

PRIMET version 1.0, manual and technical description

PRIMET version 1.0, manual and technical description

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

P. J. Van den Brink^{1,2}

M.M.S. Ter Horst¹

W.H.J. Beltman¹

J. Vlaming³

H. (Rik) van den Bosch¹

¹ Alterra, Wageningen University and Research centre, P.O. Box 47, 6700 AA Wageningen,
The Netherlands

² Wageningen University, Department of Aquatic Ecology and Water Quality Management,
Wageningen University and Research centre, P.O. Box 8080, 6700 DD Wageningen,
The Netherlands

³ Envista Consultancy, Tarthorst 1035, 6708 JJ, Wageningen, The Netherlands

Alterra-Report 1185

Alterra, Wageningen, 2005

ABSTRACT

Brink, P.J., van den, M.M.S. ter Horst, W.H.J. Beltman, J. Vlaming & H. (Rik) van den Bosch,, 2005. *PRIMET version 1.0, manual and technical description. A Decision Support System for assessing Pesticide Risks in the tropics to Man, Environment and Trade.*. Wageningen, Alterra, Alterra-Report 1185. 60 blz. 25 figs.; 1 tables.; 17 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 and soil and might also pose risks to humans via dietary exposure, in case they consume contaminated aquatic 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 is freely available at www.primet.wur.nl.

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

ISSN 1566-7197

This report can be ordered by paying € 30,- to bank account number 36 70 54 612 by name of Alterra Wageningen, IBAN number NL 83 RABO 036 70 54 612, Swift number RABO2u nl. Please refer to Alterra-Report 1185. This amount is including tax (where applicable) and handling costs.

© 2005 Alterra

P.O. Box 47; 6700 AA Wageningen; The Netherlands

Phone: + 31 317 474700; fax: +31 317 419000; e-mail: info.alterra@wur.nl

No part of this publication may be reproduced or published in any form or by any means, or stored in a database or retrieval system without the written permission of Alterra.

Alterra assumes no liability for any losses resulting from the use of the research results or recommendations in this report.

Contents

Preface	9
Summary	11
1 Introduction	13
2 Incorporated processes and calculations	15
2.1 Introduction	15
2.2 Aquatic risk assessment	15
2.2.1 Aquatic exposure assessment	15
2.2.1.1 Limitations of approach	15
2.2.1.2 Steps in calculating the aquatic exposure	16
2.2.1.3 Temperature dependent pesticide parameters	16
2.2.1.4 Calculation of the overall dissipation rate coefficient	17
2.2.1.5 Calculation of PEC^1_{water} for one application	20
2.2.1.6 Calculation of PEC^n_{water} for multiple applications	22
2.2.2 Aquatic effect assessment	22
2.2.3 Aquatic risk assessment	23
2.2.4 List of parameters needed for the aquatic risk assessment	23
2.2.4.1 Input watercourse parameters	23
2.2.4.2 Input pesticide parameters	23
2.2.4.3 Input pesticide application parameters	24
2.2.4.4 (Possible) constant parameters	24
2.2.4.5 Calculated parameters	24
2.3 Terrestrial risk assessment	25
2.3.1 Terrestrial exposure assessment	25
2.3.2 Terrestrial effect assessment	26
2.3.3 Terrestrial risk assessment	26
2.3.4 List of parameters needed for the terrestrial risk assessment	26
2.3.4.1 Input soil scenario parameters	26
2.3.4.2 Input pesticide parameters	26
2.3.4.3 Input pesticide application parameters	27
2.3.4.4 (Possible) constant parameters	27
2.3.4.5 Calculated parameters	27
2.4 Groundwater risk assessment	27
2.4.1 Groundwater exposure assessment	27
2.4.2 Groundwater effect assessment	28
2.4.3 Groundwater risk assessment	28
2.4.4 Parameters groundwater risk assessment	29
2.4.4.1 Input soil scenario parameters	29
2.4.4.2 Input pesticide parameters	29
2.4.4.3 Input pesticide application parameters	29
2.4.4.4 (Possible) constant parameters	29

2.4.4.5	Calculated parameters	29
2.5	Dietary risk assessment	30
2.5.1	Dietary exposure assessment	30
2.5.1.1	Considered food items and diet	30
2.5.1.2	Consumption via drinking water	30
2.5.1.3	Consumption via fish	30
2.5.2	Consumption via macrophytes	31
2.5.2.1	Consumption via vegetables	32
2.5.2.2	Calculation of Estimated Daily Intake	32
2.5.3	Dietary effect assessment	33
2.5.4	Dietary risk assessment	33
2.5.5	Parameters dietary risk assessment	33
2.5.5.1	Input diet scenario parameters	33
2.5.5.2	Input pesticide parameters	34
2.5.5.3	Input pesticide application parameters	34
2.5.5.4	(Possible) constant parameters	34
2.5.5.5	Calculated parameters	34
3	User manual	35
3.1	Getting Started	35
3.1.1	The start screen of PRIMET	35
3.1.2	Menu's in the menu bar	35
3.1.2.1	File	36
3.1.2.2	Tools	36
3.1.2.3	View	37
3.1.2.4	Help	37
3.1.3	The toolbar	37
3.1.4	The selection panel	37
3.2	The Home screen	37
3.2.1	Database	38
3.2.2	Manage PRA	38
3.2.3	Selection	39
3.2.4	Assessments	40
3.3	Input to a PRA	41
3.3.1	General	41
3.3.2	Pesticide	42
3.3.3	Application Scheme	44
3.3.4	The physical scenario Aquatic	45
3.3.5	Terrestrial	46
3.3.6	Groundwater	47
3.3.7	Dietary	48
3.4	Output of a PRA	50
3.4.1	Output via the Home screen; the Results screen	50
3.4.2	Output via the Compare button	52
3.5	Options	54
3.5.1	Button Options	55
3.5.2	Button Variables	55
3.5.3	Button Legend	56

3.5.4	Button Help	56
3.5.5	Button About	56
3.5.6	Button Exit	57
	Literature	59

Preface

The decision support system (DSS) described in this report can be used to assess the risks of pesticide use on aquatic and terrestrial ecosystems, groundwater and human health via dietary exposure. The DSS was developed within the scope of two projects, the MAPET and MAMAS project.

The MAPET project (MANaging Pesticides in vegetable systems in South-east Asia: combining Environment and Trade) is partly financed by the Asia Pro Eco Programme of the European Union (Contract Identification number ASI/B7-301/2598/01-2003/62752) and partly financed by partners own resources. The team consists of seven partners and is coordinated by (The Netherlands). The other partners include the Institute of Aquaculture at the University of Stirling (UK), Agricultural Economics Institute (The Netherlands), Asian Institute of Technology (Thailand), Soil Fertility Institute (China) and Hanoi Agricultural University (Vietnam).

The MAMAS project (Managing Agrochemicals in Multi-Use Aquatic Systems) is largely financed by the European Union INCO-DEV program (Contract Identification number ICA4-CT-2001-10031). The Alterra contribution is also part of the DLO Research Programme International Co-operation (North-South program) sponsored by the Dutch Ministry of Agriculture, Nature Management and Fisheries. Additional support was obtained from the Department for International Development (DFID) Aquaculture and Fish Genetics Research Programme of the United Kingdom. The team consists of seven partners and is coordinated by the Institute of Aquaculture at the University of Stirling (UK). The other partners include: Alterra (The Netherlands), University of Aveiro (Portugal), University of Peradeniya (Sri Lanka), Asian Institute of Technology (AIT, Thailand), Kasetsart University (Thailand) and National Aquatic Resources research and development Agency (NARA, Sri Lanka).

The authors want to thank all project partners with their help developing the decision support system! For more information is referred to www.mapet.nl and www.mamasproject.org.

Summary

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 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 and soil and might also pose risks to humans via dietary exposure, in case they consume contaminated aquatic products like groundwater, macrophytes and fish. To estimate these risks the PRIMET Decision Support System was developed. This DSS is able to estimate the risks of pesticide application to 1) aquatic life, 2) terrestrial life, 3) the use of groundwater as drinking water and 4) 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 on a farmers level is needed as input parameters. The risk assessment is expressed in Exposure Toxicity Ratio's (ETR) which are calculated by dividing the exposure by the safe concentration. These ETR's are calculated for the aquatic ecosystem adjacent to the field (ETR_{water}), for the soil compartment within the field (ETR_{soil}), the use of groundwater as drinking water (ETR_{gw}) and dietary exposure (ETR_{diet}). 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 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 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 and soil and might also pose risks to humans via dietary exposure, in case they consume contaminated aquatic products like groundwater, macrophytes and fish. To estimate these risks the PRIMET Decision Support System was developed. This DSS is able to estimate the risks of pesticide application to 1) aquatic life, 2) terrestrial life, 3) the use of groundwater as drinking water and 4) 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 a 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 safety 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 models (e.g. PEARL, TOXSWA, PERPEST). If ETR's are very large (e.g. >100) risks are quite certain although the methods used are based on worst-case assumptions.

For all risk assessments standard parameters of the active ingredient have to be available. This includes toxicity data, dissipation velocities, sorption characteristics, etc. For most common active ingredients the required data are included in the PRIMET 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.

To assess the risk to surface water a physical scenario has to be developed representative for the area of interest. This means that the geometry of the watercourse has to be estimated as well as water flow velocity and organic matter content of suspended solids and the sediment layer. This will involve field measurements and laboratory analysis.

For groundwater assessments a set of scenarios is included in the PRIMET database. A scenario is a combination of different blocks. Four types of building blocks exist: soil types, climates, time of application and irrigation schemes. Scenarios can only be added by the developers of PRIMET, so to do this the user has to supply the data. To add an extra scenario to the database a series of daily meteorological data for at least 5 consecutive years, a detailed soil profile description plus data on bulk density, organic matter and texture per layer are required. Besides a scenario a groundwater assessment requires information on crop and dose applied. To add a new crop to the database, data on leaf area index, soil cover and water extraction characteristics of the crop have to be delivered. Before starting the data gathering, please contact the developers of PRIMET.

For the dietary exposure assessment estimates are required of the daily fish, macrophyte and vegetable consumption. For the terrestrial assessment no additional data are required.

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, 3) the use of groundwater as drinking water and 4) 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 the human consumption of the groundwater below the treated field and the human consumption of fish and macrophytes (aquatic waterplants) present in the watercourse adjacent to the treated field as well as the cultivated crop. For all four 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 and the use of assessment 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 four 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. This PEC is an instantaneous PEC (peak concentration), not a time weighed average exposure concentration. 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 PECs four 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.

