Calculation of PEC_{soil} including Plateau Concentrations for Pesticides Dependent on FOCUS Degradation Kinetics

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User Manual ESCAPE Version 2

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Weiterentwicklung des Programms „ESCAPE“ für Higher-Tier-Simulationen zur Berechnung von PEC-Boden-Werten einschließlich Plateaukonzentrationen für Pflanzenschutzmittel (PSM) unter Einbeziehung der FOCUS-Abbaukinetiken		
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16. Kurzfassung

In diesem Projekt wurde das im Jahr 2008 erstellte Programm ESCAPE (Estimation of Soil Concentrations After PEsticide applications) zur Berechnung von zeitabhängigen Pflanzenschutzmittelkonzentrationen im Boden in folgenden Punkten weiterentwickelt:

- Porenwasserkonzentration: Neben Gesamtgehalten im Boden wurde die Möglichkeit der Berechnung von Porenwasserkonzentrationen realisiert.
- Temperaturabhängigkeit des Bioabbaus: Die bestehende Software wurde so erweitert, dass die Berücksichtigung der Temperaturabhängigkeit von Abbauraten im Boden mit den etablierten Verfahren berücksichtigt werden kann.
- Feuchteabhängigkeit des Bioabbaus: Es wurde neue eine Methode entwickelt, mit der die derzeit etablierten Verfahren zur Berücksichtigung der Feuchteabhängigkeit des Bioabbaus unabhängig von der jeweiligen Abbaukinetik in die Software integriert werden konnte.
- Erstellung von Bodenszenarien: Im Rahmen der Erweiterung werden Boden- und der Klimaparameter in „Bodenszenarien“ zusammengefasst, die der Anwender dann benutzerfreundlich für eine Simulation auswählen kann.

17. Schlagwörter

ESCAPE, Bodenkonzentration, Pflanzenschutzmittel, Wirkstoff, Metabolit, PEC-Boden, TWA, Computermodell, , Abbaukinetik, Plateaukonzentration, Standardszenario

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16. Abstract
In this project the computer model ESCAPE (Estimation of Soil Concentrations After PEsticide applications) originally developed in 2008 to calculate time dependent pesticide concentrations in soil was further developed covering following items:
- Pore water concentrations: in addition to the estimation of total contents in soil routines were implemented to calculate time dependent pore water concentrations.
- Temperature dependency of microbial degradation: in the present software additional procedures were included which allow to perform the correction of standard biodegradation rates using daily temperatures based on the established methodologies.
- Moisture dependency of microbial degradation: A new method was developed, which can be used to do soil moisture correction of the biodegradation rate based on the established methodologies and independent on the actual degradation kinetics.
- Implementation of standard scenarios: new routines were implemented which allow the defnition and use collections of weather and soil data as standard scenarios in a user friendly way.

17. Keywords

ESCAPE, soil concentration, pesticide, metabolite, degradation kinetics, PECsoil, TWA computer model, mathematical model, Plateau concentrations, standard scenarios

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1. Summary

A software called ESCAPE (**E**stimation of **S**oil **C**oncentration **A**fter **PE**sticide applications) was developed that can be used to calculate actual as well as time weighted average concentrations in soil for the parent compound and additional metabolites. In addition to SFO kinetics (single first order) the software is able to consider hockey stick – kinetics (HS), FOMC- kinetics (first order multi compartment) and DFOP- kinetics (double first order in parallel). ESCAPE can handle singular and multiple applications over a simulation period of 10 years. The user may also enter irregular application pattern within a year. ESCAPE considers different soil depths and performs corrections of actual rates dependent on the current crop interception automatically. Visualisation of results is carried out graphically (diagram showing the simulated concentrations vs. time) and tabularly based on time intervals as defined by EU or national regulations.

In the new version 2.0 of ESCAPE in addition to traditional total contents also pore water concentrations can be calculated. Furthermore, degradation rates can be corrected based on actual soil moisture and temperature data. Finally, realistic worst case scenarios based on specific information on soil cores and climate data sets containing daily weather series can be used for the calculations.

2. Background

Within the registration of pesticides time dependent concentrations in soil have to be calculated for all active ingredients and their main metabolites. Traditionally these estimations are performed considering first order degradation kinetics as described in the FOCUS-document *Soil persistence models and EU registration* finalised in 1997. Calculated actual (PEC_{act}) and time weighted average concentrations ($PEC_{TWA)}$ are used for comparisons with respective results of eco-toxicity tests as the base for the risk assessment of these substances in soil.

As first order degradation means that the half life of a compound is only a function of the rate constant and therefore constant over time and independent on the actual soil concentration, this kinetics has many advantages especially when complicated application pattern with different application amounts, rates or times have to be considered.

However, in the final report of the FOCUS working group on degradation kinetics which came out recently (FOCUS 2006) additional degradation kinetics were described, which are often more suitable to describe the fate of pesticides in soil than the traditional methodology based on single first order degradation (FOCUS nomenclature: SFO: S*ingle First Order)*. Additional recommended kinetics are e.g. HS: *hockey stick*, DFOP: *double first order in parallel*, or FOMC: *first order multi compartment*.

For single applications FOCUS Degradation Kinetics published algorithms allowing the calculation of time dependent concentrations in soil for parent and metabolite compounds. Unfortunately, for complicated application pattern with irregular application timing and rates currently no bug-free and user-friendly is available that can be used to calculated actual and average concentrations in soil. Additionally, tools to estimate plateau concentrations are currently not available. The commonly used leaching models (PELMO, PEARL) are also not appropriate, as long as they consider first order degradation in soil only. The main difficulty is the non-existence of simple mathematical solutions for the concentration dependency for more complicated application pattern. However, consideration of non-kinetic sorption modules in these models could be an alternative.

In contrast to simple first order kinetics the strategy of handling residues from earlier applications has to be defined clearly when using more complicated degradation kinetics.

To consider also soil concentrations based on different weather conditions the degradation rates can be corrected based on temperature and soil moisture.

