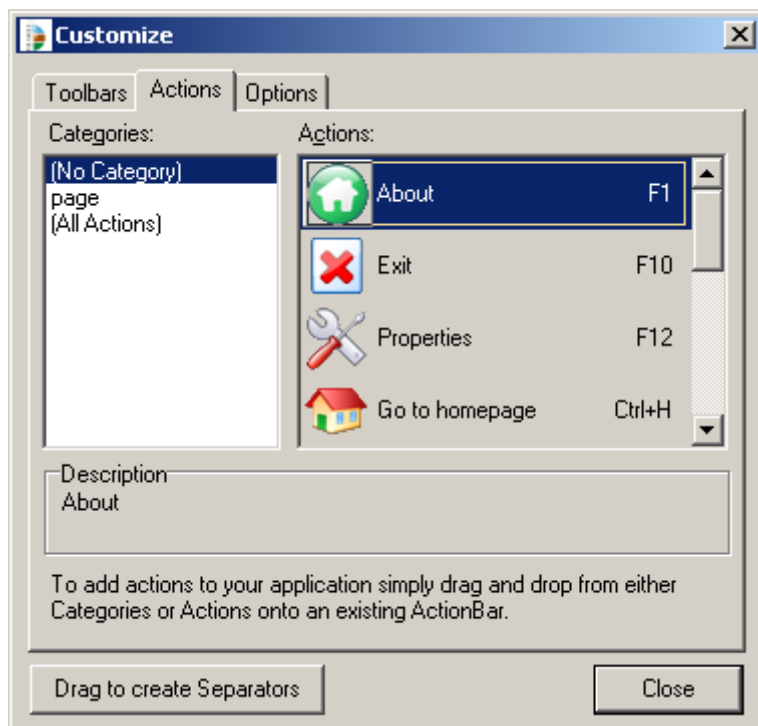


Figure 2. *Customize toolbar dialog' in PRIMET*

On the first tab ("Toolbars") in Figure 2 the visibility of the toolbar in PRIMET is set. The second tab ("Actions") is used to add buttons to or remove buttons from the toolbar. Individual buttons can be added to the toolbar by dragging them from the field 'Actions' and dropping them in the toolbar. Buttons are removed from the toolbar by dragging them from the toolbar and dropping them anywhere in the application. The third tab ("Options") is used to personalize the menu and toolbar but is not yet in use.

3.3.2.3 View

With the View menu the user can call the input screens for pesticide, application scheme and the six physical scenarios. These input screens are described in more detail in section 3.5. input to a PRA.

3.3.2.4 Help

The command 'Help' and the command 'About' are described in more detail in section 3.7 Options. By clicking on the command 'Go to homepage' the homepage of the PRIMET model (<http://www.primet.wur.nl>) will start-up in your internet browser.

3.3.3 The toolbar

The toolbar below the menu bar can be customized by the user. Buttons can be added or removed. How to do this is explained in section 3.2.3.2. Tools.

3.3.4 The selection panel

The selection panel contains two sub panels: 'Main' and 'Options'. Clicking on the grey title buttons will show the buttons of the sub level. The sub level 'Main' buttons are described in sections 3.4 and 3.5. The buttons in the 'Options' sub level is described in section 3.7.

The use of the selection panel is optional because its options can also be called using options in the menu bar or in the Home screen (3.2). The selection panel can be hidden by clicking on the menu command 'show selection panel' under the menu 'View' in the menu bar.

3.4 The Home screen

The Home screen can be accessed from the main menu with the button:



The Home screen (Figure 3) is the main screen of PRIMET. It can be used to select the PRIMET database, the active ingredients database and the MonQI database, to manage PRA's (Pesticide Risk Assessment) and it shows the results of the different risk assessments expressed as the ETR (Exposure Toxicity Ratio) after selection of input to the assessment types.

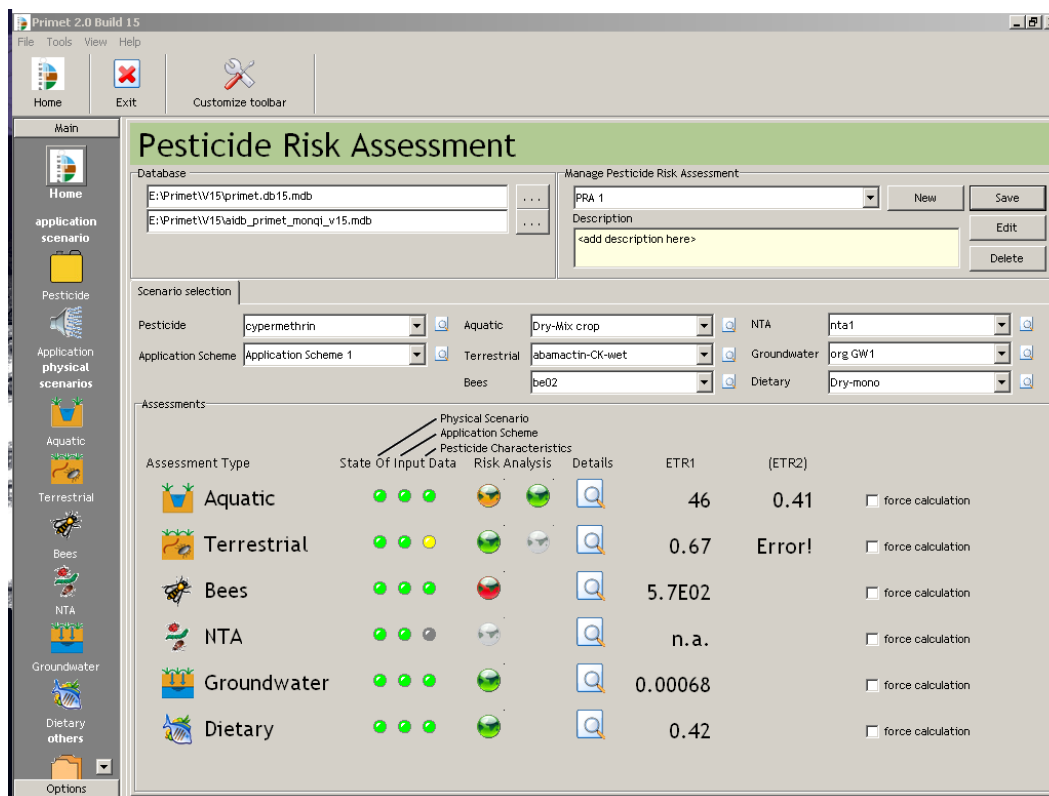


Figure 3. The Home screen

3.4.1 Databases used in PRIMET


PRIMET is distributed with two Microsoft Access databases. At the first start, PRIMET will ask where the databases are located. As default the following databases will be connected:

1. PRIMET database (primet_db_v2.mdb)
2. Active Ingrediënt (aidb_primet_v2.0.mdb)

In PRIMET 2.0 there is an option to connect a third database, namely:

3. MonQI Result Database (monqi_db_mdb).

This database is not connected as default. These data are project dependent and have to be collected by the user itself. For more information see section 3.5.10.