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 $DegT50_{water}$ was determined (K), see Eq. (4)
- $k_w(T)$ = degradation rate coefficient at ambient temperature (1/d)
- $k_w(T_{refkw})$ = degradation rate coefficient at reference temperature (1/d)
- E = molar Arrhenius activation energy (J/mol)
- R = universal gas constant (≈ 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:

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

(Van den Berg and Boesten, 1998) with,

- T = ambient temperature in scenario (K)
- T_{refP} = reference temperature, at which $P(T_{refP})$ was determined (K)
- $P(T)$ = saturated vapour pressure of substance at ambient temperature (Pa)
- $P(T_{refP})$ = saturated vapour pressure of substance at reference temperature (Pa)
- ΔH_p = enthalpy of vaporization (J/mol)
- R = universal gas constant (≈ 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:

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

(Van den Berg and Boesten, 1998) with,

- T = ambient temperature in scenario (K)
- T_{refC} = reference temperature, at which $C_{sol}(T_{refC})$ was determined (K)
- $C_{sol}(T)$ = solubility of substance in water at ambient temperature (g/m^3)
- $C_{sol}(T_{refC})$ = solubility of substance in water at reference temperature (g/m^3)
- ΔH_{sol} = enthalpy of dissolution (J/mol)
- R = universal gas constant (≈ 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 (section 2.2.1.5)

Degradation rate

The $DegT50_{water}$ is an input parameter for PRIMET, from which $k_w(T_{refkw})$ can be calculated using Eq. (4):

$$k_w(T_{refkw}) = \frac{Ln(2)}{DegT50_{water}} \quad (4)$$

with,

$k_w(T_{refw})$ = degradation rate coefficient at reference temperature (1/d)

$DegT50_{water}$ = 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):

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

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

with,

O_x = width of the water surface (m)

b = water depth of watercourse (m)

b = bottom width of watercourse (m)

s_1 = side slope, horizontal/vertical (-)

A = cross section of water layer (m²)

According to Liss and Slater (1974), exchange coefficients of the pesticide in air (k_g) and water (k_l) 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);
- M_{CO_2} = molecular weight of CO₂ (= 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_{g,H_2O} of 720 m/d).
- M_{H_2O} = molecular weight of H₂O (= 18 g/mol);
(Adriaanse, 1996; Beltman and Adriaanse, 1999).

The Henry coefficient can be calculated by:

$$K_H = \frac{P(T) \cdot M_{pesticide}}{R \cdot T \cdot C_{sol}(T)} \quad (10)$$

(Adriaanse, 1996) with,

- K_H = dimensionless Henry coefficient (-)
- $P(T)$ = saturated vapour pressure of substance at ambient temperature (Pa)
- $M_{pesticide}$ = molecular weight of the pesticide under investigation (g/mol)
- R = universal gas constant (≈ 8.3144 J/mol K)
- T = ambient temperature in scenario (K)
- $C_{sol}(T)$ = solubility of substance in water at ambient temperature (g/m³)

If the $C_{sol}(T)$ 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,

τ = residence time (d)
 L = length of the watercourse (m)
 v = flow velocity (m/d)

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

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

with,

k_{τ} = dilution rate coefficient (1/d)
 τ = residence time (d)

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):

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

with,

k^* = overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)
 $k_m(T)$ = degradation rate coefficient at ambient temperature (1/d)
 k_v = volatilization rate coefficient (1/d)
 k_{τ} = dilution rate coefficient (1/d)

Where the overall half-life DT50* then becomes:

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

with,

k^* = overall dissipation rate coefficient accounting for degradation, volatilization and dilution (1/d)
 $DT50^*$ = overall half-life accounting for degradation, volatilization and dilution (d)

2.2.1.5 Calculation of PEC_{water}^1 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):

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

with,

- c^* = total mass concentration in water layer ($\text{mg}/\text{m}^3 = \mu\text{g}/\text{L}$)
- M = dose applied ($\text{g a.i.}/\text{ha}$)
- $\%drift$ = percentage of spray drift (%)
- 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 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 watercourse (m)
- b = bottom width of watercourse (m)
- s_1 = side slope, horizontal/vertical (-)
- 1 = length of watercourse

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

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

(Adriaanse, 1996) with,

- PEC_{water}^f = 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 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)

2.2.2 Aquatic effect assessment

For the effect assessment a 'safe' concentration is calculated from toxicity values for some standard test species and an assessment 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 assessment factor (e.g. EU, 1997). The assessment factor is needed to extrapolate from a 50% effect to no effect and to account for interspecies variation. The No Effect Concentration is calculated using:

$$NEC_{water} = \text{lowest value of:} \\ \begin{aligned} &0.01 \text{ LC50 or EC50 fish} \\ &0.01 \text{ LC50 or EC50 } Daphnia \\ &0.1 \text{ EC50 algae} \end{aligned} \quad (20)$$

with,

- NEC_{water} = No Effect Concentration for the water compartment ($\mu\text{g/L}$)
- LC50 = concentration that kills 50% of the test organisms ($\mu\text{g/L}$)
- EC50 = concentration that affects 50% of the test organisms (immobilisation in case of *Daphnia* and fish and growth inhibition in case of algae; $\mu\text{g/L}$)
- 0.01 = assessment factor
- 0.1 = assessment factor

2.2.3 Aquatic risk assessment

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

$$ETR_{water}^n = PEC_{water}^n / NEC_{water} \quad (21)$$

ETR_{water}^n = Exposure Toxicity Ratio due to n applications (-)

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

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

If	$ETR_{water}^n < 1$	No Risk (indicated by a green colour)
	$1 < ETR_{water}^n < 100$	Possible risk (orange)
	$ETR_{water}^n > 100$	Risk (red)

2.2.4 List of parameters needed for the aquatic risk assessment

2.2.4.1 Input watercourse parameters

T	= ambient temperature in scenario (K)
L	= length of the watercourse (m)
v	= flow velocity (m/d)
h	= water depth of watercourse (m)
b	= bottom width of watercourse (m)
s_1	= side slope, horizontal/vertical (-)
ss	= mass concentration of suspended solids in water (kg/L)
$m_{om,ss}$	= mass fraction organic matter in suspended solids (g/g)

2.2.4.2 Input pesticide parameters

T_{refkw}	= reference temperature, at which $K_w(T_{ref})$ or $DegT50_{water}$ was determined (K)
T_{refP}	= reference temperature, at which $P(T_{refP})$ was determined (K)
$P(T_{refP})$	= saturated vapour pressure of substance at reference temperature (Pa)
T_{refC}	= reference temperature, at which $C_{sol}(T_{refC})$ was determined (K)
$c_{sol}(T_{refC})$	= solubility of substance in water at reference temperature (g/m^3)
$DegT50_{water}$	= half-life for degradation in water (d)
$M_{pesticide}$	= molecular weight of the pesticide under investigation
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	= concentration that kills 50% of the test organisms ($\mu\text{g/L}$)
EC50	= concentration that affects 50% of the test organisms ($\mu\text{g/L}$)

2.2.4.3 Input pesticide application parameters

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

2.2.4.4 (Possible) constant parameters

E	= molar Arrhenius activation energy (= 54000 J/mol)
R	= universal gas constant (≈ 8.3144 J/mol*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

$k_d(T_{ref})$	= degradation rate coefficient at reference temperature (1/d)
$P(T)$	= saturated vapour pressure of substance at ambient temperature (Pa)
$k_d(T)$	= degradation rate coefficient at ambient temperature (1/d)
$c_{sol}(T)$	= 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 = μ g/L)
V_1	= ratio between volume and surface of watercourse (m)
K_{om}	= sorption coefficient on organic matter (L/kg). Only when K_{oc} is available
PEC_{water}^1	= momentary water concentration from a single application (μ g/L)
PEC_{water}^n	= momentary water concentration from n applications (μ g/L)
NEC_{water}	= No Effect Concentration for the water compartment (μ g/L)
ETR_{water}^n	= Exposure Toxicity Ratio due to n applications (-)

2.3 Terrestrial risk assessment

2.3.1 Terrestrial exposure assessment

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 5 cm of the soil.

$$C_{soil} = \frac{0.1 \cdot M}{DEPTHF} \quad (22)$$

with,

C_{soil} = concentration in the upper 5 cm of the soil (mg pesticide/m³ soil)

0.1 = correction factor to convert from g/ha to mg/m²

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

DEPTHF = depth of the field is 0.05 (m)

The Predicted Environmental Concentration (PEC) for the soil compartment after one application is:

$$PEC_{soil}^1 = \frac{C_{soil}}{\rho_b} \quad (23)$$

with,

PEC_{soil}^1 = concentration in the upper 5 cm of the soil from one application (mg pesticide/kg soil)

C_{soil} = concentration in the upper 5 cm of the soil (mg pesticide/m³ soil)

ρ_b = dry bulk density soil (kg soil/m³ soil)

The average bulk dry densities recorded by Koorevaar et al. (1983) for different surface soils are:

Sandy soils: 1600 kg/m³

Clay soils: 1100 kg/m³

Loamy soils: 1100 kg/m³

Peat soils: 250 kg/m³

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

$$PEC_{soil}^n = PEC_{soil}^1 \frac{1 - e^{-n \cdot k_s \cdot \Delta t}}{1 - e^{-k_s \cdot \Delta t}} \quad (24)$$

with,

PEC_{soil}^n = concentration in the upper 5 cm of the soil from n applications (mg pesticide/kg soil)

n = number of applications (-)

k_s = degradation rate coefficient in soil (1/d), where $k_s = \ln(2)/\text{DegT50}$

Δt = time interval between applications (d)

2.3.2 Terrestrial effect assessment

For the effect assessment a ‘safe’ concentration is calculated from toxicity values and, in case of earthworms, an assessment factor (EU, 1997). The assessment factor is needed to extrapolate from a 50% effect to no effect. The No Effect Concentration is calculated using:

$$NEC_{soil} = \text{lowest value of:} \\ \text{LD30 or ED30 beneficial arthropods or} \\ \text{0.1 x LD50 earthworms} \quad (25)$$

NEC_{soil} = No Effect Concentration for the soil compartment (mg/kg)
LD30 = concentration that kills 30% of the test organisms (mg/kg)
ED30 = concentration that affects 30% of the test organisms (mg/kg)
LD50 = concentration that kills 50% of earthworms (mg/kg)
0.1 = assessment factor