This version of ESCAPE is finally able to consider pore water concentrations as e.g. recommended by EFSA.

3. Methodology

3.1. Degradation models considered by ESCAPE

ESCAPE considers in total 4 different degradation kinetics SFO: (S*ingle First Order),* HS (*Hockey Stick)*, DFOP: (*Double First Order in Parallel) and* FOMC: F*irst Order Multi Compartment)*. All models are available for parent compounds. However, the identification of a suitable model for the description of the formation and degradation of metabolites are much more complex. As the description of the concentration curve of a single metabolite depends on a correct description of the degradation of the parent substance and of the degradation of the metabolite itself. Due to the parallel formation of metabolites only two of the four available models can be used also for metabolites namely the SFO and the DFOP kinetics. The other models are not conceptually correct for a metabolite that is gradually formed over a period of time (FOCUS 2006).

3.1.1. SFO (Single first order)-kinetics

SFO is the most simple degradation model using only a single parameter, the constant rate constant (unit: 1/d) leads to a simple exponential equation of pesticide concentration with time. The main assumption behind that model is that the pesticide concentration is small compared to the number of degrading micro-organisms or water molecules (if the compound is degraded by hydrolysis). The model is so simple and easy to work with because at any time the degradation of pesticide with time is directly proportional to the current concentration in soil as expressed in the following equation*(1*):

$$\frac{dC}{dt} = -k_{SFO}\, C \qquad (1)$$

C: pesticide concentration (mg/kg)

k_{SFO}: rate constant (1/d)

As explained earlier after integration of equation *(1*) an exponential term is obtained for SFO-kinetics as shown in the next equation *(2)*:

$$C = C_0 * exp(-k_{SFO} * t) \qquad (2)$$

C: pesticide concentration at time t (mg/kg)

C_0 concentration at time $t=0$ (mg/kg)

Independent on the initial concentration the same time is always needed to reduce the concentrations to a fixed extend (e.g. 50 % or 90 %). Therefore simple and easy to interpret DT50 or DT90 values can be obtained when considering SFO-kinetics as presented in the next equations.

$$DT50 = \frac{\ln(2)}{k_{SFO}} \qquad (3) \qquad DT90 = \frac{\ln(10)}{k_{SFO}} \qquad (4)$$

The SFO model can be used within ESCAPE for calculating the fate of parent compounds as well as for metabolites. An example simulations is presented in Figure 1.

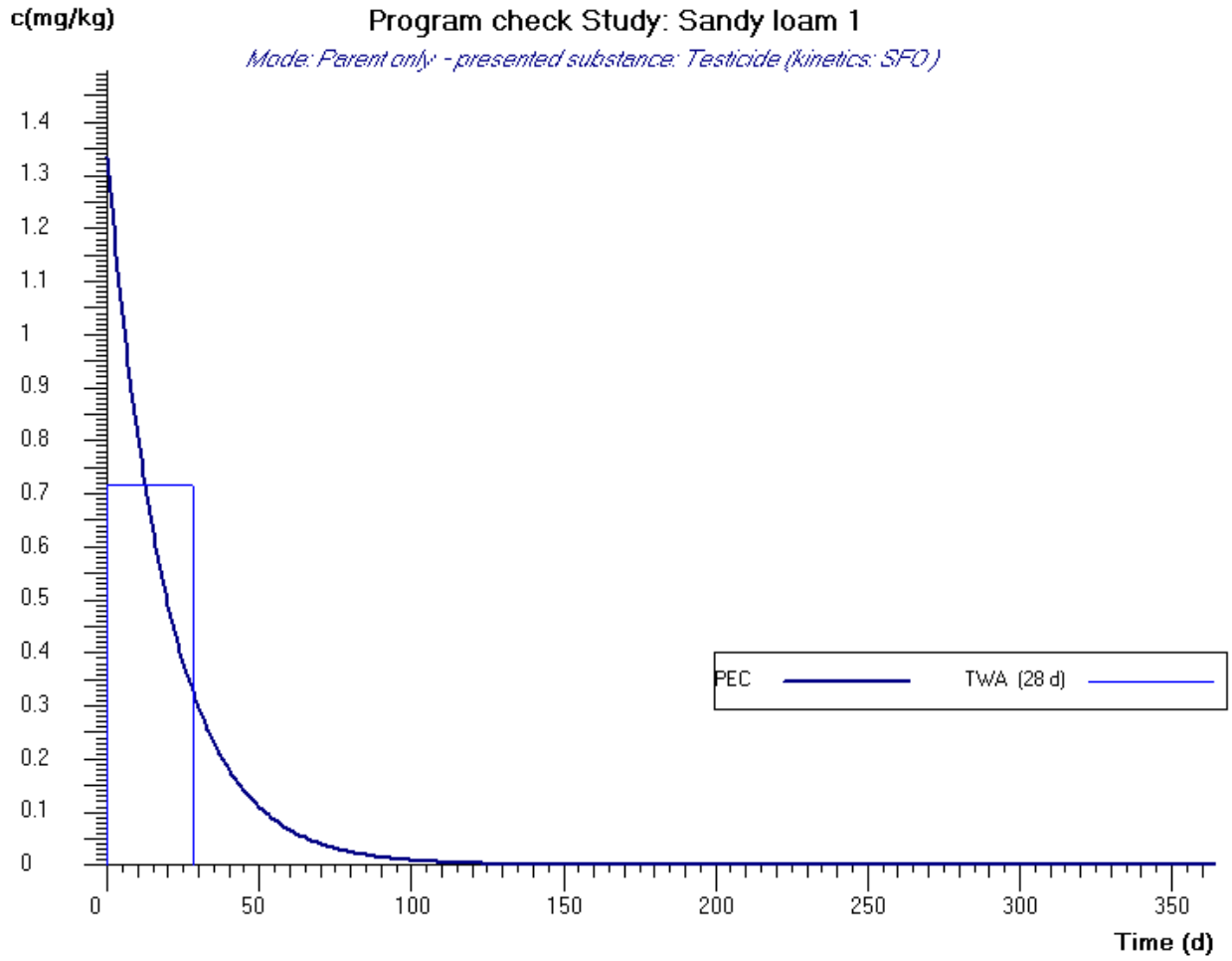


Figure 1: SFO-model (1 kg/ha, k_{SFO} = 0.05 d^{-1}, soil depth: 5 cm)