The database can be selected from a browse screen. Click on the grey button with the three dots  to select one of the databases (Figure 4). This will prompt a new screen, to locate the database. In the title of the screen you can read which database is mentioned (Primet, AI or MonQI). If the database type is not the right one, the database will not be accepted by PRIMET. If the database is not accepted, you can try it again with the buttons behind the database names.

Note that a PRIMET database needs to be selected because it contains configuration information what PRIMET needs. It is therefore not possible to select an arbitrary

empty MS access database. If you wish to start with an empty database it is advised to remove existing data in the forms of PRIMET. Subsequently you can remove all the PRA's, application scenarios and physical scenarios you won't need.

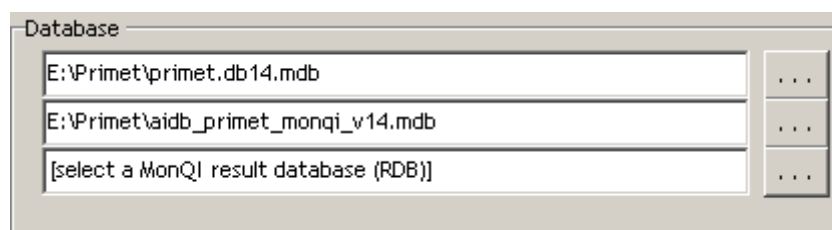


Figure 4. The Database section in the Home screen of PRIMET

3.4.2 Manage Pesticide Risk Assessment (PRA)

In the section 'Manage PRA' existing PRA's (Pesticide Risk Assessment) can be selected from a list, they can also be edited or deleted and new PRA's can be created (Figure 5).

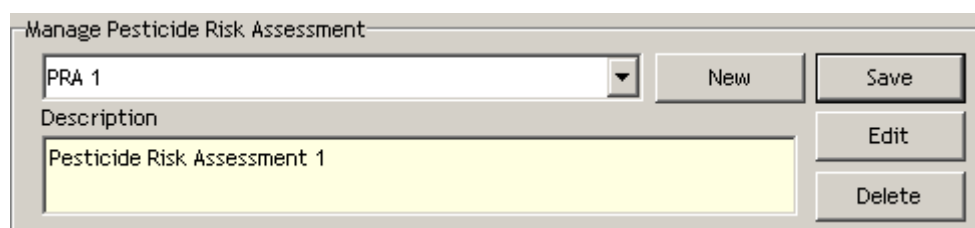


Figure 5. The Manage PRA section in the Home screen of PRIMET

An existing PRA can be selected from the pick list. A new PRA can be generated by clicking on the button 'New'. The screen shown in Figure 6 appears. The name filled in the box 'PRA' will be added to the pick list of the 'Manage PRA' section in the Home screen of PRIMET. The description typed in the field 'Description' will appear in the yellow box shown in Figure 5.

It is important to realise that the physical scenarios and the six assessment types properties belonging to the PRA, are only saved to the database after clicking the 'Save' button.

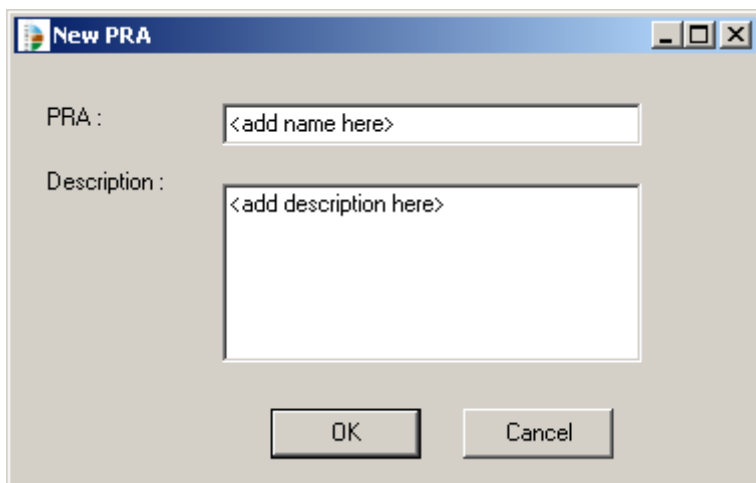


Figure 6. New(Edit) PRA screen of PRIMET

3.4.3 Selection of scenarios

A PRA needs input from eight different components. They can be selected in the Scenario selection section in the Home screen of PRIMET (Figure 7).

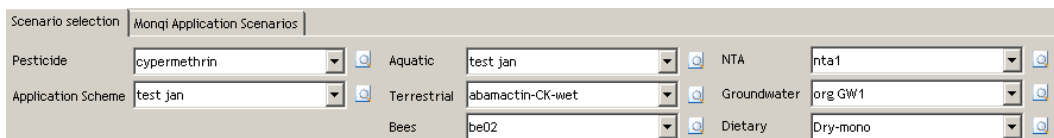


Figure 7. The Scenario selection section in the Home screen of PRIMET

Every component (i.e. Pesticide, Application Scheme etc.) has its own pick list from which the pesticide and the different scenarios can be selected. The button with the picture of a magnifying-glass can be used to switch to the input screens of the different components directly. The input screens are discussed in more detail in section 3.5.

3.4.4 Assessments

The Assessments section in the Home screen of PRIMET gives information about the status of the input data and a brief summary of the output. The information about input and output is given per assessment type.

The three 'lights' below 'State of Input Data' are an indication whether all input data are present in the PRA. If the lights are green, all data necessary for generating output is available. If one or more lights have a grey colour, some input data are missing and output cannot be generated (i.e. Figure 8, Terrestrial scenario; one or more pesticides characteristics are missing). If the light is yellow, only ETR1 can be calculated (data are missing to calculate ETR2).

The globes below ‘Risk Analysis’ enable the user to quickly check the risk calculated for each individual assessment. A green colour indicates there is no risk, orange indicates that there is a potential risk and a red colour indicates there is a risk (more detailed information about the calculation can be found in Chapter 2). A grey coloured globe signifies that some input data are missing and that the risk calculation cannot be performed.

Clicking on the button with the magnifying glass below ‘Details’ will open a new screen showing all input data and all output data including the output data of intermediate calculations of the assessment (these output screens will be discussed in section 3.5). The risk is expressed in ETR (Exposure Toxicity Ratio) and given below ‘ETR’. If some input data are missing the ETR cannot be calculated and the value n.a. (not available) is assigned to the ETR. To enforce a new calculation, you can use the option box ‘force calculation’. PRIMET will calculate till the point that relevant data are missing.