2.3.3 Terrestrial risk assessment

The risk, expressed in Exposure Toxicity Ratio (ETR) as a result of all stacked applications is:

$$ETR_{soil} = PEC_{soil}^n / NEC_{soil} \quad (26)$$

ETR_{soil} = Exposure Toxicity Ratio due to application (-)
 PEC_{soil}^n = concentration in the upper 5 cm of the soil from n applications (mg pesticide/kg soil) =
 NEC_{soil} = No Effect Concentration for the soil compartment (mg/kg)

If $ETR_{soil} < 1$ No Risk (green)
 $1 < ETR_{soil} < 100$ Possible risk (orange)
 $ETR_{soil} > 100$ Risk (red)

2.3.4 List of parameters needed for the terrestrial risk assessment

2.3.4.1 Input soil scenario parameters

ρ_b = dry bulk density soil (kg soil/m³ soil)

2.3.4.2 Input pesticide parameters

LD30 = concentration that kills 30% of the test organisms (mg/kg)
ED30 = concentration that affects 30% of the test organisms (mg/kg)
LD50 = concentration that kills 50% of the test organisms (mg/kg)

2.3.4.3 Input pesticide application parameters

M = dose applied (g a.i. ha⁻¹)

2.3.4.4 (Possible) constant parameters

0.05 = depth of the field (m)

2.3.4.5 Calculated parameters

C_{soil} = concentration in the upper 5 cm of the soil (mg pesticide/m³ soil)
 PEC_{soil}^f = concentration in the upper 5 cm of the soil (mg pesticide/kg soil)
 NEC_{soil} = No Effect Concentration for the soil compartment (mg/kg)
 ETR_{soil} = Exposure Toxicity Ratio due to application (-)
 PEC_{soil}^n = concentration in the upper 5 cm of the soil from n applications (mg pesticide/kg soil)

2.4 Groundwater risk assessment

2.4.1 Groundwater exposure assessment

Since for leaching no meta-model is available like for the surface water, leaching is incorporated in PRIMET by using tables produced by the PEARL model (Leistra et al., 2001). The most important parameters determining leaching are scenario, crop, $DegT50_{soil}$, K_{om} and dose applied. PEARL is ran with different combinations of K_{om} and $DegT50_{soil}$ for different scenarios and different crops and pesticide doses to calculate the annual average concentration in soil moisture at 1 m depth. An interpolation program is ran within the PRIMET tool to give the user the opportunity to calculate the annual average concentration at 1 m depth for specific values for K_{om} and $DegT50_{soil}$ given a certain scenario, crop and application dose.

Limitations

The program to run PEARL in sequence for different combinations of K_{om} - $DegT50_{soil}$ only works for PEARL 1.1.1.

Input

The input that has to be provided by the user of PRIMET are K_{om} , $DegT50_{soil}$, scenario, crop and dose. The user can, however, only choose between fixed values of dosages present in the PRIMET model and only between a certain number of crops. A scenario is a description of the location (weather and soil parameters), irrigation and time of application. Use $M_{stacked}$ i.e. the summation of all dosages applied during a growing season as dose.

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

$$K_{om} = \frac{K_{oc}}{1.724} \quad (27)$$

(FOCUS, 2001) with,

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

2.4.2 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 Tolerable Daily Intake (TDI) which is calculated from toxicity studies performed with e.g. rats:

$$TDI = \frac{NOEL \text{ or } NOAEL}{AF} \quad (28)$$

with,

TDI = Tolerable Daily Intake (mg/kg*d)
 $NOEL$ = No Observed Effect Level (mg/kg*d)
 $NOAEL$ = No Observed Adverse Effect Level (mg/kg*d)
 AF = assessment factor to account for interspecies and intraspecies extrapolation, adequacy of study, nature and severity of effect. Normally a value of 100 is used (-)

The Acceptable Daily Intake (ADI) as set by the FAO (JMPR, 2003) can also be used as a good estimate for the TDI. The TDI is converted to a Drinking Water Standard using (WHO, 1996):

$$DWS = \frac{TDI \cdot bw \cdot P}{C_{water}} \quad (29)$$

with,

DWS = Drinking Water Standard (mg/L)
 TDI = Tolerable Daily Intake (mg/kg*d)
 bw = course weight (60 kg for adults)
 P = fraction of the TDI allocated to drinking-water (default 0.1)
 $ConsWater$ = daily drinking-water consumption (2 litres for adults, L/d).

2.4.3 Groundwater risk assessment

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

$$ETR_{gw} = \frac{PEC_{gw}}{DWS \cdot 1000} \quad (30)$$

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 $ETR_{gw} < 1$ No Risk (green)
 $1 < ETR_{gw} < 100$ Possible risk (orange)
 $ETR_{gw} > 100$ Risk (red)

2.4.4 Parameters groundwater risk assessment

2.4.4.1 Input soil scenario parameters

Scenario = a scenario is a description of the location (weather and soil parameters), crop, irrigation and time of application. From picklist.

2.4.4.2 Input pesticide parameters

$DegT50_{soil}$ = overall half-life in soil (d)
 K_{om} = sorption coefficient on 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
 NOEL = No Observed Effect Level ($\text{mg/kg}\cdot\text{d}$)
 NOAEL = No Observed Adverse Effect Level ($\text{mg/kg}\cdot\text{d}$)
 AF = assessment factor

2.4.4.3 Input pesticide application parameters

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

2.4.4.4 (Possible) constant parameters

bw = course weight (60 kg for adults)
 P = fraction of the TDI allocated to drinking-water (default 0.1)
 $ConsWater$ = daily drinking-water consumption (2 litres for adults, L/d).

2.4.4.5 Calculated parameters

PEC_{gw} = annual average concentration leaching from the soil profile at 1 m depth ($\mu\text{g/L}$)
 TDI = Tolerable Daily Intake ($\text{mg/kg}\cdot\text{d}$)

DWS = Drinking Water Standard (mg/L)
 ETR_{gw} = Exposure Toxicity Ratio due to application (-)

2.5 Dietary risk assessment

2.5.1 Dietary exposure assessment

2.5.1.1 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.

2.5.1.2 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:

$$EDI_{dw} = \frac{PEC_{gw} \cdot C_{water}}{bw \cdot 1000} \quad (31)$$

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 ($\mu\text{g/L}$)

$ConsWater$ = daily drinking-water consumption (2 litres for adults, L/d)

bw = course weight (60 kg for adults)

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

2.5.1.3 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_{water}^1 or, in case

of multiple applications, the PEC_{water}^n as calculated in the surface water risk assessment, and bioconcentration factors (BCF) values for the different pesticides:

$$PEC_{\text{fish}} = \frac{PEC_{\text{water}}^n \cdot BCF}{1000} \quad (32)$$

with,

- PEC_{fish} = concentration in the fish (mg pesticide/kg fish)
- 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
- 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):

$$BCF = 10^{(0.85 \cdot \text{Log}(K_{ow}) - 0.70)} \quad (33)$$

with,

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

The EDI for fish can now be calculated using:

$$EDI_{\text{fish}} = \frac{PEC_{\text{fish}} \cdot C_{\text{fish}}}{bw} \quad (34)$$

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)
- C_{fish} = daily fish consumption (kg/d).
- bw = course weight (60 kg for adults)

2.5.2 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_{water}^1 or, in case of multiple application the PEC_{water}^n as calculated in the surface water risk assessment, and sorption coefficient values (K_d) for the different pesticides:

$$PEC_{\text{mf}} = \frac{PEC_{\text{water}}^n \cdot K_d}{1000} \quad (35)$$

with,

- PEC_{mf} = concentration in the macrophytes (mg pesticide/kg macrophyte)
- 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 ($C_{sol}(T)$) using the following relation as determined by Crum et al. (1999):

$$K_d = 3.20 - 0.65 \cdot \log[C_{sol}(T)] \quad (36)$$

with,

K_d = sorption coefficient for macrophytes (L/kg)

$C_{sol}(T)$ = solubility of substance in water at ambient temperature (g/m^3)

$C_{sol}(T)$ is calculated using Eq. (3). The EDI for fish can now be calculated using:

$$EDI_{mf} = \frac{PEC_{mf} \cdot C_{mf}}{bw} \quad (37)$$

with,

EDI_{mf} = Estimated Daily Intake due to eating of macrophytes ($\text{mg}/\text{kg} \cdot \text{d}$)

PEC_{mf} = concentration in the macrophytes (mg pesticide/ kg macrophyte)

C_{mf} = daily macrophyte consumption (kg/d).

bw = course weight (60 kg for adults)

2.5.2.1 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:

$$EDI_{vegetem} = \frac{PEC_{vegetem} \cdot C_{vegetem}}{bw} \quad (38)$$

with,

$EDI_{vegetem}$ = Estimated Daily Intake due to eating of a defined vegetable item ($\text{mg}/\text{kg} \cdot \text{d}$)

$PEC_{vegetem}$ = concentration in the defined vegetable item (mg pesticide/ kg macrophyte)

$C_{vegetem}$ = daily consumption of the vegetable item (kg/d).

2.5.2.2 Calculation of Estimated Daily Intake

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

$$EDI = EDI_{dw} + EDI_{fish} + EDI_{mf} + EDI_{veg} \quad (39)$$

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)

2.5.3 Dietary effect assessment

The effect standard is based on the Tolerable Daily Intake (TDI) which is calculated from toxicity studies performed using Eq. (28). The Acceptable Daily Intake (ADI) as set by the FAO (JMPR, 2003) can also be used as a good estimate for the TDI. Like TDI, 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.

2.5.4 Dietary risk assessment

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

$$ETR_{diet} = \frac{EDI}{TDI} \quad (40)$$

- ETR_{diet} = Exposure Toxicity Ratio due to application (-)
- EDI = Estimated Daily Intake (mg/kg*d)
- TDI = Tolerable Daily Intake (mg/kg*d)

- | | | |
|----|------------------------|------------------------|
| If | $ETR_{diet} < 1$ | No Risk (green) |
| | $1 < ETR_{diet} < 100$ | Possible risk (orange) |
| | $ETR_{diet} > 100$ | Risk (red) |

2.5.5 Parameters dietary risk assessment

2.5.5.1 Input diet scenario parameters

- PEC_{gw} = annual average concentration leaching from the soil profile at 1 m depth ($\mu\text{g/L}$)
- PEC_{water}^n = momentary water concentration from n applications ($\mu\text{g/L}$)
- C_{fish} = daily fish consumption (kg/d).
- C_{mf} = daily macrophyte consumption (kg/d).
- $C_{vegetem}$ = daily consumption of the vegetable item (kg/d).