3.1.2. FOMC (First Order Multi Compartment)-kinetics

The FOMC model was suggested by Gustafson and Holden (1990) with a mechanistic background. As soil is a heterogeneous medium with many regions of different degradation capacity. Therefore it is reasonable to divide the soil into a large number of sub-compartments each with a different first order degradation rate. Assuming the rate constants follow a γ–distribution an analytical solution can be found to describe this degradation model mathematically as shown in equation *(5)*.

$$C = \frac{C_0}{\left(\frac{t}{\beta}+1\right)^{\alpha}} \qquad (5)$$

C: pesticide concentration at time t (mg/kg)

C_0 concentration at time $t=0$ (mg/kg)

α: 1st fitting parameter

ß: 2nd fitting parameter

The FOMC model is a very simple biphasic degradation approach which needs only two fitting parameter. The differential form of this model is shown in equation (6):

$$\frac{dC}{dt} = \frac{\alpha}{\beta}\ C\left(\frac{t}{\beta}+1\right)^{-1} \qquad (6)$$

A disadvantage of this approach is that in contrast to the SFO-model the degradation depends on time (see the difference between equation (1) and (5)). Therefore the model cannot be used in transport models (e.g. leaching) where pesticide movement is simulated. However, this is not a problem when parent compounds are simulated with ESCAPE and only single applications are considered, because the whole pesticide amount is released into a single compartment without further movement. For multiple applications it must be defined how residues from previous applications should be handled.
Due to the permanent formation of metabolites during the simulation the FOMC-model is also not suitable for these degradation products.

However, DT50 and DT90 values can be easily expressed based on the two fitting parameters α and ß as shown in the next equations.

$$\text{DT50} = \beta\left[2^{\left(\frac{1}{\alpha}\right)}-1\right] \qquad (7)$$

$$\text{DT90} = \beta\left[10^{\left(\frac{1}{\alpha}\right)}-1\right] \qquad (8)$$

An example for a time dependent soil concentrations using the FOMC model is presented in Figure 2

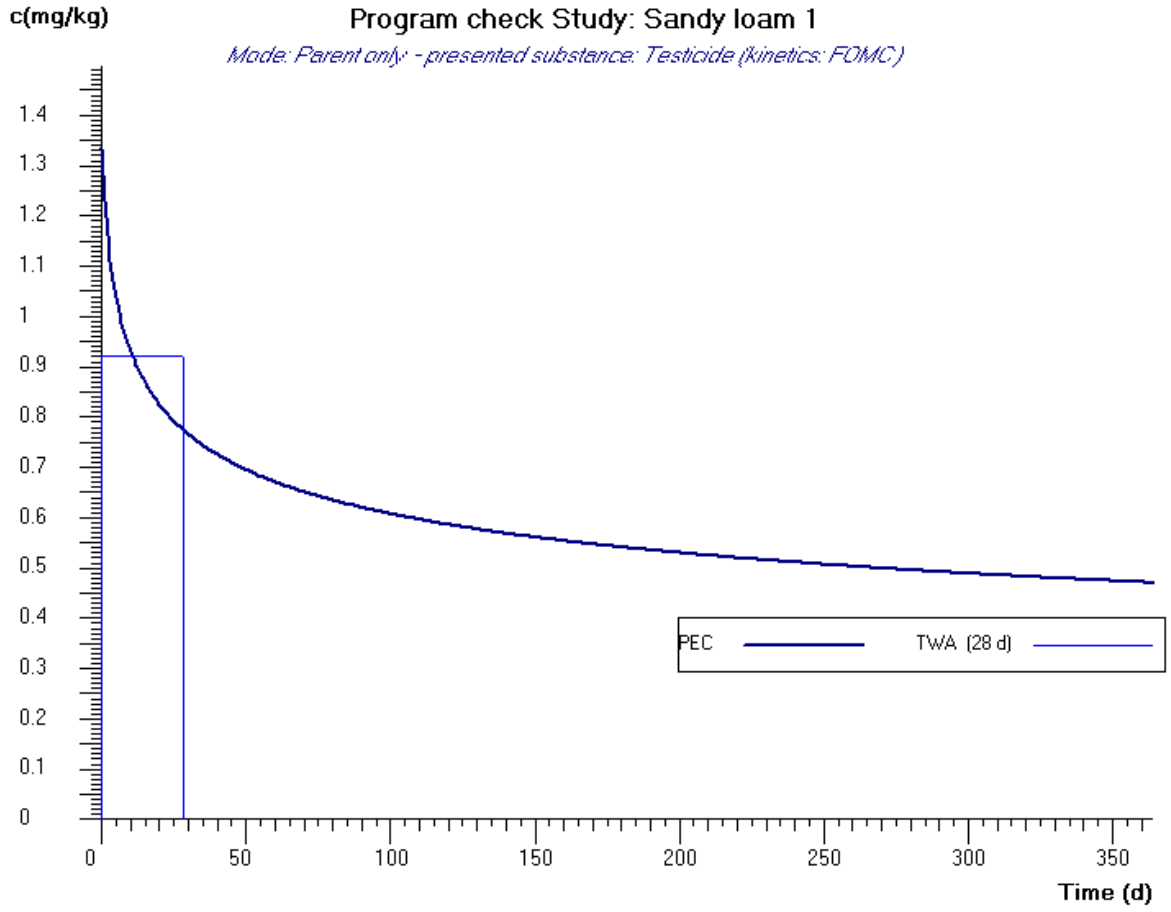


Figure 2: FOMC-model (1 kg/ha, α = 0.2, ß = 2, , soil depth: 5 cm)