For some assessment types it is possible to calculate an ETR2. In case of aquatic and terrestrial assessment ETR2 gives the ETR’s for chronic risk. In case of non target arthropods ETR2 gives the risk off-field (ETR1 gives the risk in-field).











































Assessment Type	Physical Scenario Application Scheme Pesticide Characteristics				ETR1	(ETR2)	
	State Of Input Data	Risk Analysis	Details				
 Aquatic	  	 			57	0.13	<input type="checkbox"/> force calculation
 Terrestrial	  	 			0.67	Error!	<input type="checkbox"/> force calculation
 Bees	  	 			5.7E02		<input type="checkbox"/> force calculation
 NTA	  	 			n.a.		<input type="checkbox"/> force calculation
 Groundwater	  	 			0.0015		<input type="checkbox"/> force calculation
 Dietary	  	 			0.44		<input type="checkbox"/> force calculation

Figure 8. The Assessments section in the Home screen of PRIMET

3.5 Input to a PRA

3.5.1 General

Every input screen contains two sections: ‘Select and Manage’ and ‘Input data’. In the ‘Select and Manage’ section existing pesticides or scenarios can be selected from a list, they can also be edited or deleted and new pesticides or scenarios can be generated. The ‘Select and manage’ section (Figure 9) is more or less analogous to the ‘Manage PRA’ section in the Home screen.

It is possible to edit the values of the default data. The default value for the active ingredients can always be rollback with the ‘restore values’ button. To keep the original values, you can also create a new item with the ‘new’ button. It is also possible to delete items with the ‘delete’ button.

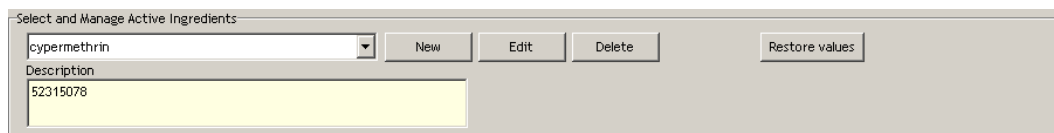


Figure 9. The Select and Manage Active Ingredients section in the input screens of PRIMET

In the section 'Input data' data can be typed in to the boxes. The boxes can have different colours. The meaning of these colours is explained in Figure 10.

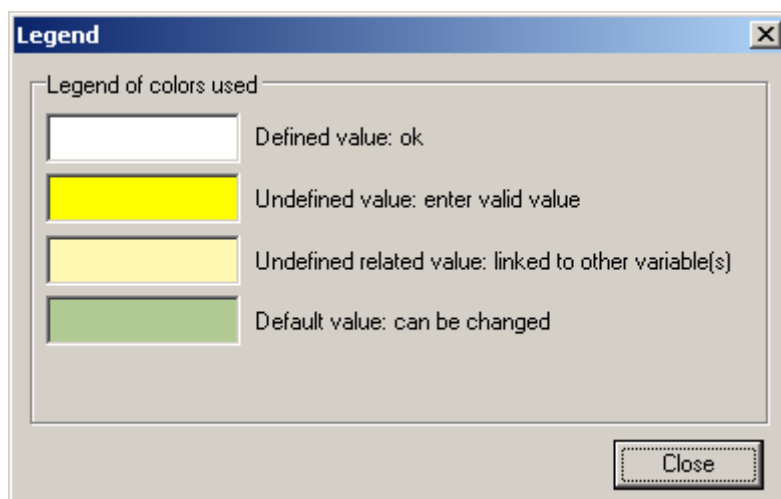


Figure 10. The 'show legend' screen (under tools), explaining the meaning of the colours of the boxes in the input screen

A blue button with a question mark is placed in front of every input box (Figure 11). Moving the mouse cursor over the blue button will display a pop-up box containing relevant information about the parameter like: range and unit. When you click on the blue button two little grey buttons with arrows appear behind the input box. With these buttons you can alter the number of decimals visible in the input box.

Do realize however, that PRIMET performs the calculations with the numbers given in the database and not with the numbers displayed on the input screens. So the number of decimals stored in the database is determining for the output of the calculations.

The numbers between brackets behind the values gives relations between other values, i.e. EC50 algae are related with L(E)C50 daphnia en L(E)C50 fish (the lowest value is used for the No Effect concentration water).



Figure 11. Input boxes and their options in the input screens of PRIMET

Sections 3.5.2 – 3.5.9 do NOT explain the individual parameters given in the screens because the user can obtain this information using the blue button with the question mark and because a more elaborate explanation of the parameters is already given in Chapter 2) of this report.

3.5.2 Pesticide

The Pesticide input screen can be accessed from the main menu with the button:



The 'Select and Manage' section can be used to generate a new pesticide or modify or delete existing ones.

The 'Input data' section of the Pesticide input screen consists of six parts: Aquatic, Bees, Groundwater, Dietary, Terrestrial and NTA (Figure 12). They correspond to the physical scenarios and the six assessment types shown in the Home screen. The subdivision is made to show the user which pesticide input data is relevant for which assessment. It is therefore possible some pesticide input parameters are displayed twice or more in the 'Input data' section. The PRIMET software takes this into account: if for instance the user enters a value for 'SOL(Tref)' in the 'Aquatic' section this number is automatically copied to the 'SOL(Tref)' box in the Dietary section.

Select and Manage Active Ingredients	
cypermethrin	New Edit Delete Restore values
Description: 52315078	

Input data	
Aquatic	
DT50water	3 d
EC50 algae	1.3 (3) mg/L
Koc	8.678E4 (1) L/kg
KOM	5.034E4 (1) L/kg
L(E)C50 daphnia	5.872E-5 (3) mg/L
L(E)C50 fish	0.00128 (3) mg/L
Mpesticide	416.3 g/mol
NOEC Daphnia	0.0001664 (6) mg/L
NOEC fish	(6) mg/L
SOL(Tref)	0.009 mg/L
TrefSOL	293 K
Trefkw	293 K
TrefVP	293 K
VP(Tref)	0.00023 Pa
Bees	
LD50 bee	0.035 µg/bee
Groundwater	
ADI (user)	0.05 (7) mg/kg*d
DT50soil	68 (2) d
EF mammals	100 (7) -
Koc	8.678E4 (1) L/kg
KOM	5.034E4 (1) L/kg
NOEL mammal	10 (7) mg/kg*d
Dietary	
ADI (user)	0.05 (7) mg/kg*d
EF mammals	100 (7) -
Log(Kow)	5.5 L/kg
NOEL mammal	10 (7) mg/kg*d
SOL(Tref)	0.009 mg/L
Terrestrial	
DT50soil	68 (2) d
LC50earthworms	100 mg/kg
NOEC earthworms	mg/kg
NTA	
LR50 nta	-

Figure 12. Pesticide input screen of PRIMET

Furthermore there are some pesticide input parameters which can be calculated from other pesticide input parameters, like K_{OM} and K_{OC} . Usually K_{OC} information is more readily available; however K_{OM} is needed in the calculations. K_{OM} can be calculated from the K_{OC} and vice versa. This is implemented in PRIMET. If a value for K_{OC} is

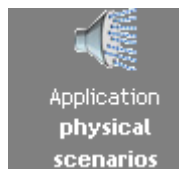
entered, PRIMET converts the K_{OC} to the K_{OM} and the correct value for K_{OM} is automatically loaded in the input box for K_{OM} and vice versa. The user has the possibility to fill in one of the relating parameters instead of having to make the conversion him/herself. There are four types of combinations of input parameters which are related in the way described above. They are given in Table 1. PRIMET calculates only the parameters of the left-hand side formulas.