2.5.5.2 Input pesticide parameters

- K_{ow} = Octanol-water partitioning coefficient (L/kg)
 $C_{sol}(T)$ = solubility of substance in water at ambient temperature (g/m^3)
 TDI = Tolerable Daily Intake ($\text{mg}/\text{kg}\cdot\text{d}$)

2.5.5.3 Input pesticide application parameters

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

2.5.5.4 (Possible) constant parameters

- $ConsWater$ = daily drinking-water consumption (2 litres for adults, L/d).
 bw = course weight (60 kg for adults)

2.5.5.5 Calculated parameters

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

3 User manual

3.1 Getting Started

3.1.1 The start screen of PRIMET

PRIMET is distributed as an executable with a Microsoft Access database. The executable (PRIMET.exe) and the database (PRIMET.mdb) may be placed anywhere on the pc, preferably in the same directory. To start the program, double-click the executable in the file manager. The start screen will be displayed (Figure 1).

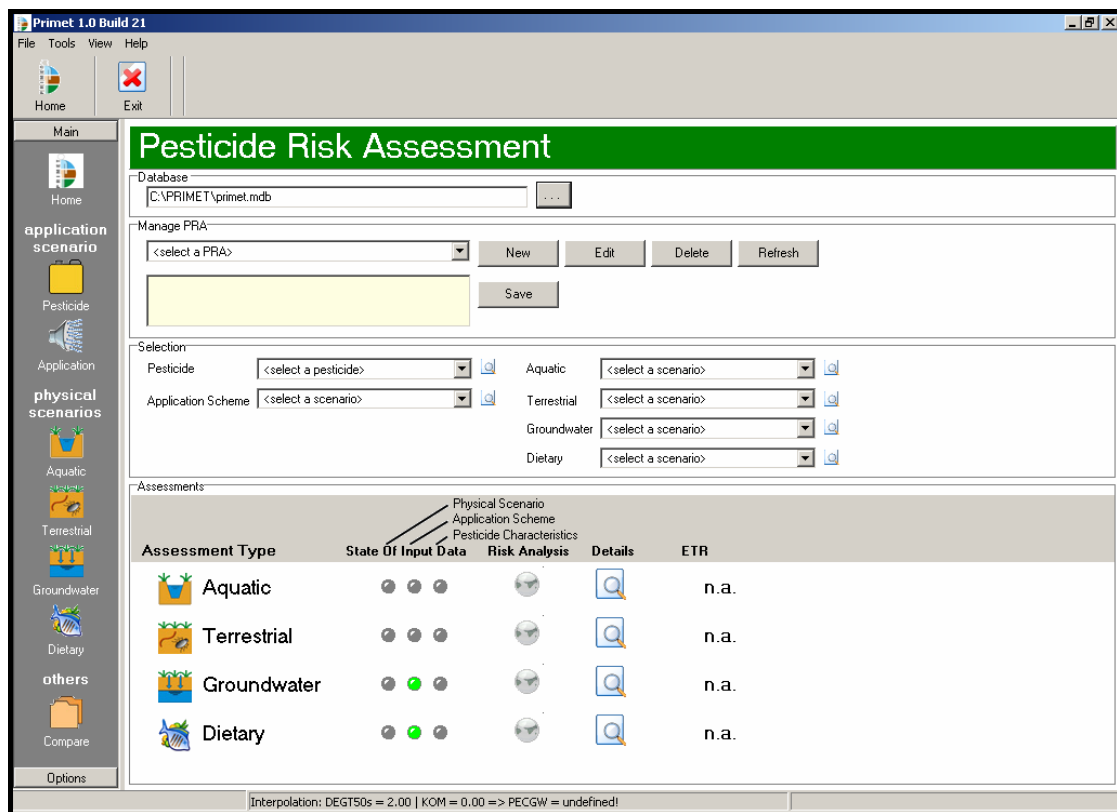


Figure 1. The start screen of PRIMET

The start screen consists of a menu bar at the top of the screen (section 3.1.2), a toolbar just below the menu bar (section 3.1.3), a selection panel at the left hand side of the screen (section 3.1.4) and a large main section in the centre of the screen (chapter 3.2).

3.1.2 Menu's in the menu bar

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

3.1.2.1 File

The 'File' menu includes two menu commands: 'select database' and 'exit'. The 'select database' option is described in more detail in section 3.2.1. A click on the 'exit' command will close PRIMET.

3.1.2.2 Tools

The commands in the menu 'Tools' are all, except for 'Customize toolbar', described in more detail in chapter 3.5. Clicking on the command 'Customize toolbar' will show Figure 2.

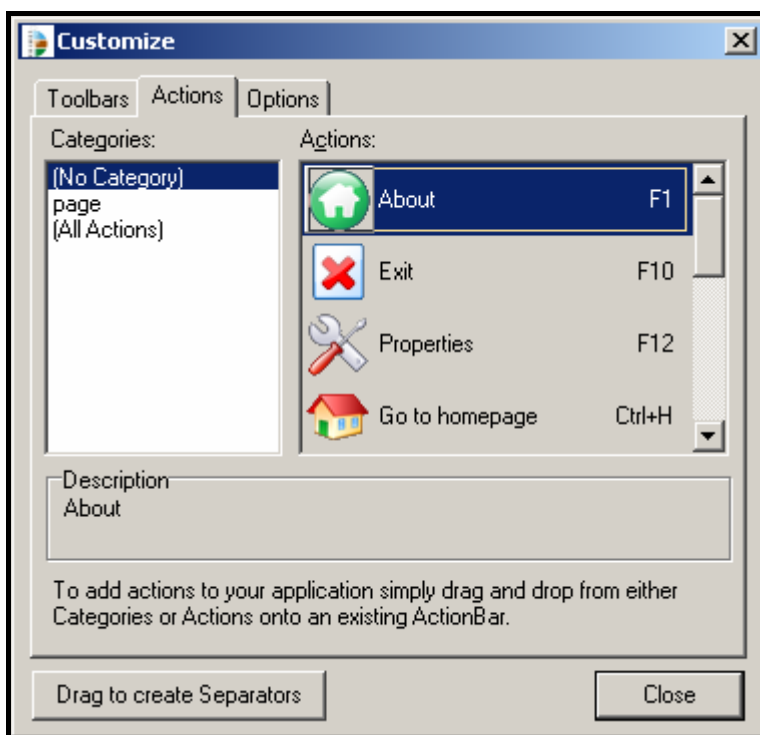


Figure 2. 'Customize toolbar dialog' in PRIMET

On the first tab ("Toolbars") in Figure 2 the visibility of the toolbar in PRIMET is set. The second tab 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 is used to personalize the menu and toolbar but is not yet in use.

3.1.2.3 View

With the command 'Show Selection Panel' the user can hide or display the selection panel. With the other commands the user can call the input screens for pesticide, application scheme and the four physical scenarios. These input screens are described in more detail in chapter 3.3.

3.1.2.4 Help

The command 'Help' and the command 'About' are described in more detail in section 3.5. 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.

3.1.3 The toolbar

The tool bar below the menu bar can be customized by the user. Buttons can be added or removed. How to do this is explained in section 3.1.2.2.

3.1.4 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 discussed in chapters 3.3 and 3.4. The buttons in the 'Options' sub level are discussed in chapter 3.5.

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 (chapter 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.

3.2 The Home screen

The Home screen can be accessed from different locations in PRIMET:

- Menu bar → menu 'View' → option 'Home'
- Tool bar → button 'Home' (if added to toolbar, see section 3.1.2.2)
- Selection Panel → button 'Main' → button 'Home'

The Home screen (Figure 3) is the main screen of PRIMET. It can be used to select the PRIMET database, to manage PRAs (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.

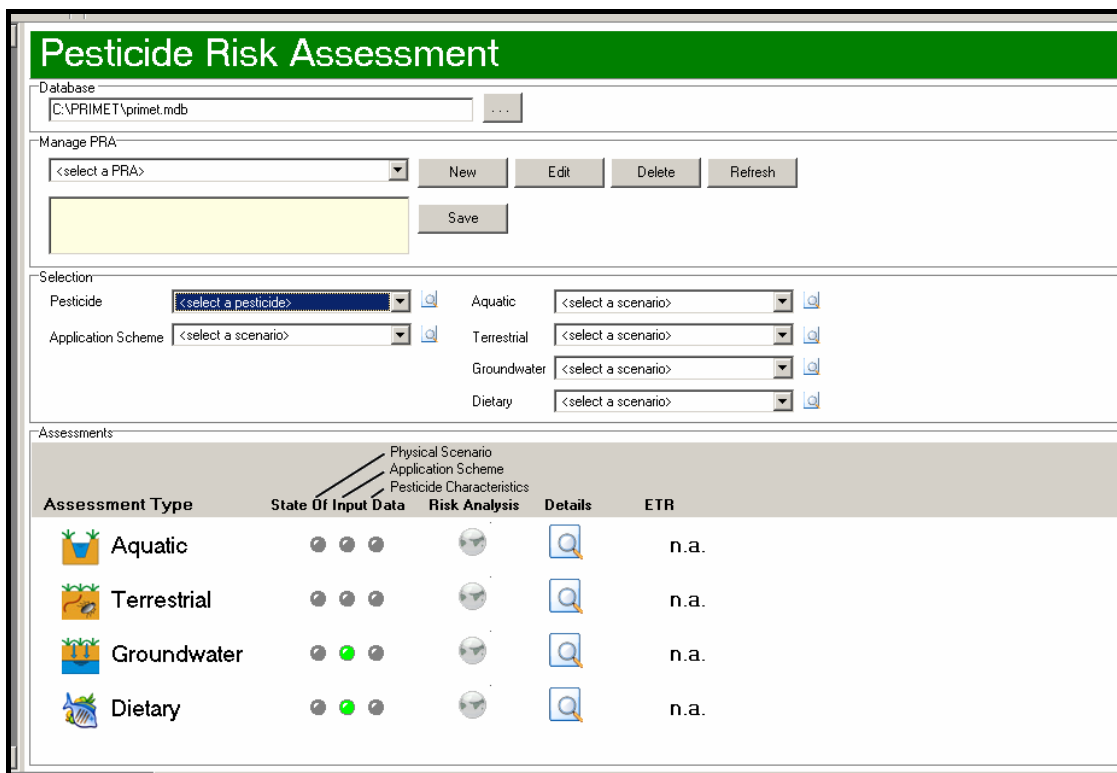


Figure 3. The Home screen

3.2.1 Database

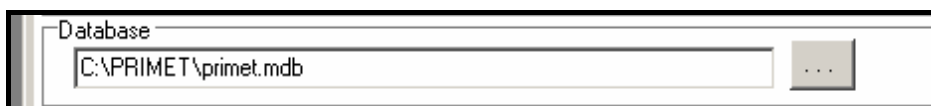


Figure 4. The Database section in the Home screen of PRIME T

The database can be selected from a browse screen. Click on the grey button with the three dots to select the PRIME T database (Figure 4). Note that a PRIME T database needs to be selected because it contains configuration information PRIME T needs. It is therefore not possible to select an arbitrary empty MS access database. If you wish to start with an empty database you can copy the existing PRIME T database, change its name and select this database in PRIME T. Subsequently you can remove all the PRA's, application scenarios and physical scenarios you won't need.