3.1.3. DFOP (Double First Order in Parallel)-kinetics

DFOP is a bi-exponential model that describes degradation by a sum of two normal first-order degradation each in different part of the soil compartment. It needs in total 3 parameters (one more than the FOMC-model), namely the two different first order rate constants and the fraction of the pesticides being degraded according to the first rate constant. The equation of the DFOP-model is presented in equation ***(9)***.

$$C = C_0 \ [\ g * exp(-k_1 * t) + (1- g) * exp(-k_2 * t)\ ] \qquad (9)$$

C: pesticide concentration at time t (mg/kg)

C_0 concentration at time $t=0$

g fraction of the pesticide applied to the first compartment

k_1: rate constant in the first compartment (1/d)

k_2: rate constant in the second compartment (1/d)

With its two different exponentials terms the model is too complicated to define a differential equation or to calculate DT50 and DT90 values based on the three fitting parameters k_1, k_2, and g. These parameters have to be found by iterative procedures.
However, an example for the DFOP-model (that can be used for parent compounds as well as for metabolites) is presented in Figure 3

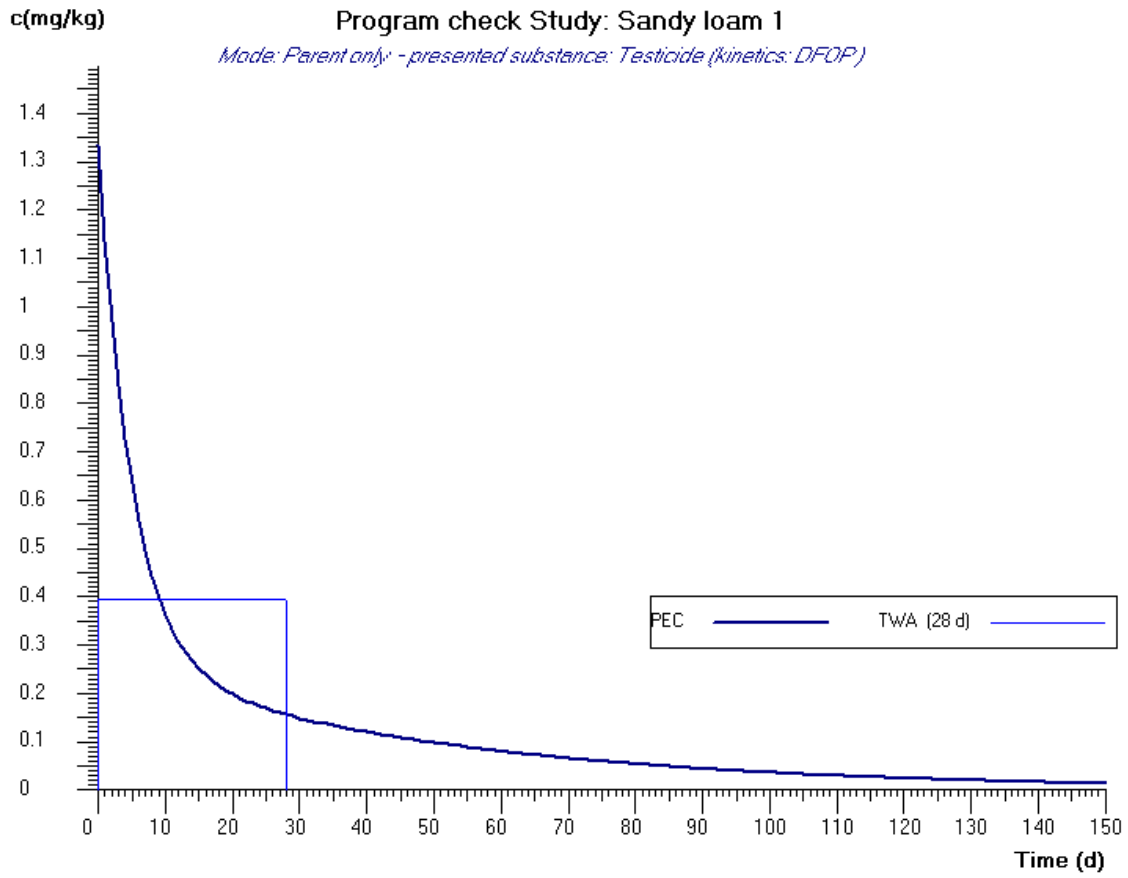


Figure 3: DFOP-model (1 kg/ha, k_1 = 0.2 d^{-1}, k_2 = 0.02 d^{-1}, , g = 0.8, soil depth: 5 cm)

3.1.4. HS(Hockey Stick)-kinetics

In contrast to the DFOP model the hockey stick kinetics consist of two sequential first order declines. First the pesticide completely degrades according to the first degradation rate. At a certain time degradation switches completely to a second degradation rate. To describe the HS-model the same number of parameters (three) is needed as for the DFOP-model. A mathematical description of this model is presented in equation *(10))*

$$C = C_0 * exp(-k_1 * t) \qquad for\ t \leq t_b$$
$$C = C_0 * exp(-k_1 * t_b) * exp[-k_2 * (t-t_b)] \qquad for\ t > t_b$$

*)

C: pesticide concentration at time t (mg/kg)

C_0 concentration at time $t=0$ (mg/kg)

t_b breakpoint (when rate constant changes)

k_1: rate constant before $t = t_b$ (1/d)

k_1: rate constant after $t = t_b$ (1/d)

The HS-model can be expressed also by its underlying differential equation as presented in equation *(11)*:

$$\frac{dC}{dt} = -k_1 C \qquad for\ t \leq t_b$$
$$\frac{dC}{dt} = -k_2 C \qquad for\ t > t_b \qquad (11)$$

A disadvantage of the HS-model is that the degradation depends on time because of the breakpoint t_b. Therefore the model can hardly be used in transport model (e.g. leaching) where pesticide movement is simulated. However, this is not a problem when parent compounds are simulated with ESCAPE and only single applications are considered, because the whole pesticide amount is released into a single compartment without further movement. For multiple applications it must be defined how residues from previous applications should be handled.