Table 1 Relating parameters in the Pesticide input screen

assessment	parameters	Formula
<input type="radio"/> Aquatic <input type="radio"/> Aquatic	<input type="radio"/> $K_w(T_{refkw})$ <input type="radio"/> DT50	$K_w(T_{refkw}) = \frac{Ln(2)}{DT50}$
<input type="radio"/> Aquatic/Groundwater <input type="radio"/> Aquatic/Groundwater	<input type="radio"/> K_{OM} <input type="radio"/> K_{OC}	$K_{om} = \frac{K_{oc}}{1.724}$
<input type="radio"/> Soil <input type="radio"/> Soil/Groundwater	<input type="radio"/> K_s <input type="radio"/> DT50 _{soil}	$K_s = \frac{Ln(2)}{DT50_{soil}}$
<input type="radio"/> Groundwater/Dietary	<input type="radio"/> ADI <input type="radio"/> NOAEL	$ADI = \frac{NOAEL}{AF}$

3.5.3 Application Scheme

The Application Scheme input screen can be accessed from the main menu with the button:



The ‘Select and Manage’ section can be used to generate a new Application Scheme or modify or delete existing ones.

The ‘Input data’ section of the Application Scheme input screen contains five parts: Aquatic, Terrestrial, NTA, Bees and Groundwater, corresponding to the physical scenarios and the assessment types with the same name (Figure 13).

Analogous to the Pesticide input screen input some parameters are displayed twice in the ‘Input data’ section and if one parameter in one part of the section (i.e. Dt in Aquatic) is entered, the same value will automatically be loaded in the box of the same parameter in the other part of the section (i.e. Dt in Terrestrial).

The assessments NTA, Bees and Groundwater are mentioned for the individual parameters for the application (i.e. dose, number of applications and drift). The other

global parameters can be accessed on the specific schemes. For using a MonQI application as single application, see section 3.5.10.

Figure 13. Application Scheme input screen of PRIMET

3.5.4 The physical scenario Aquatic

The Aquatic assessment input screen can be accessed from the main menu with the button:



The Aquatic assessment input screen is shown in Figure 14. The 'Select and Manage' section can be used to generate a new Aquatic scenario or modify or delete existing ones.

In the 'Input data' section the user can fill in the values for the different parameters belonging to the scenario.

The blue buttons with a question mark together with the picture in the right hand side of the screen can be used to gain information about the parameters.

Physical Scenario: Aquatic assessment input data

Select and Manage Aquatic Scenarios

Dry-Mix crop

New

Edit

Delete

Description

Dry season - mix crop at kokprachadee

Scenario

b	<div>?</div> 1.17	m
EF water, acute-algae	<div>?</div> 0.1	-
EF water, acute-Daphnia	<div>?</div> 0.01	-
EF water, acute-fish	<div>?</div> 0.01	-
EF water, chronic-Daphnia	<div>?</div> 0.1	-
EF water, chronic-fish	<div>?</div> 0.1	-
h	<div>?</div> 0.34	m
L	<div>?</div> 96.75	m
mom	<div>?</div> 0.6946	g/g
s1	<div>?</div> 0.51	-
ss	<div>?</div> 0.01	kg/L
T	<div>?</div> 304.8	K
v	<div>?</div> 0.001	m/d

Input parameters physical description

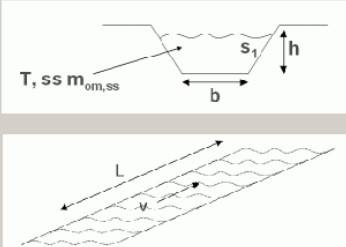


Figure 14. The Aquatic scenario input screen of PRIMET

3.5.5 Terrestrial

The Terrestrial assessment input screen can be accessed from the main menu with the button:



The Terrestrial assessment input screen is shown in Figure 15. The 'Select and Manage' section can be used to generate a new Terrestrial scenario or modify or delete existing ones.

In the 'Input data' section the user can fill in the values for the different parameters belonging to the scenario.

The blue buttons with a question mark and the picture at the right hand side of the screen provide information about the parameters.

Physical Scenario: Terrestrial assessment input data

Select and Manage Terrestrial Scenarios

te01

Description

Input data

Scenario

Depth (D)	<input type="text" value="0.05"/>	m
EF soil-acute	<input type="text" value="0.1"/>	-
EF soil-chronic	<input type="text" value="0.2"/>	-
Bulk density (PB)	<input type="text" value="1.3"/>	kg/dm3 soil

Input parameters physical description

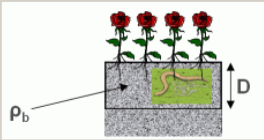


Figure 15. The Terrestrial scenario input screen of PRIMET

3.5.6 Bees

The Bees assessment input screen can be accessed from the main menu with the button:



The Bees assessment input screen is shown in Figure 16. The 'Select and Manage' section can be used to generate a new Bees scenario or modify or delete existing ones.

The 'Input data' section only exists of the extrapolation correction factor for effect assessment of bees, to convert from $\mu\text{g}/\text{bee}$ to g/ha (default value = 50).

Figure 16. The Bees scenario input screen of PRIMET

3.5.7 NTA

The NTA assessment input screen can be accessed from the main menu with the button:



The NTA assessment input screen is shown in Figure 17. The ‘Select and Manage’ section can be used to generate a new NTA scenario or modify or delete existing ones.

The ‘Input data’ section only exists of the extrapolation factor for effect assessment of non target arthropods (default value = 2) and the vegetation distribution factor (default value = 10)

Physical Scenario: Non-Target Anthropod assessment input data

Select and Manage NTA Scenarios

nta1 [New] [Edit] [Delete]

Description

Input data

Scenario	
EF nta	2 -
veg	10 -

Figure 17. The NTA scenario input screen of PRIMET

3.5.8 Groundwater

The Groundwater assessment input screen can be accessed from the main menu with the button:



The Groundwater assessment input screen is shown in Figure 18. The 'Select and Manage' section can be used to generate a new Groundwater scenario or modify or delete existing ones.

A meta-model of PEARL is used and the user has to select a region as described in section 2.6.1. After selecting the right scenario, you can copy the resulting values to the Groundwater scenario with the copy button on the right-hand side from the Pearl scenario selection screen.

In the part 'Scenario' of the 'Input data' section the user has to fill in values for the different parameters (i.e. bw , $ConsWater$ etc., see section 2.6.1) required to calculate the ETR_{gw} .