3.2.2 Manage 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).

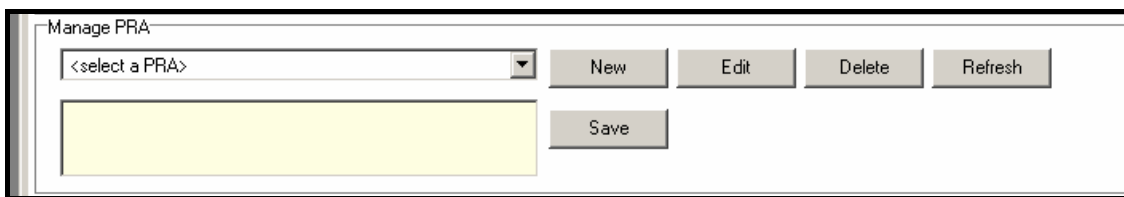


Figure 5. The Manage PRA section in the Home screen of PRIMET

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 tot 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.

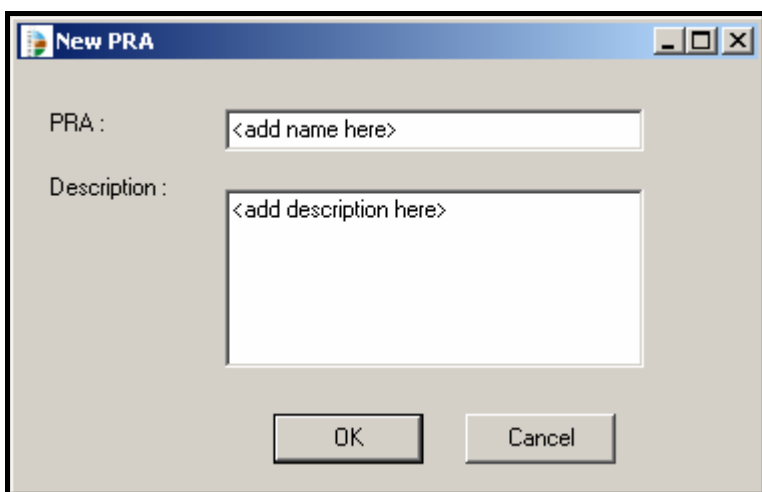


Figure 6. New/Edit PRA screen of PRIMET

It is important to realise that a PRA is only added to the database after clicking the 'Save' button.

3.2.3 Selection

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

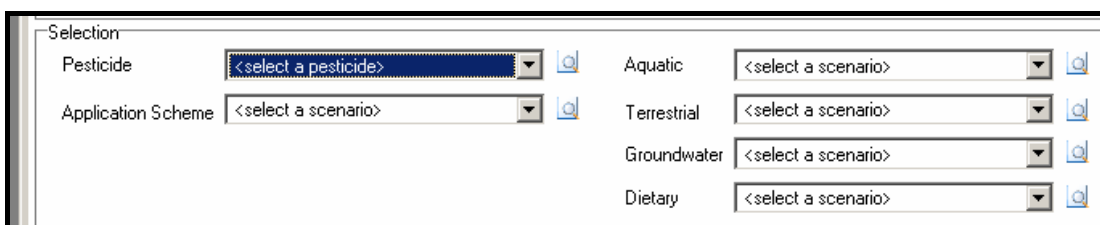


Figure 7. The Selection section in the Home screen of PRIMET

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 chapter 3.3.

3.2.4 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 is 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 is missing and output cannot be generated (i.e. Figure 8, Terrestrial; input data to the physical scenario is missing).

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 chapter 3.4.1). The risk is expressed in ETR (Exposure Toxicity Ratio) and given below 'ETR'. If some input data is missing the ETR cannot be calculated and the value n.a. (not available) is assigned to the ETR.

















Assessment Type	State Of Input Data	Risk Analysis	Details	ETR
 Aquatic				6.3
 Terrestrial				n.a.
 Groundwater				4.3E-06
 Dietary				1.7E02

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

3.3 Input to a PRA

3.3.1 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.

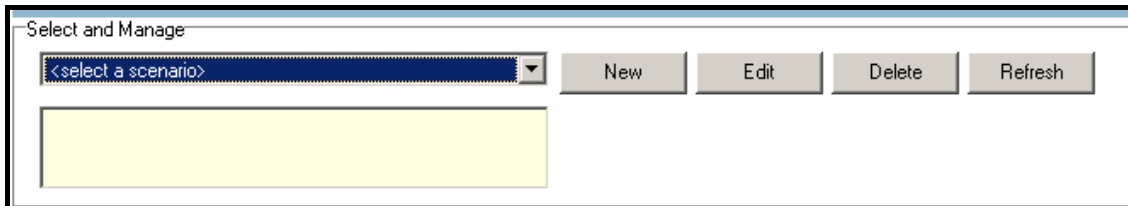


Figure 9. The Select and Manage section in the input screens of PRIMET

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.

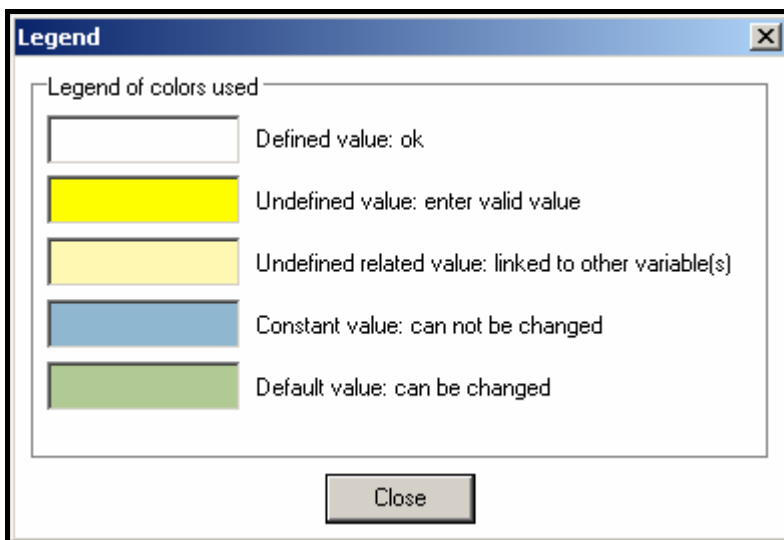


Figure 10. The Legend screen, explaining the meaning of the colours of the boxes in the input screen

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.



csol(TrefC)		<input type="text" value="8"/>	g/m3
Kow		<input type="text" value="32.3594"/>	L/kg

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

Sections 3.3.2 – 3.3.7 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.

3.3.2 Pesticide

The Pesticide input screen can be accessed from several locations:

- Menu bar → menu 'View' → option 'Pesticide'
- Tool bar → button 'Pesticide' (if added to toolbar, see section 3.1.2.2)
- Selection Panel → button 'Main' → button 'Pesticide'
- Home screen → section 'Selection' → button with magnifying glass behind 'Pesticide'

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 four parts: Aquatic, Groundwater, Dietary and Terrestrial. They correspond to the physical scenarios and the four 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 'csol(TrefC)' in the 'Aquatic' section this number is automatically copied to the 'csol(TrefC)' box in the Dietary section.

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.

Table 1 Relating parameters in the Pesticide input screen

assessment	parameters	Formula
<ul style="list-style-type: none"> ○ Aquatic ○ Aquatic 	<ul style="list-style-type: none"> ○ $K_w(T_{refkw})$ ○ DegT50 	$K_w(T_{refkw}) = \frac{\ln(2)}{\text{DegT50}}$
<ul style="list-style-type: none"> ○ Aquatic/Groundwater ○ Aquatic/Groundwater 	<ul style="list-style-type: none"> ○ K_{OM} ○ K_{OC} 	$K_{om} = \frac{K_{oc}}{1.724}$
<ul style="list-style-type: none"> ○ Soil ○ Soil/Groundwater 	<ul style="list-style-type: none"> ○ K_s ○ DegT50_{soil} 	$K_s = \frac{\ln(2)}{\text{DegT50}_{soil}}$
<ul style="list-style-type: none"> ○ Groundwater/Dietary 	<ul style="list-style-type: none"> ○ TDI ○ NOEL 	$TDI = \frac{NOEL}{AF}$

3.3.3 Application Scheme

The Application Scheme input screen can be accessed from several locations:

- Menu bar → menu 'View' → option 'Application'
- Tool bar → button 'Application' (if added to toolbar, see section 3.1.2.2)
- Selection Panel → button 'Main' → button 'Application'
- Home screen → section 'Selection' → button with magnifying glass behind 'Application Scheme'

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 two parts: Aquatic and Terrestrial, both 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 Groundwater and Dietary are not mentioned in the Application Scheme input screen. The reason for this is that the Dietary assessment does not need input of an application scheme and for the Groundwater assessment the application scheme is part of the PEARL scenario (chapter 2 incorporated processes and calculations).

Figure 13. Application Scheme input screen of PRIMET

3.3.4 The physical scenario Aquatic

The Aquatic assessment input screen can be accessed from several locations:

- Menu bar → menu 'View' → option 'Aquatic'
- Toolbar → button 'Aquatic' (if added to toolbar, see section 3.1.2.2)
- Selection Panel → button 'Main' → button 'Aquatic'
- Home screen → section 'Selection' → button with magnifying glass behind 'Aquatic'

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.