Due to the permanent formation of metabolites during the simulation no breakpoint can be given for these degradation products and the HS-model is therefore also not suitable for these problems.

However, DT50 and DT90 values can be expressed based on the three fitting parameters k_1, k_1, and t_b as shown in equations (12) and (13).

$$\text{DT50} = \frac{\ln(2)}{k_1} \qquad \text{for } DT50 \leq t_b$$

$$\text{DT50} = \frac{\ln(2) - k_1 * t_b}{k_2} \qquad \text{for } DT50 > t_b \qquad (12)$$

$$\text{DT90} = \frac{\ln(10)}{k_1} \qquad \text{for } DT50 \leq t_b$$

$$\text{DT90} = \frac{\ln(10) - k_1 * t_b}{k_2} \qquad \text{for } DT50 > t_b \qquad (13)$$

An example for a time dependent soil concentrations using the HS-model is presented in Figure 4.

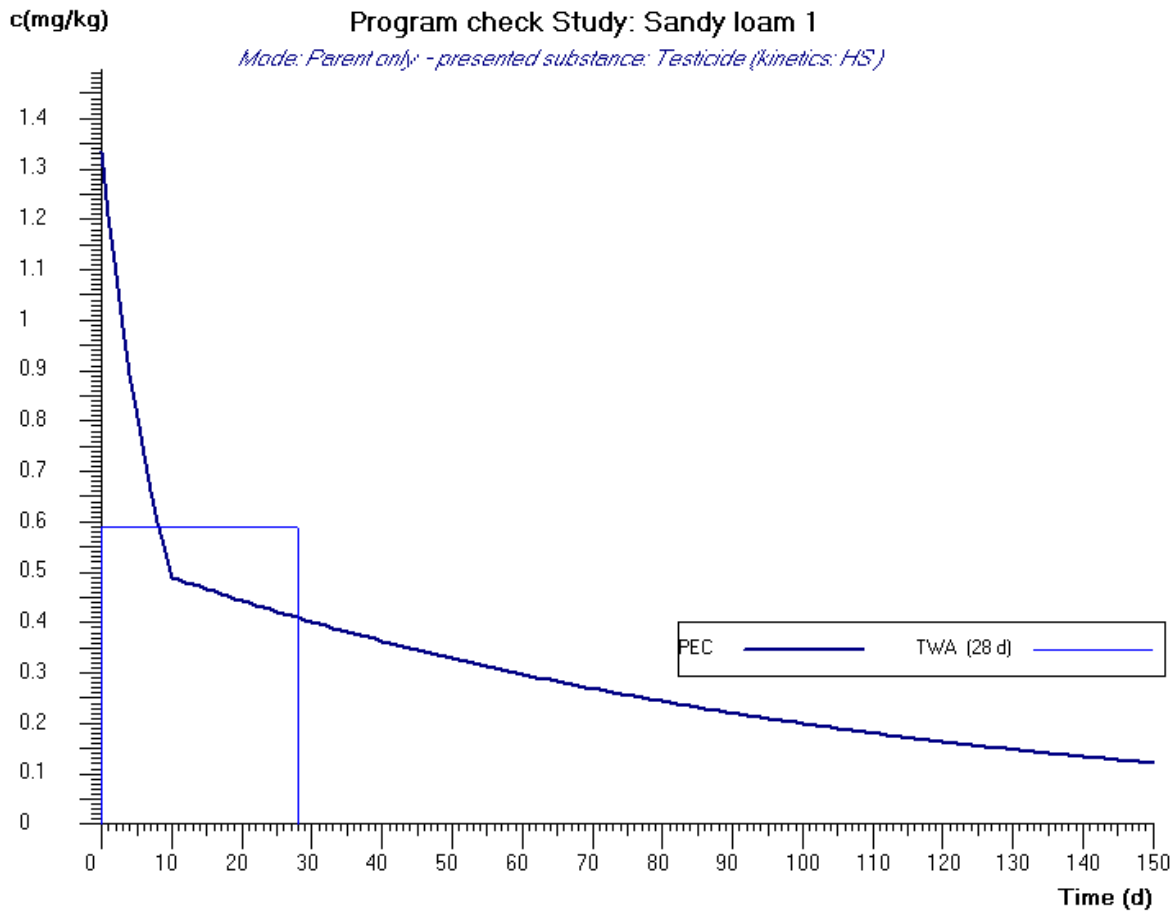


Figure 4: HS- model (1 kg/ha, k_1 = 0.1 d^{-1}, k_2 = 0.01 d^{-1}, t_b = 10 d, soil depth: 5 cm)

3.2. Temperature and soil moisture correction of degradation constants

Dependent on the actual soil moisture and temperature conditions ESCAPE corrects the standard degradation rate.
Temperature correction is done based on the Q10-approach according to following equation:

$$k = k_0 \cdot Q_{10}^{\frac{T - T_{Ref}}{10}}$$

4)

k: actual rate constant

k_0: rate constant at T_{Ref} (°C)

Q_{10}: Q10-factor (-)

T: current temperature (°C)

The Q_{10}-factor, the temperature at reference conditions T_{Ref}, and the rate constant at reference conditions must be given by the user, whereas the current temperature is taken from the weather file by ESCAPE.