Physical Scenario: Groundwater assessment input data

Select and Manage Groundwater Scenarios

org GW1

New

Edit

Delete

Description

Mixed vegetable crop- Thailand- Dry season

Input data

Select PEARL scenario

meta model

spring : TW

Description

temperate and wet: mean annual rainfall > 0.8 m/yr, mean annual temperature < 12.5 °C

Resulting values

4.72

0.39

0.58

Copy >>

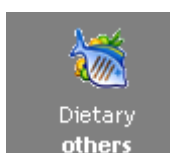
Scenario

a0	?	4.72	-
a1	?	0.39	-
a2	?	0.58	-
bw	?	60	kg
ConsWater	?	2	L/d
DGW	?	1	m
Fom	?	0.019	kg/kg
P	?	0.1	-
Bulk density (PB)	?	1	kg/dm3 soil
Pr	?	1500	m/yr
theta	?	0.25	m3 /m

Figure 18. The Groundwater scenario input screen of PRIMET

3.5.9 Dietary

The Dietary assessment input screen can be accessed from the main menu with the button:



The Dietary assessment input screen is shown in Figure 19. The 'Select and Manage' section can be used to generate a new Dietary scenario or modify or delete existing ones.

In the 'Input data' section the user can fill in the values for the different parameters relevant to the scenario.

The blue buttons with a question mark can be used to obtain information about the parameters.

The parameters PEC_{gw} and $PEC_{n\ water}$ can be derived from other scenarios, but they also may be specified by the user. If you want to specify these parameters yourself, values for the parameters have to be filled in the boxes of these parameters shown at

the left-hand side of the screen. The values filled in these boxes will always overrule the values derived from other scenarios.

Input data		
Scenario		
bw	60	kg
ConsFish	1	kg/d
ConsMF	1	kg/d
ConsWater	2	L/d
ConsVeg	1	kg/d
PECgw (user)		(5) µg/L
PECnwater (user)		(4) µg/L
PECvegitem	1	mg pesticide / kg vegetable

values derived from other scenarios

PECgw	0.2278	(GW)
PECn water	0.0268	(AQ)


User defined values will over-rule these calculated values.

Figure 19. The Dietary scenario input screen of PRIMET

Something to be aware of is that the value for $PEC_{n\ water}$ derived from other scenarios is only visible at the right-hand side of the Dietary input screen if a PRA is selected in the Home screen containing a complete Aquatic and Groundwater scenario (all parameters have a value). If not all values filled in for the groundwater and aquatic scenario, no values can be derived for PEC_{gw} and $PEC_{n\ water}$.

3.5.10 MonQI scenario's

If you want to work with specific MonQI scenarios, you first have to select a MonQI results database. How to organize a correct MonQI database; see <http://www.monqi.org>.

First a MonQI database has to be selected in the home screen. If the third database option is not visible, the MonQI database option has to be selected. Choose the option 'Use MonQI Result Database' in the PRIMET properties via Tools >> Properties. The database can be selected with the  button on the Home screen. After that the 'Monqi Application Scenarios' tab, see figure 20 has to be chosen from the Home screen. To perform a MonQI Scenario run the three steps given in the screen have to be followed.

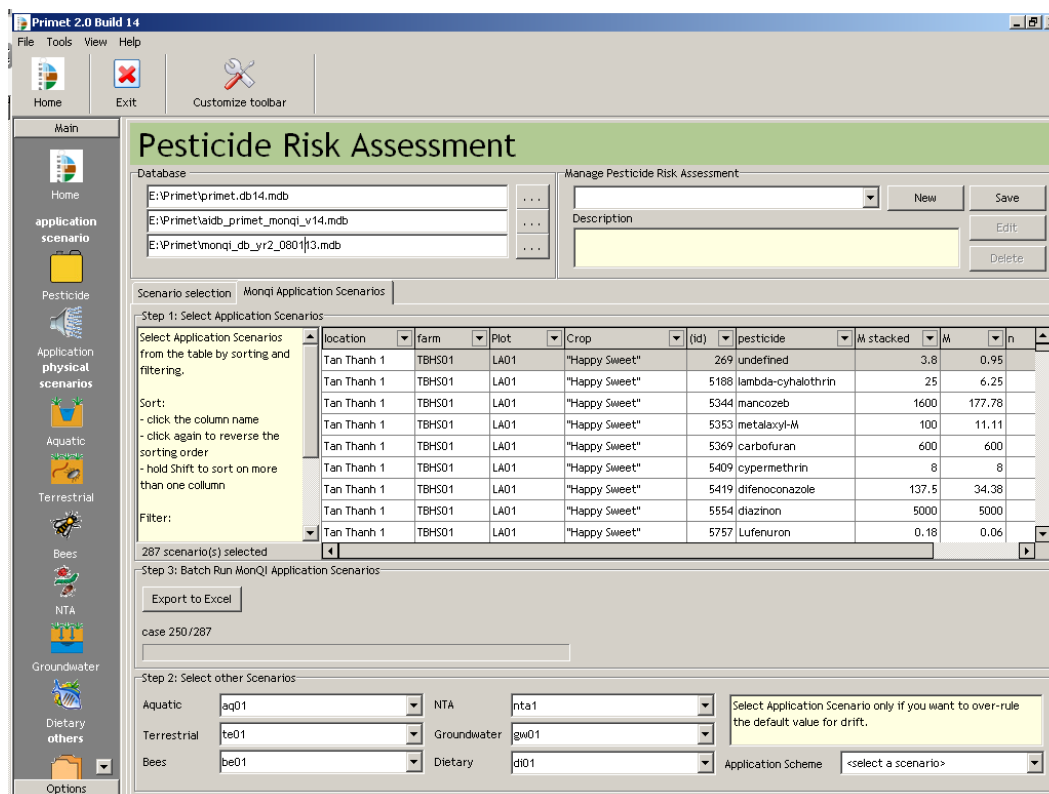


Figure 20. The MonQI Application Scenarios on the Home screen of PRIMET

Step 1.

The scenarios can be filtered on each column for a specific scenario-run in the same way as a filter selection in MS Excel. The complete instructions on how to do this is explained in the left-hand side of the matrix of MonQI scenarios.

Step 2.

Chose a complete scenario for seven components in the same way as for a single PRA, see Figure 21. The pesticide is already given in the MonQI Scenarios. If an 'Application Scheme', will not be selected the default value for drift will be taken.

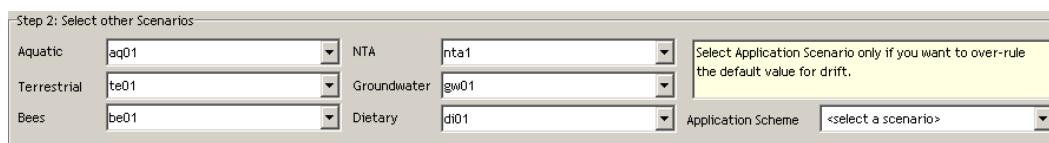


Figure 21. Selection of The Dietary scenario input screen of PRIMET

Step 3. To see the calculated results, press the **Export to Excel** button. PRIMET will ask to select a location and filename to save the results as a MS Excel sheet. After that PRIMET will show the results. The first rows of the sheet contain information about the selected farms en scenarios.