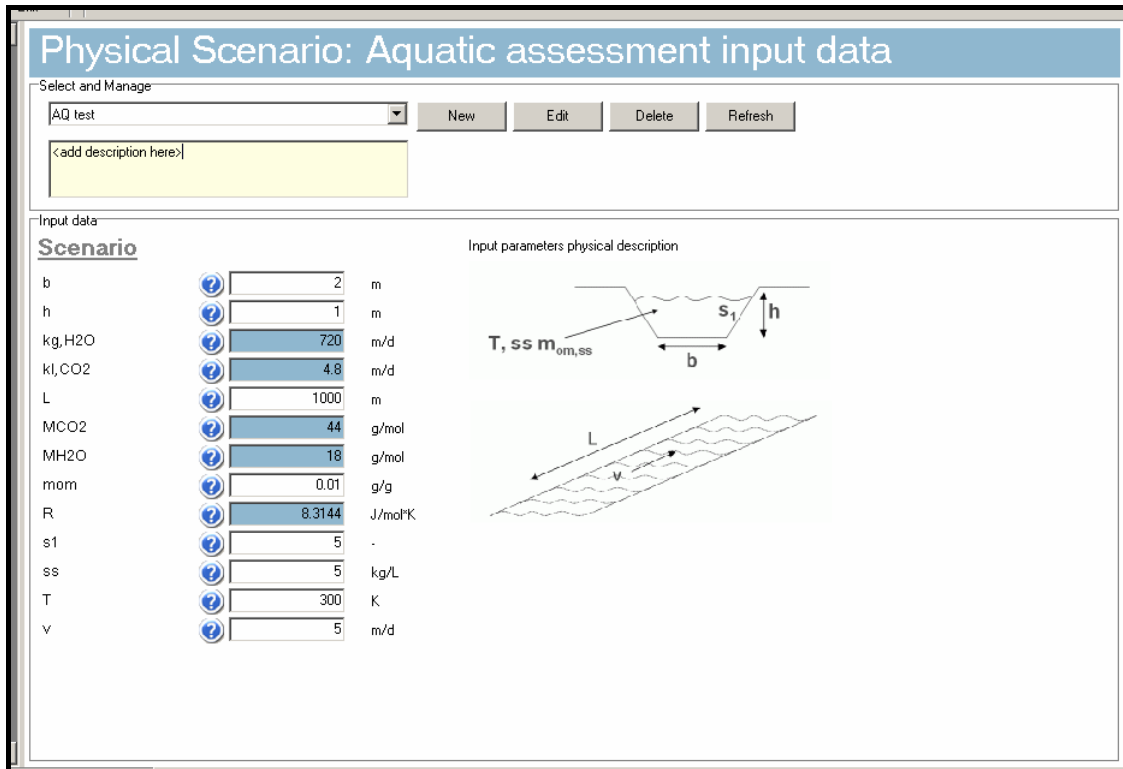


Figure 14. The Aquatic scenario input screen of PRIMET

3.3.5 Terrestrial

The Terrestrial assessment input screen can be accessed from several locations:

- Menu bar → menu 'View' → option 'Terrestrial'
- Tool bar → button 'Terrestrial' (if added to toolbar, see section 3.1.2.2)
- Selection Panel → button 'Main' → button 'Terrestrial'
- Home screen → section 'Selection' → button with magnifying glass behind 'Terrestrial'

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.

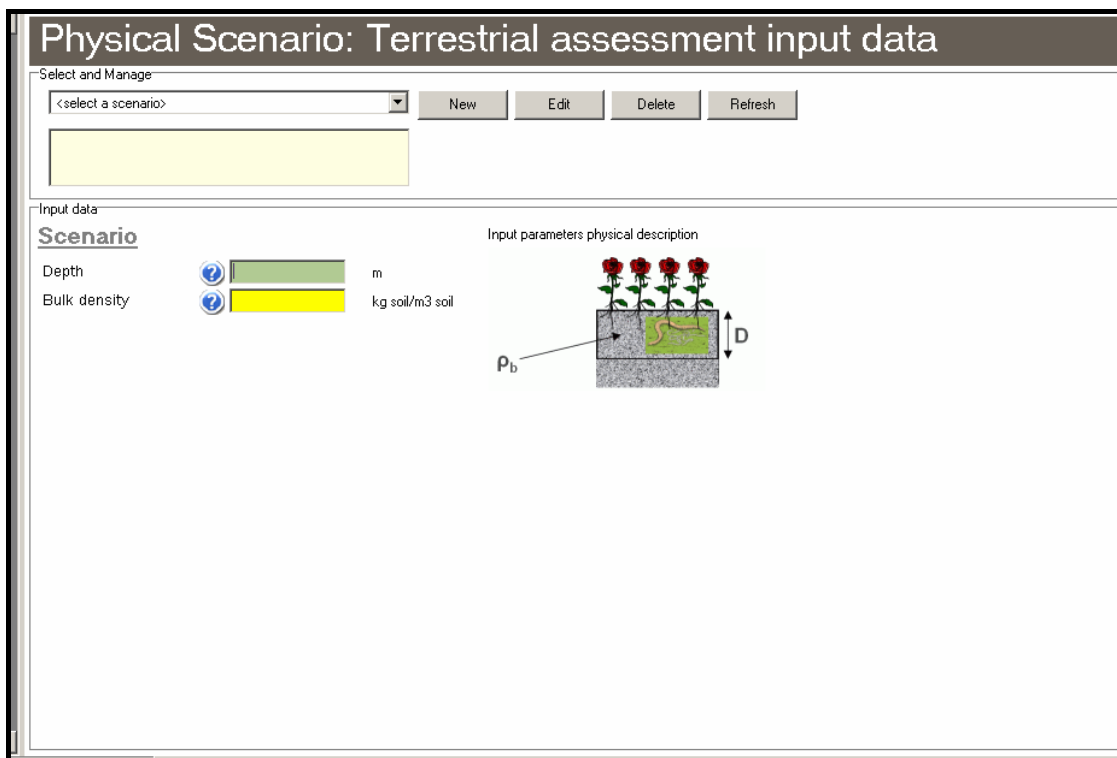


Figure 15. The Terrestrial scenario input screen of PRIMET

3.3.6 Groundwater

The Groundwater assessment input screen can be accessed from several locations:

- Menu bar → menu 'View' → option 'Groundwater'
- Tool bar → button 'Groundwater' (if added to toolbar, see section 3.1.2.2)
- Selection Panel → button 'Main' → button 'Groundwater'
- Home screen → section 'Selection' → button with magnifying glass behind 'Groundwater'

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

In the 'Input data' section the user has to select a PEARL scenario first. PEARL simulations are done for different PEARL scenarios and different combinations of K_{OM} and $DegT50_{soil}$. An interpolation program is run by PRIMET to calculate the PEC_{gp} for specific values of K_{OM} and $DegT50_{soil}$ defined in the Pesticide input screen. A PEARL scenario consists of a scenario, a crop and a dose.

The scenario is defined by the location (weather and soil parameters), irrigation and time of application. The user can only choose between values for doses fixed by the PRIMET team and a certain number of crops.

In the part 'Scenario' of the 'Input data' section the user has to fill in values for the different parameters (i.e. bw , $ConsWater$ and P , see section 2.4.4.4) required to calculate the ETR_{gw} .

Figure 16. The Groundwater scenario input screen of PRIMET

3.3.7 Dietary

The Dietary assessment input screen can be accessed from several locations:

- Menu bar → menu 'View' → option 'Dietary'
- Tool bar → button 'Dietary' (if added to toolbar, see section 3.1.2.2)
- Selection Panel → button 'Main' → button 'Dietary'
- Home screen → section 'Selection' → button with magnifying glass behind 'Dietary'

The Dietary assessment input screen is shown in Figure 17. 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.

Physical Scenario: Dietary assessment input data

Select and Manage
 DI1 [New] [Edit] [Delete] [Refresh]

<add description here>

Input data

Scenario

bw	?	60	kg
ConsFish	?	2	kg/d
ConsMF	?	2	kg/d
ConsVeg	?	2	kg/d
ConsWater	?	2	L/d
PECgw (user)	?	(6)	µg/L
PECnwater (user)	?	(7)	µg/L
PECvegitem	?	1E3	mg pesticide/kg macrophy

values derived from other scenarios

PECgw	2.19E-15	(GW)
PECn water	40.7	(AQ)

Figure 17. 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). This is illustrated in Figure 18. The screens in Figure 18 are both part of the DI1 Dietary scenario shown in Figure 17. In the 'Input data' section shown above in Figure 18 a PRA containing a complete Aquatic and Groundwater scenario was selected in the Home screen. In the 'Input data' section shown below in Figure 18 no PRA was selected in the Home screen. The boxes in the part 'values derived from other scenarios' stay empty. However if a PRA is generated later on and the DI1 scenario is part of the PRA and the DI1 scenario is checked again in the Dietary scenario input screen, you will see that the boxes in the part 'values derived from other scenarios' are filled.

Input data

Scenario

bw	?	<input style="width: 90%;" type="text" value="60"/>	kg	
ConsFish	?	<input style="width: 90%;" type="text" value="2"/>	kg/d	
ConsMF	?	<input style="width: 90%;" type="text" value="2"/>	kg/d	
ConsVeg	?	<input style="width: 90%;" type="text" value="2"/>	kg/d	
ConsWater	?	<input style="width: 90%;" type="text" value="2"/>	L/d	
PECgw (user)	?	<input style="width: 90%;" type="text" value="(6)"/>	μg/L	
PECnwater (user)	?	<input style="width: 90%;" type="text" value="(7)"/>	μg/L	
PECvegitem	?	<input style="width: 90%;" type="text" value="1E3"/>	mg pesticide/kg macrophy	

values derived from other scenarios

PECgw	<input style="width: 90%;" type="text" value="2.19E-15"/>	(GW)
PECn water	<input style="width: 90%;" type="text" value="40.7"/>	(AQ)

Input data

Scenario

bw	?	<input style="width: 90%;" type="text" value="60"/>	kg	
ConsFish	?	<input style="width: 90%;" type="text" value="2"/>	kg/d	
ConsMF	?	<input style="width: 90%;" type="text" value="2"/>	kg/d	
ConsVeg	?	<input style="width: 90%;" type="text" value="2"/>	kg/d	
ConsWater	?	<input style="width: 90%;" type="text" value="2"/>	L/d	
PECgw (user)	?	<input style="width: 90%;" type="text" value="(6)"/>	μg/L	
PECnwater (user)	?	<input style="width: 90%;" type="text" value="(7)"/>	μg/L	
PECvegitem	?	<input style="width: 90%;" type="text" value="1E3"/>	mg pesticide/kg macrophy	

values derived from other scenarios

PECgw	<input style="width: 90%;" type="text" value="undefined"/>	(GW)
PECn water	<input style="width: 90%;" type="text" value="undefined"/>	(AQ)