Soil moisture equation is done based on the Walker-model as shown in following equation.

$$k = k_0 \cdot \left(\frac{\Theta}{\Theta_0} \right)^f$$

5)

k: actual rate constant

k_0: rate constant at T_{Ref} (°C)

f: moisture exponent (-)

Θ: current soil moisture (m³/m³)

Θ_0: soil moisture at reference conditions (pF 2) = *field capacity* (m³/m³)

The soil moisture exponent (field capacity, pF 2) must be given by the user, whereas the current soil moisture and the rate constant at reference conditions content is calculated by ESCAPE based on the weather conditions and considering worst case assumptions according to following equation.

$$\Theta_t = MAX\left\{MIN\left[\Theta_{t-1} + \frac{R - ET_{Pot}}{d}, \Theta_{FC}\right], \Theta_{WP}\right\} \qquad 16)$$

Θ_t: soil moisture at the current simulation day (m³/m³)

Θ_{t-1}: soil moisture at the previous simulation day (m³/m³)

ET_{Pot}: potential evapotranspiration at the current simulation day (cm)

R: Rainfall at the current simulation day (cm)

Θ_{FC}: soil moisture at field capacity (m³/m³)

Θ_{WP}: soil moisture at wilting point (m³ / m³)

d soil depth (cm)

The functions MAX and MIN in the equation guarantee that only soil moisture contents are calculated between field capacity and wilting point. Run-off or drainage are not considered as transport processes for soil water. The equation is nevertheless conservative because it is assumed that actual evapotranspiration is always as high as the potential evapotranspiration. The temperature and soil moisture correction has been originally developed for first order kinetics only. For the biphasic kinetics they have to be adapted. ESCAPE uses a time-step normalisation approach to do the soil moisture and temperature correction independent on the actual degradation kinetics. In this method a normalised ‘day length’ is calculated based on daily variations in soil temperature and moisture content using the equations and assumptions presented above. The procedure is described in detail in FOCUS 2006. For example a daily soil temperature of 25^{o}C (Q10 =2.2) and moisture content of 20% (vs. 25% for pF2) gives a normalised day length of 1.27 days at 20^{o}C and pF2. The daily values are calculated and the cumulative time between sampling points.

3.3. Calculation modes considered by ESCAPE

ESCAPE can be used in four different calculation modes namely:

- parent compound only
- parent compound and a single metabolite
- parent compound and two metabolites formed in parallel
- parent compound and two metabolites formed in a sequence

Dependent on the calculation mode not all degradation models presented in chapter 3.1 are available.

3.3.1. Simulation considering the parent compound only

For the parent compound ESCAPE calculates actual and time weighted average concentrations based on all four kinetic models presented in chapter 3.1:

- SFO (single first order)
- FOMC (first order multi compartment)
- DFOP (double first order in parallel)
- HS (hockey stick)

In this mode ESCAPE considers a single compartment usually. Also if multiple applications are simulated only a single compartment is used and internal counter is always set to "*0*" after a new application has been released.
However, if multiple applications are to be simulated and the user wants to keep residues from previous applications separately (important for the FOMC- or the HS-kinetics only) additional compartments are created for each new application as shown in Figure 5. Within each compartment there is only a single concentration defined per time and there is no transport considered between these compartments. The soil concentration is calculated as the sum of all pesticide residues at a given time.

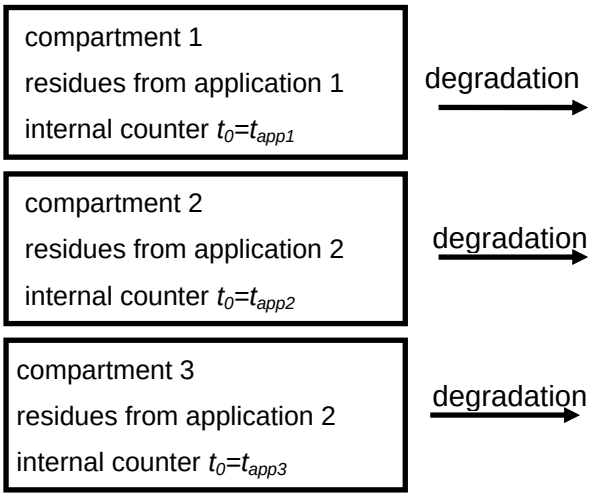


Figure 5: A series of compartments if residues from different applications are kept separately

3.3.2. Simulation considering the parent compound and a single metabolite

In this mode ESCAPE considers two compartments (for the parent compound and for the metabolite) as shown in Figure 6.

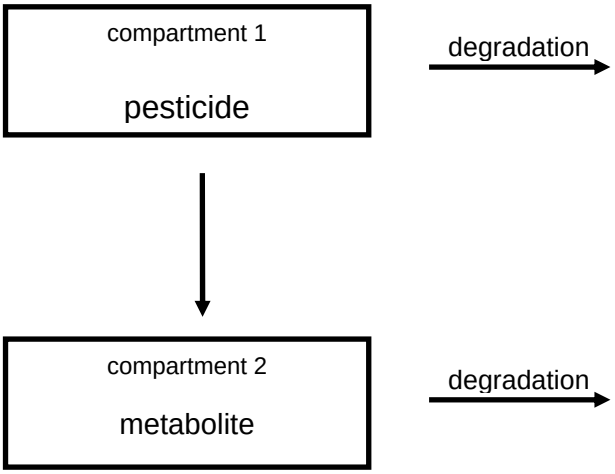


Figure 6: Two compartments for parent and metabolite

The calculation of the formation of the metabolite is done based on the time dependent degradation of the parent compound, the formation fraction of the metabolite, and the differences in the molar masses according to equation ***(17***).

$$R_{form} = \frac{R_{deg} * f * M_{met}}{M_{par}} \qquad (17)$$

R_{form}: actual formation of the metabolite (g/ha)

R_{deg}: actual degradation of the parent compound (g/ha)

f: formation fraction of the metabolite (-)

M_{par}: molecular mass of the parent compound (g/mol)

M_{met}: molecular mass of the metabolite (g/mol)

Again, for the parent compound ESCAPE calculates actual and time weighted average concentrations based on all four kinetic models presented in chapter 3.1.
However, as the degradation in the degradation models FOMC and HS depends on the time since application, but these times cannot be defined for the formation of metabolites (the formation takes place over the whole simulation period instantaneously), these two models cannot be selected for metabolites.
The user can decide to keep pesticide residues from different applications separately also in this calculation mode (see Figure 5 and the explanation in chapter 3.3.1).

3.3.3. Simulation considering the parent compound and two parallel metabolites

In this mode ESCAPE considers three compartments (each for the parent compound and for the two metabolites) as shown in Figure 7.