MonQI Application Scheme

In order to view an individual MonQI application, you can copy a specific MonQI farm and application to a new Application Scenario. A new scenario have to be made (i.e. Monqi scenario 1) and a record from the MonQI scenario matrix has to be selected, see Figure 22. With the **Copy >>** button it is possible to copy the application parameters into the new application scenario in PRIMET.

Application Scheme

Select and Manage Application Scenarios

Monqi scenario 1 [New] [Edit] [Delete]

Description

Input data

Select MonQI scenario

farm	PLOT	CROP	pesticide	M stacked	M	n	Dt
TBHS01	LA01	"Happy Sweet"	cypermethrin	8	8	1	
TBHS01	LA04	"Happy Sweet"	cypermethrin	60	30	2	25
TBHS01	LA05	"Happy Sweet"	cypermethrin	42.6667	21.3333	2	25
TBHS01	LA06	"Happy Sweet"	cypermethrin	20	20	1	
TBHS01	LA07	"Happy Sweet"	cypermethrin	26	13	2	36

[Copy >>] Filter by Pesticide as selected on Home page

Aquatic

%drift-ditch [?] [2.77] %

Dt [?] [25] d

M [?] [30] g a.i./ha

n [?] [2] -

NTA

%drift [?] [2.77] %

M [?] [30] g a.i./ha

n [?] [2] -

Terrestrial

Dt [?] [25] d

M [?] [30] g a.i./ha

n [?] [2] -

Bees

M [?] [30] g a.i./ha

Groundwater

M stacked [?] [60] g a.i./ha

Figure 22. Selection of a specific MonQI using for copying into a new scenario in PRIMET

3.6 Output of a PRA

3.6.1 Output via the Home screen; the Results screen

The section 'Assessments' in the Home screen contains an entry to the screens with detailed output per assessment. Clicking on the button with the magnifying glass (Figure 8) below 'Details' will open a new screen (Results; Figure 23) showing, per assessment, all input data and all output data including the results of intermediate calculations.

Only the structure and possibilities of the Results screen will be discussed in this section, because the structure is the same for the Results screens of all six assessments, the Result screen of one assessment (Terrestrial) is chosen as an example (Figure 23). The parameters are discussed neither as they are already described in detail in Chapter 2 of this report.

Results: Physical Scenario: Terrestrial assessment input data						
Summary						
type	topic	name	label	value	unit	description
OUTPUT	SC	ETRSOIL_A	ETR soil-acute	0.778	-	Acute Exposure Toxicity Ratio due to n applications
OUTPUT	SC	ETRSOIL_C	ETR soil-chronic	*undefined*	-	Chronic Exposure Toxicity Ratio due to application
OUTPUT	SC	NECSOIL_A	NEC soil acute	10	mg/kg	No Effect Concentration for the soil compartment
OUTPUT	SC	NECSOIL_C	NEC soil chronic	*undefined*	mg/kg	No Effect Concentration for the soil compartment
OUTPUT	SC	PECNSOIL	PECnsoil	7.78	mg pesticide/kg	Concentration in the upper part of soil (depending on the depth of the soil) from
Log						
Errors occurred!						
Scenario						
GetValue: No value defined for ETRSOIL_C, part of "Terrestrial".						
Values						
type	topic	name	label	value	unit	description
Pesticide:						
INPUT	PE	DT50S	DT50soil	68	d	Overall half-life in soil due to degradation
INPUT	PE	LC50_T_E	LC50earthworms	100	mg/kg	Dose that affects 50% of the earthworms
INPUT	PE	NOEC_T_E	NOEC earthworms	*undefined*	mg/kg	No observed effect concentration of earthworms
INTER	PE	KS	ks	0.01019	1/d	Degradation rate coefficient in soil, where ks = ln(2)/DEG50soil
INPUT	AP	DT	Dt	7	d	Time interval between applications
INPUT	AP	M	M	1000	g a.i./ha	Individual dose applied
INPUT	AP	N	n	6	-	Number of applications
INPUT	SC	DEPTHF	Depth (D)	0.05	m	Depth of the field
INPUT	SC	EF_S_A	EF soil-acute	0.1	-	extrapolation factor for acute effect assessment of earthworms

Figure 23. The Results screen of PRIMET

The Results screen contains three sections: Summary, Log and Values. The input of the sections becomes visible if you click in the grey bar with the name of the section in it.

The Summary section contains all output variables of the scenario and their calculated value. The Log section is usually empty, but displays error messages when input or intermediate data is missing. The Values section contains all input, output and intermediate parameters and their values.

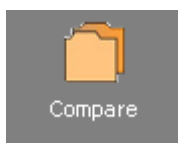
The structure of the Summary and Values sections is the same. The sections contain seven columns: type, topic, name, label, value, unit and description.

The column 'type' indicates if the parameter is input data, output of an intermediate calculation or output data. The column 'topic' informs the user about whether the parameter is defined by the pesticide (PE), the application scheme (AP) or the physical scenario (SC).

Furthermore the Result screen contains two buttons below in the screen: 'Print' and 'Export'. Clicking on the button 'Print' will sent a print command to the printer, which will print the Results screen. The button 'Export' can be used to export the data in the Results screen to a MS Excel file.

3.6.2 Output via the Compare button

The Compare screen can be opened from the main menu with the button:



In this screen the results of up to three Pesticide Risk Assessments can be compared.

Figure 24. The Compare screen of PRIMET

The selection column of one PRA is shown in detail in Figure 24. The column contains two sections: Settings and Results. The input of the sections becomes visible if you click on the grey bar with the name of the section in it.

The Settings section (Figure 25, left-hand side) contains several pick lists. There are two possibilities.

1. The user can select a PRA from the first pick list and the other parts of the PRA will be selected automatically
2. The user may specify the separate parts defining a PRA (i.e. application scheme, pesticide, physical scenarios).

The Results section contains input data, output of an intermediate calculation or output data of all four assessments. The label, value and unit of the parameters are given in the Results section.

You can hide or show the data of an assessment by clicking on the coloured bar with the name of the assessment in it. Depending on the size of your screen it might be necessary to hide the data of the other assessments to make the data of the Dietary assessment. The vertical grey bars on the right hand side can be used to scroll up and down the data.