Figure 18. Both screens are part of the DI1 Dietary scenario show in Figure 17. Above screen is shown when a PRA containing a complete Aquatic and Groundwater scenario is selected in the Home screen. Screen below is shown when no PRA is selected in the Home screen

3.4 Output of a PRA

3.4.1 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 19) 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 four assessments, the Result screen of one assessment (Terrestrial) is chosen as an example (Figure 19). 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	label	value	unit	description
OUTPUT	SC	ETRsoil	8.8	-	Exposure Toxicity Ratio due to application
OUTPUT	SC	NECsoil	0.31	mg/kg	No Effect Concentration for the soil compartment
OUTPUT	SC	PECnsoil	2.7	mg pesticide/kg	Concentration in the upper 5 cm of the soil from one application
Log					
Values					
type	topic	label	value	unit	description
INPUT	PE	DegT50soil	52	d	Overall half-life in soil
INPUT	PE	ED30	*undefined*	mg/kg	Dose that affects 30% of the test organisms
INPUT	PE	ED50earthworms	3.1	mg/kg	Dose that affects 50% of the earthworms
INPUT	PE	ks	0.01333	1/d	Degradation rate coefficient in soil, where $k_s = \ln(2)/DEG50soil$
INPUT	AP	Dt	7	d	Time interval between applications
INPUT	AP	M	1E03	g a.i./ha	Individual dose applied
INPUT	AP	n	3	-	Number of applications
INPUT	SC	Depth	0.05	m	Depth of the field
INPUT	SC	Bulk density	2E3	kg soil/m ³ soil	Dry bulk density soil
INTER	SC	Csoil	1999.99997019	mg pesticide/m ³	Concentration in the upper 5 cm of the soil
INTER	SC	PEC1soil	0.99999998509	mg pesticide/kg	Concentration in the upper 5 cm of the soil from one application
OUTPUT	SC	ETRsoil	8.8	-	Exposure Toxicity Ratio due to application
OUTPUT	SC	NECsoil	0.31	mg/kg	No Effect Concentration for the soil compartment
OUTPUT	SC	PECnsoil	2.7	mg pesticide/kg	Concentration in the upper 5 cm of the soil from one application

Figure 19. 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 six columns: type, topic, 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.

3.4.2 Output via the Compare button

The Compare screen can be opened (Figure 20) through the ‘Compare’ button found in the selection panel. In this screen the results of up to three Pesticide Risk Assessments can be compared.

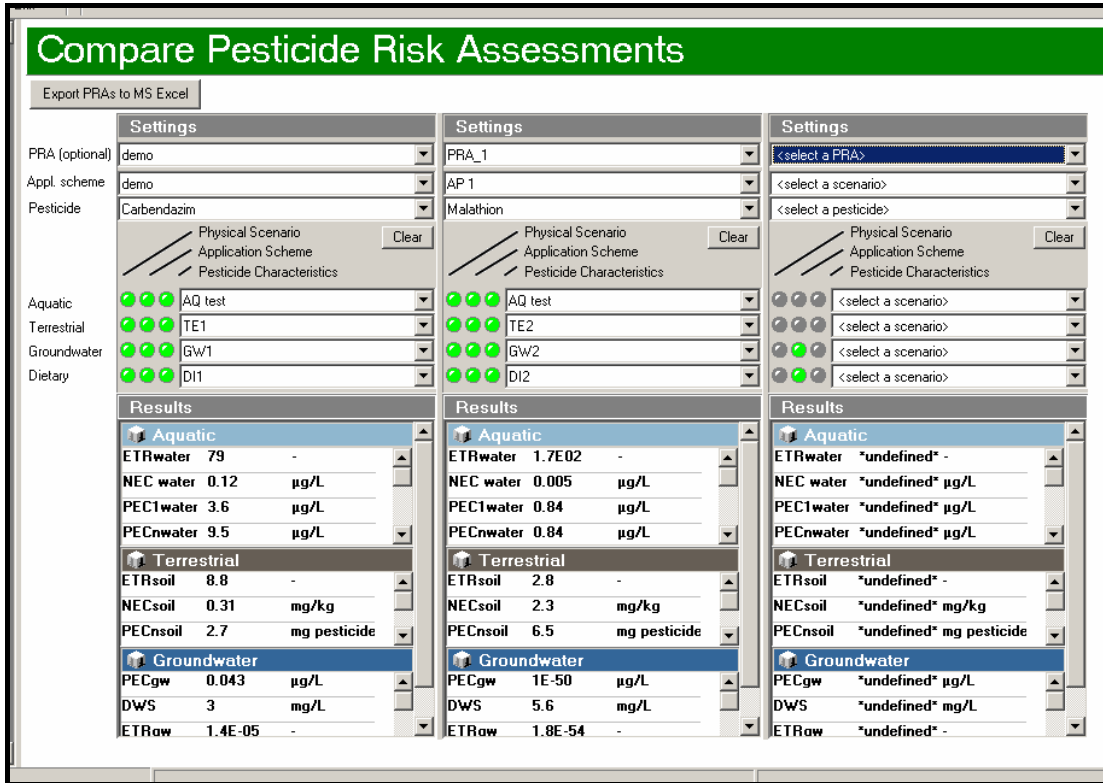


Figure 20. The Compare screen of PRIMET

The selection column of one PRA is shown in detail in Figure 21. 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 21, 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.

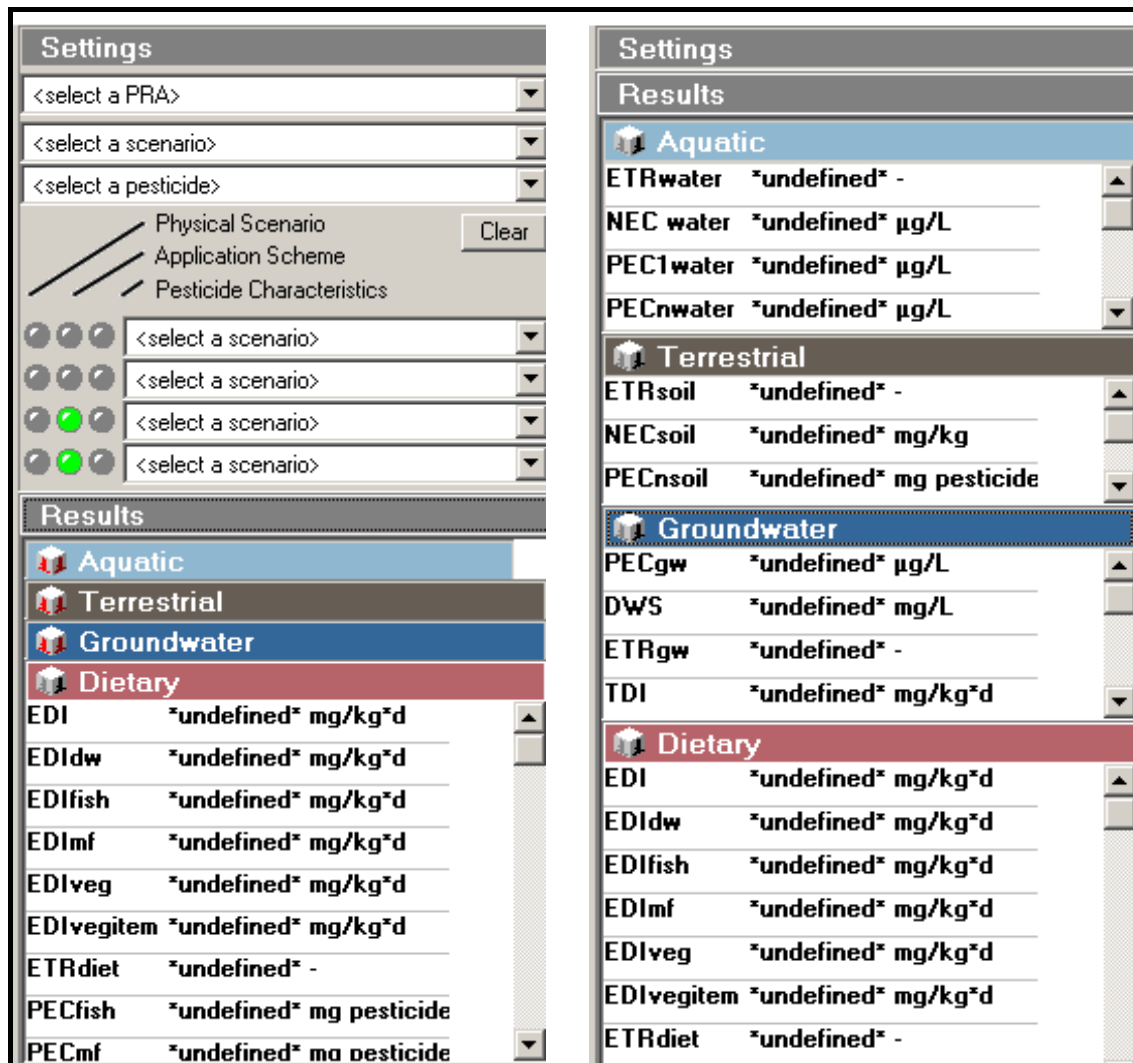


Figure 21. Selection column of a PRA is lifted out of the Compare screen

The Compare screen also contains a button (Figure 20, button: 'Export PRAs to MS Excel') which makes it possible to export the data to a MS excel file. An extra column containing the description of the parameter is added to the Excel file

3.5 Options

The functionalities of the buttons in the Options section of the Status bar (Figure 22) are discussed in this chapter.



Figure 22. The buttons in the Options section of the Selection Panel

3.5.1 Button Options

The PRIMET properties screen (Figure 23) appears after clicking the button Options.