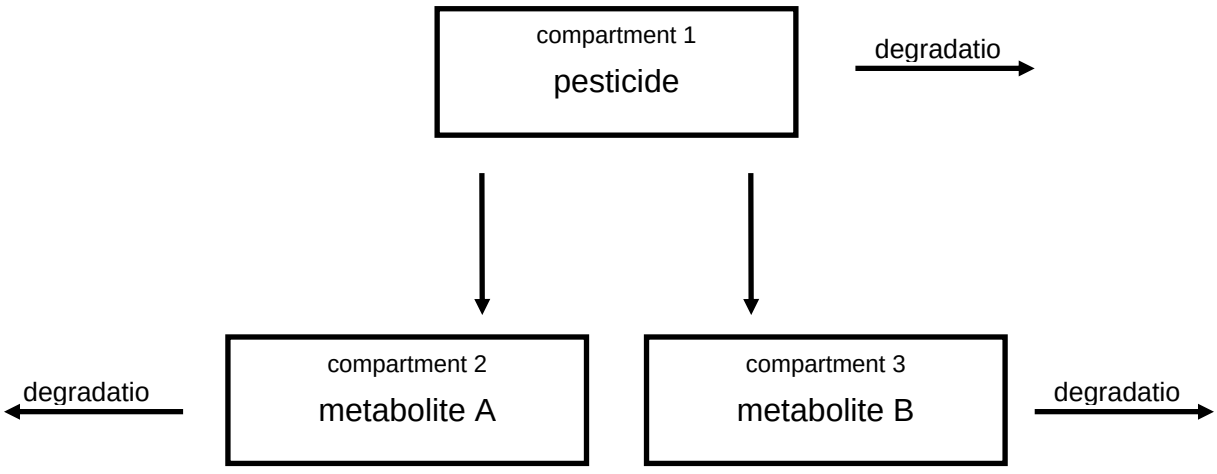


Figure 7: Three compartments for parent and two parallel metabolites

The calculation of the formation of the two metabolites is done based on the time dependent degradation of the parent compound, the formation fraction of the metabolite, and the differences in the molar masses according to equation *(18)*.

$$R_{formA,\,B} = \frac{R_{deg} * f_{A,\,B} * M_{metA,\,B}}{M_{par}} \qquad \textbf{(18)}$$

$R_{formA,B}$:	actual formation of the metabolite A or B (g/ha)
R_{deg}:	actual degradation of the parent compound (g/ha)
$f_{A,B}$:	formation fraction of the metabolite A or B (-)
M_{par}:	molecular mass of the parent compound (g/mol)
$M_{metA,B}$:	molecular mass of the metabolite A or B (g/mol)

For the parent compound ESCAPE calculates actual and time weighted average concentrations based on all four kinetic models presented in chapter 3.1.
However, as the degradation in the degradation models FOMC and HS depends on the time since application, but these times cannot be defined for the formation of metabolites (the formation takes place over the whole simulation period instantaneously), these two models cannot be selected for metabolites.
The user can decide to keep pesticide residues from different applications separately also in this calculation mode (see Figure 5 and the explanation in chapter 3.3.1)

3.3.4. Simulation considering the parent compound and two metabolites in a sequence

In this mode ESCAPE considers three compartments (for the parent compound and for the two metabolites) as shown in Figure 8.

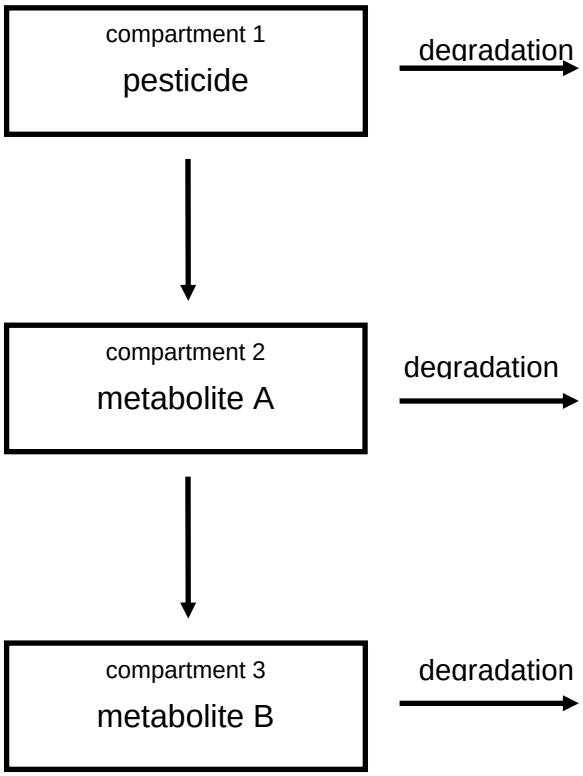


Figure 8: Three compartments for parent and two metabolites in a sequence

The calculation of the formation of metabolite A is done based on the time dependent degradation of the parent compound, the formation fraction of metabolite A, and the differences in the molar masses according to equation (19**)**.

$$R_{form} = \frac{R_{deg} * f * M_{met}}{M_{par}} \qquad (19)$$

R_{form}: actual formation of metabolite A (g/ha)
R_{deg}: actual degradation of the parent compound (g/ha)
f: formation fraction of metabolite A (-)
M_{par}: molecular mass of the parent compound (g/mol)
M_{met}: molecular mass of metabolite A (g/mol)

The calculation of the formation of metabolite B is done based on the time dependent degradation of metabolite A, the formation fraction of metabolite B, and the differences in the molar masses according to equation (20).

$$R_{formB} = \frac{R_{degA} * f_B * M_{metB}}{M_{metA}} \qquad (20)$$

R_{formB}: actual formation of metabolite B (g/ha)
R_{degA}: actual degradation of metabolite A (g/ha)
f_B: formation fraction of metabolite B (-)
M_{metA}: molecular mass of metabolite A (g/mol)
M_{metB}: molecular mass of metabolite B (g/mol)

For the parent compound ESCAPE calculates actual and time weighted average concentrations based on all four kinetic models presented in chapter 3.1.
However, as the degradation in the degradation models FOMC and HS depends on the time since application, but these times cannot be defined for the formation of metabolites (the formation takes place over the whole simulation period instantaneously), these two models cannot be selected for metabolites.
The user can decide to keep pesticide residues from different applications separately also in this calculation mode (see Figure 5 and the explanation in chapter 3.3.1).