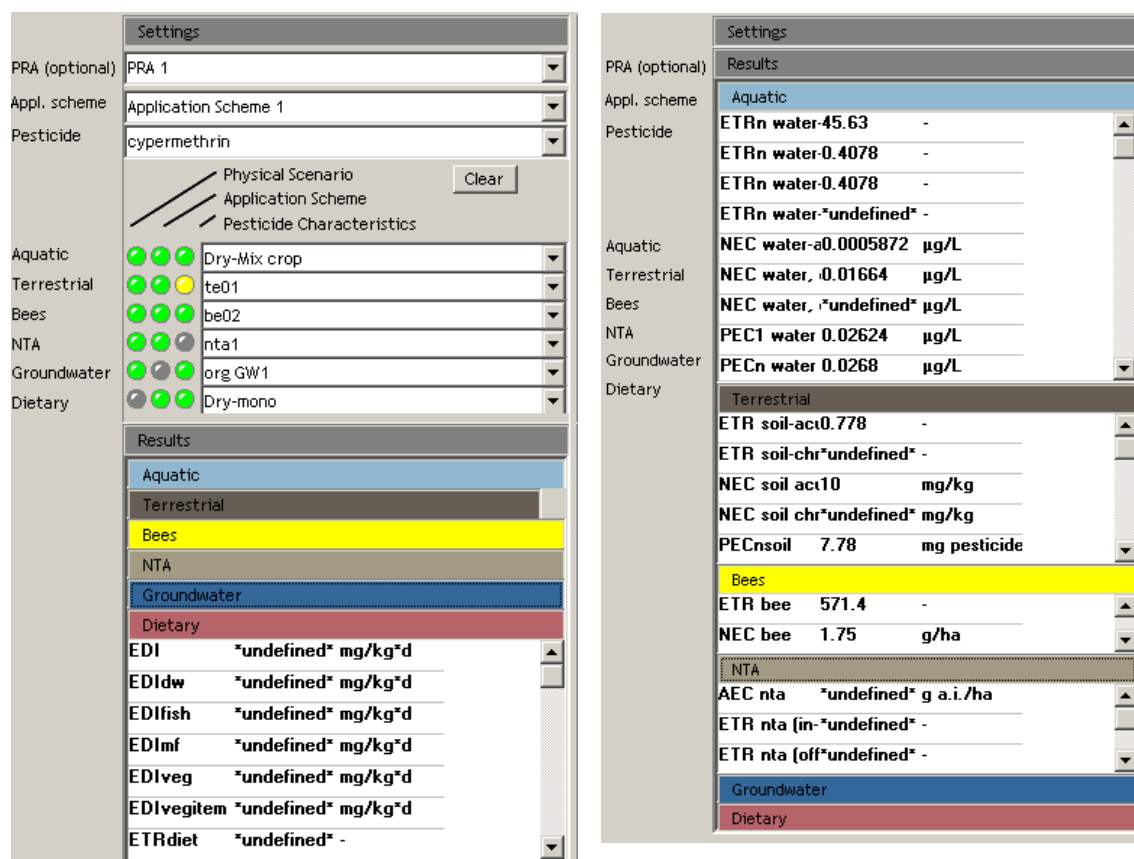


Figure 25. Selection column of a PRA is lifted out of the Compare screen. Clicking on the header will shrink of

The Compare screen also contains a button [Export PRAs to MS Excel](#) to export the data to a MS excel file. An extra column containing the description of the parameter is added to the Excel file

3.7 Options

The functionalities of the buttons in the Options section of the Status bar (Figure 26) are discussed in this Chapter.

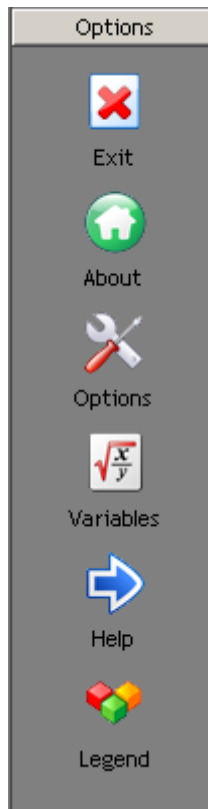


Figure 26. The buttons in the Options section of the Selection Panel

3.7.1 Button Exit

Clicking on the Exit button will close PRIMET.

3.7.2 Button About

A click on the 'About' button shows the About PRIMET screen. The screen contains three tabs: About PRIMET, Authors and Licence.

The About PRIMET tab gives information about the version and specifies some links to homepages of the companies and projects related to PRIMET. The tab Authors gives the email addresses of the authors of PRIMET. The Licence tab gives relevant information about the terms and conditions for using PRIMET.

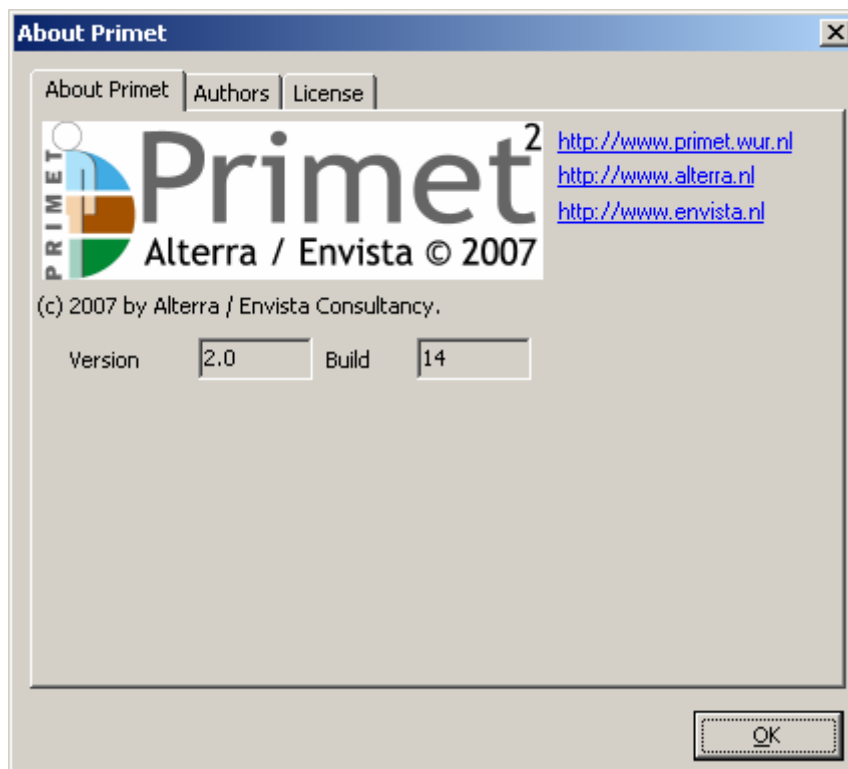


Figure 27. The About PRIMET screen

3.7.3 Button Options

The PRIMET properties screen (Figure 28) appears after clicking the button Options.