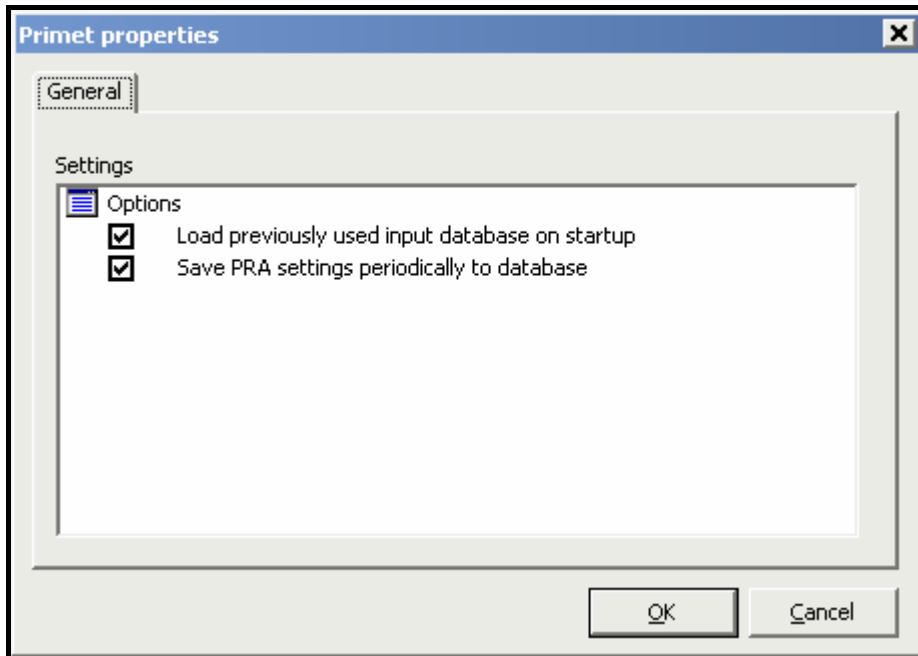


Figure 23. The PRIMET properties screen

Standard the options ‘Load previously used input database on startup’ and ‘Save PRA settings periodically to database’ are selected.

3.5.2 Button Variables

In the Configure Variables 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.

It is possible to modify these figures. However: **DO NOT CHANGE ANYTHING IF YOU DO NOT KNOW WHAT YOU ARE DOING!**

If you are sure that you should make an adjustment then changing the data is possible after you double-clicked on the text in the white text box below the grey bar with the text ‘Configure Variables’. The yellow rows in the table change colour to green. The data can now be edited. Double-clicking a second time on the text in the white text box will change the table to non changeable again.

Note that the ‘name’ of the parameter can not and should not be changed as that will prevent the model from looking up the correct values for its calculations.

Configure Variables									
Variable configuration									
DO NOT CHANGE IF YOU DO NOT KNOW WHAT YOU'RE DOING									
Changing the values in this table will change the appearance of the variables and their presentation on the other pages.									
Restart the program to make the changes visible.									
name	label	unit	descr	constant	default	range_min	range_max	precision	decimals
A	A	m ²	Cross section of water layer						
AF	AF	-	Assessment factor		100	0	10000	3	1
B	b	m	Bottom width of water body			0.05	100	3	2
BCF	BCF	L/kg	BioConcentration Factor						
BW	bw	kg	Body weight (60 kg for adults)		60	30	90	0	0
CFISH	ConsFish	kg/d	Daily fish consumption			0	5	2	2
CMF	ConsMF	kg/d	Daily macrophyte consumption			0	5	2	2
CSOIL	Csoil	mg pesticide/r	Concentration in the upper 5 cm of the						
CSOLT	Csol(T)	g/m ³	Solubility of substance in water at ambie			1E-6	2000000	4	4
CSOLTREFC	csol(TrefC)	g/m ³	Solubility of substance in water at refer			1E-6	2000000	4	4
CTDT	c*	mg/m ³ = mg/L	Total mass concentration in water layer						
CVEGIT	ConsVeg	kg/d	Daily consumption of the vegetable item			0	5	2	2
CWATER	ConsWater	L/d	Daily drinking-water consumption (2 litre		2	1		3	0
DEGT50S	DegT50soil	d	Overall half-life in soil				1000000	2	2
DEGT50W	DegT50	d	Half-life for degradation in water			0.1	1000000	4	1
DEPTHF	Depth	m	Depth of the field		0.05	0.01	0.3	2	2
DHP	DHP	J/mol	Enthalpy of vaporization	95000			95000	5	0
DHSOL	DHsol	J/mol	Enthalpy of dissolution	27000		27000	27000	5	0
DRIFT	%drift	%	Percentage of spray drift			0	100	2	2
DT	Dt	d	Time interval between applications				1000	1	1
DT50	DT50*	d	Overall half-life accounting for degradat					2	2
DWS	DWS	mg/L	Drinking Water Standard					2	2
E	E	J/mol	Molar Arrhenius activation energy	54000		54000	54000	5	0
EC50I	EC50invertebrates	µg/L	Concentration that affects 50% of the te			0	2000000000	4	2
EC50P	EC50primary prod	µg/L	Concentration that affects 50% of the te			0	2000000000	4	2

Figure 24. The Configure Variables screen

3.5.3 Button Legend

Clicking on this button will show the Legend screen. This screen is already discussed in section 3.3.1 of this report.

3.5.4 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.

3.5.5 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.

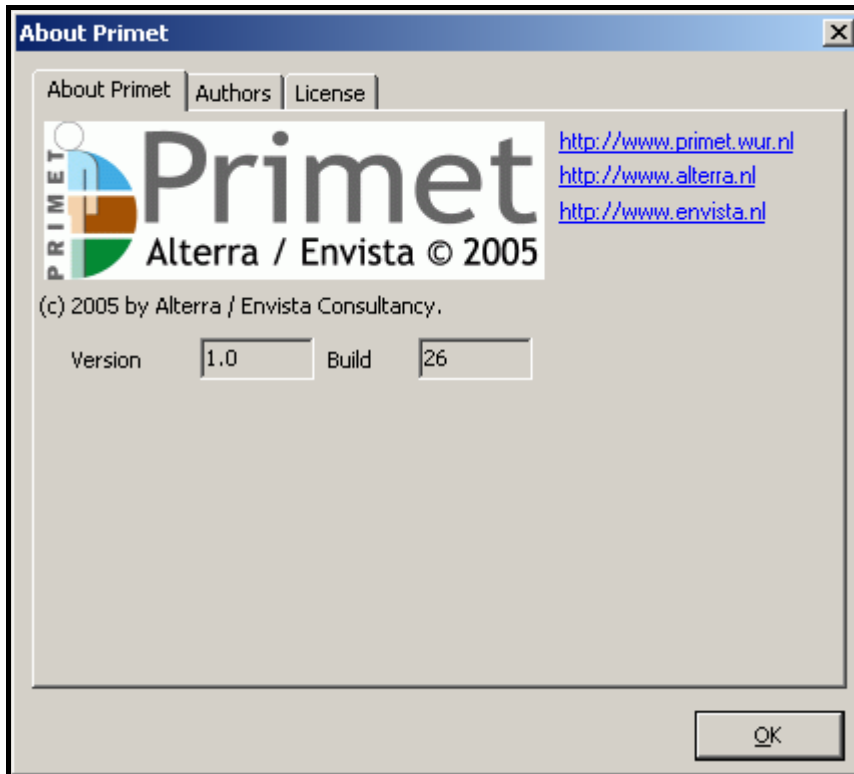


Figure 25. The About PRIMET screen

3.5.6 Button Exit

Clicking on the Exit button will close PRIMET.

Literature

Adriaanse, P.I. (1996). Fate of pesticides in field ditches: the TOXSWA simulation model. Winand Staring Centre, Report 90, Wageningen, The Netherlands.

Adriaanse, P.I., W.H.J. Beltman, E. Westein, W.W.M. Brouwer & S. van Nierop (1997). A proposed policy for differentiated hazard evaluation of pesticides in surface waters. Exposure concentrations simulated by TOXSWA and ecotoxicological hazards of pesticides in field ditches and main watercourses. Winand Staring Centre, Report 141, Wageningen, The Netherlands

Beltman, W.H.J. & P.I. Adriaanse (1999) Users Manual for TOXSWA 1.2.; simulation of pesticide fate in small surface waters., Winand Staring Centre, Techn. Doc. 54, Wageningen, The Netherlands.

Bowman B.T. & W.W. Sans (1985). Effect of temperature on the water solubility of insecticides. *J. Environ. Sci. and Health*, B20: 625-631.

Crum, S.J.H., A.M.M. Van Kammen-Polman and M. Leistra (1999). Sorption of nine pesticides to three aquatic macrophytes. *Archives of Environmental Contamination and Toxicology* 37: 310-316.

EU (1997). Council Directive 97/57/EC of September 21, 1997; Establishing annex VI to Directive 91/414/EEC Concerning the placing of plant protection products on the market. *Official Journal of the European Communities* L265: 87-109.

FOCUS Soil Modeling Workgroup (1997). Soil persistence models and EU registration. DG VI, European Commission, Doc. 7617/VI/96, Brussels, Belgium.

FOCUS (2001). FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC. Report, EC Document Reference SANCO/4802/2001-rev.1. Report of the FOCUS Working Group on Surface Water Scenarios, Brussels, Belgium.

JMPR (2003). Report of: 2003 Joint FAO/WHO meeting on pesticide residues. Geneva, 15–24 September 2003 www.fao.org/ag/agp/agpp/pesticide/jmpr/pm_jmpr.htm

Koorevaar, P., G. Menelik & C. Dirksen (1983). *Elements of soil physics*. Elsevier, Amsterdam, The Netherlands.

Leistra, M., A.M.A. van der Linden, J.J.T.I. Boesten, A. Tiktak & F. van den Berg (2001). PEARL model for pesticide behaviour and emissions in soil-plant systems; Description of the processes in FOCUS PEARL v 1.1.1. Alterra, Report 013, Wageningen The Netherlands.

Liss, P.S. & P.G. Slater (1974). Flux of gases across the air-sea interface. *Nature* 24: 181-184.

OECD (1993). OECD guidelines for the testing of Chemicals. Organisation for Economic Co-operation and Development, Paris, France.

Smit, A.A.M.F., F. van den Berg & M. Leistra (1997). Estimation method for the volatilization of pesticides from allow soil. Environmental Planning Bureau Series 2, Agricultural Research Department, Wageningen, The Netherlands.

Van den Berg F. & J.J.T.I. Boesten (1998). Pesticide Leaching and Accumulation model (PEST-LA) version 3.4. Description and user's guide. Winand Staring Centre, Techn. Doc. 43, Wageningen, The Netherlands.

Veith GD, DL de Foe and BV Bergstedt. 1979. Measuring and estimating the bioconcentration of chemicals in fish. *J. Fish. Res. Board Can.* 36: 1040-1048.

WHO (1996). Guidelines for drinking-water quality, 2nd ed. Vol. 2. Health criteria and other supporting information. World Health Organization, Geneva, Switzerland.

WHO (2003). GEMS/Food regional diets: Regional per capita consumption of raw and semi-processed agricultural commodities. The Global Environment Monitoring System/Food Contamination Monitoring and Assessment Programme (GEMS/Food), Food Safety Department, World Health Organization, Geneva, Switzerland.