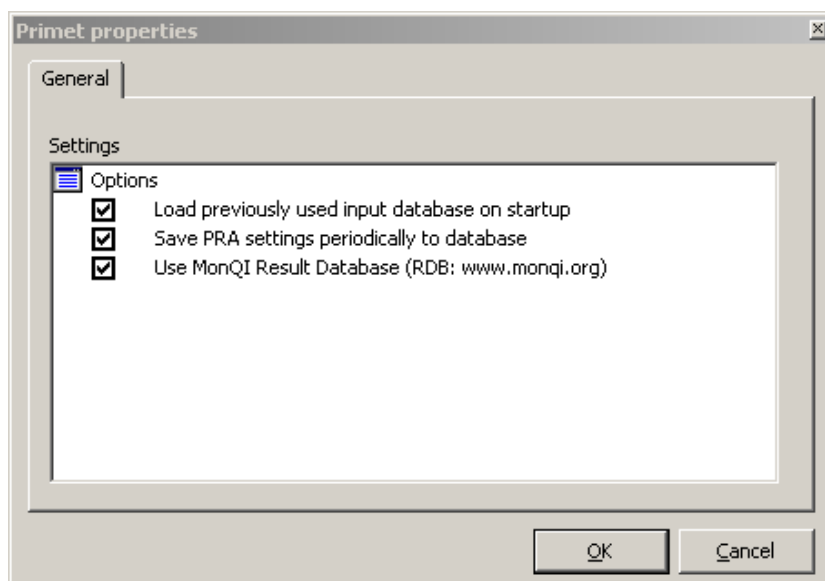
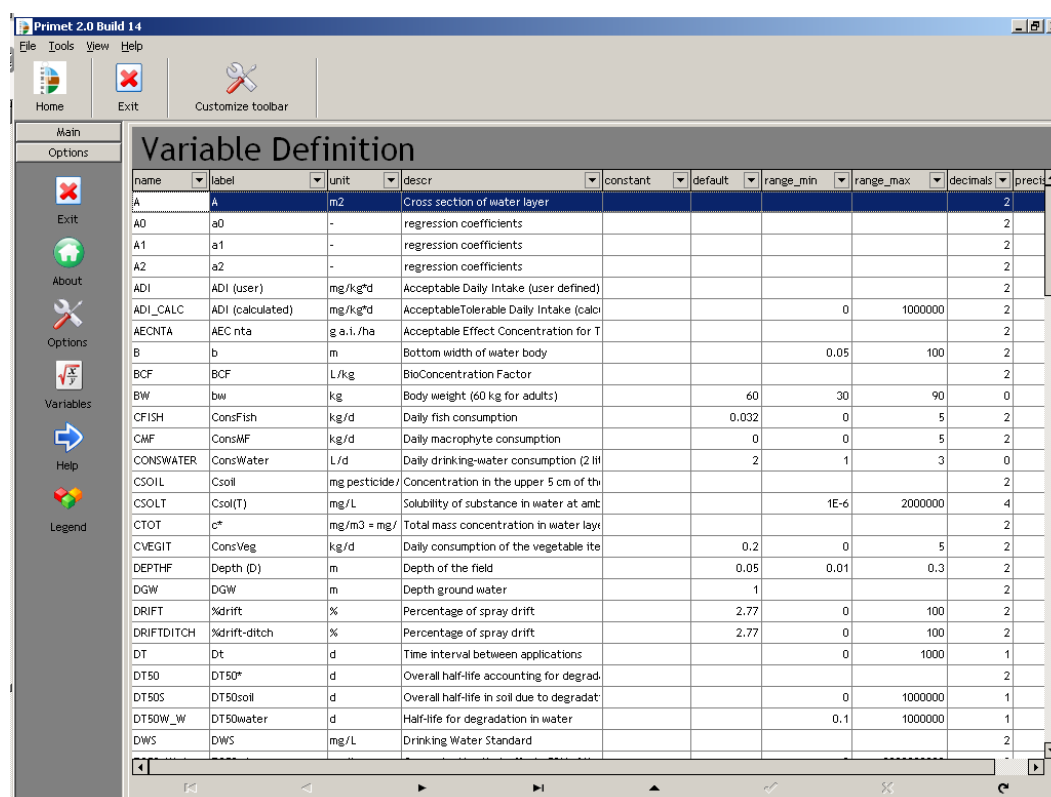


Figure 28. The PRIMET properties screen

If you want to work with a MonQI database, then select the option 'Use MonQI Result Database'. This option is default unselected. Standard the options 'Load previously used input database on start-up' and 'Save PRA settings periodically to database' are selected.

3.7.4 Button Variables

In the Variable Definition screen the user is able to check background information of the different parameters of PRIMET. If a parameter is a constant, its value is given in the table. In addition the range, precision (number of figures in which the value is expressed) and the number of decimals with which the value is displayed are specified in the table.



name	label	unit	descr	constant	default	range_min	range_max	decimals	prec
A	A	m2	Cross section of water layer						2
A0	a0	-	regression coefficients						2
A1	a1	-	regression coefficients						2
A2	a2	-	regression coefficients						2
ADI	ADI (user)	mg/kg*d	Acceptable Daily Intake (user defined)						2
ADI_CALC	ADI (calculated)	mg/kg*d	AcceptableTolerable Daily Intake (calculated)			0	1000000		2
AECNTA	AEC nta	g a.i./ha	Acceptable Effect Concentration for T						2
B	b	m	Bottom width of water body			0.05	100		2
BCF	BCF	L/kg	BioConcentration Factor						2
BW	bw	kg	Body weight (60 kg for adults)		60	30	90		0
CFISH	ConsFish	kg/d	Daily fish consumption		0.032	0	5		2
CMF	ConsMF	kg/d	Daily macrophyte consumption		0	0	5		2
CONSWATER	ConsWater	L/d	Daily drinking-water consumption (2 lit)		2	1	3		0
CSOIL	Csoil	mg pesticide/	Concentration in the upper 5 cm of the						2
CSOLT	Csol(T)	mg/L	Solubility of substance in water at ambient			1E-6	2000000		4
CTOT	c*	mg/m3 = mg/	Total mass concentration in water layer						2
CVEGIT	ConsVeg	kg/d	Daily consumption of the vegetable intake		0.2	0	5		2
DEPTH	Depth (D)	m	Depth of the field		0.05	0.01	0.3		2
DGW	DGW	m	Depth ground water		1				2
DRIFT	%drift	%	Percentage of spray drift		2.77	0	100		2
DRIFTDITCH	%drift-ditch	%	Percentage of spray drift		2.77	0	100		2
DT	Dt	d	Time interval between applications			0	1000		1
DT50	DT50*	d	Overall half-life accounting for degradation						2
DT50S	DT50soil	d	Overall half-life in soil due to degradation			0	1000000		1
DT50W_W	DT50water	d	Half-life for degradation in water			0.1	1000000		1
DWS	DWS	mg/L	Drinking Water Standard						2

Figure 29. The Variable Definition screen

3.7.5 Button Help

A click on the Help button should reveal the Help file. However the Help file is not yet implemented in this version of PRIMET.

3.7.6 Button Legend

Clicking on this button will show the Legend screen. This screen is already discussed in section 3.5.1 of this report.

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