3.4. Calculation of the total content in soil

3.4.1. Initial concentrations

At the beginning of a simulation ESCAPE calculates the initial concentration in soil. For the calculation two soil parameters (soil depth and soil density) and two parameters related to the application pattern (application rate and crop interception) are used. Thus, the initial pesticide concentration is calculated based on these four variables according to equation *(21*):

$$C_0 = \frac{R * Ic}{d} \qquad (21)$$

C_0: initial pesticide concentration (mg/kg)

R: application rate (mg/m²)

d: soil depth (m)

ρ: soil density (kg/m³)

Ic: crop interception (-)

3.4.2. Time dependent concentrations

As analytical solutions are not available for many situations especially when the formation of metabolites is considered ESCAPE generally calculates time dependent concentrations numerically in a stepwise approach assuming a minimum time step of one day. Independent on the degradation kinetics the concentrations of the parent compound is calculated based on the initial concentrations at day $t=0$ and using the integrated mathematical descriptions of the models as explained earlier in chapter 3.1 for all degradation models.

Dependent on the degradation model it may be important whether or not residues from different application are kept separately.

Figure 9 shows the time dependent concentration if residues from different applications are not separated. Due to the fast degradation shortly after applications for this example of a FOMC-kinetics no accumulation in soil is calculated.

If, as a second option, residues from different applications are kept separately an initial concentration and an individual starting point will be defined for every application according to equation *(21*).

The actual concentration in soil is then calculated as the sum of all pesticide residues from previous applications. This is demonstrated exemplarily for the FOMC-kinetics in equation *(22*). The idea of this approach is, that new applications do not change the rate of

degradation of residues from previous applications, but instead degrade with the same rate as they had done without new applications.

$$C_j = \sum_{i=1}^{napp} \left(\frac{C_{0i}}{\left(\frac{Max(j - t_i, 0)}{\beta} + 1 \right)^{\alpha}} \right) \qquad (22)$$

C_j: pesticide concentration at time j (mg/kg)

j: current simulation day

i: application number

$napp$: total number of applications

t_i: day of application i

C_{0i}: initial concentration of application i at time t_i (mg/kg)

Max: Maximum function

α: 1st fitting parameter

β: 2nd fitting parameter

However as shown in Figure 10, dependent on the rate parameters this equation may lead to a situation where never any final plateau is reached even after many pesticide applications. Instead an unrealistic infinite increase of concentration with time is calculated.
Therefore, a third option was implemented:
Residues from different application are separated within one year, but all residues are joined and degraded together with the actual residues after the first application in the new year occurred (see the example in Figure 11). Option 3 guarantees a final plateau after many applications, but at a higher level than with the first option (shown in Figure 9). Of course, there will be no difference between option 1 and option 3, if only a single application per year is simulated or the degradation models SFO or DFOP are used.

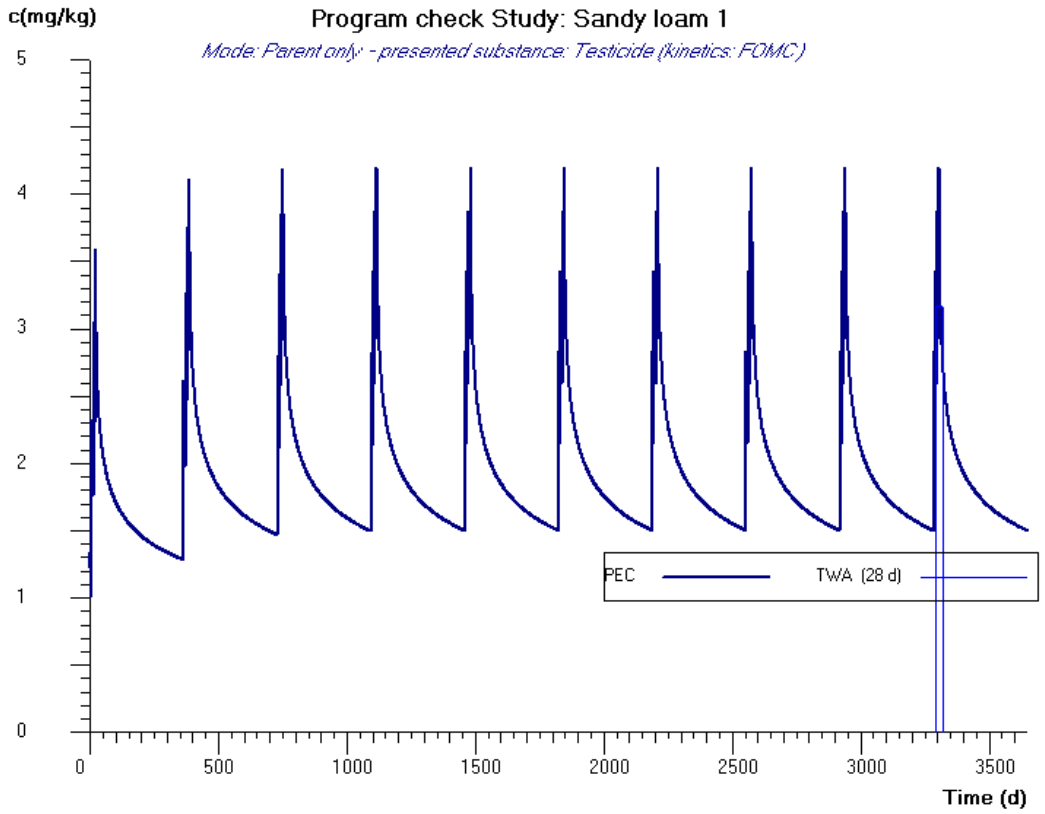


Figure 9: FOMC-model (10*4 applications, α=0.2, ß=2), separating of residues switched off

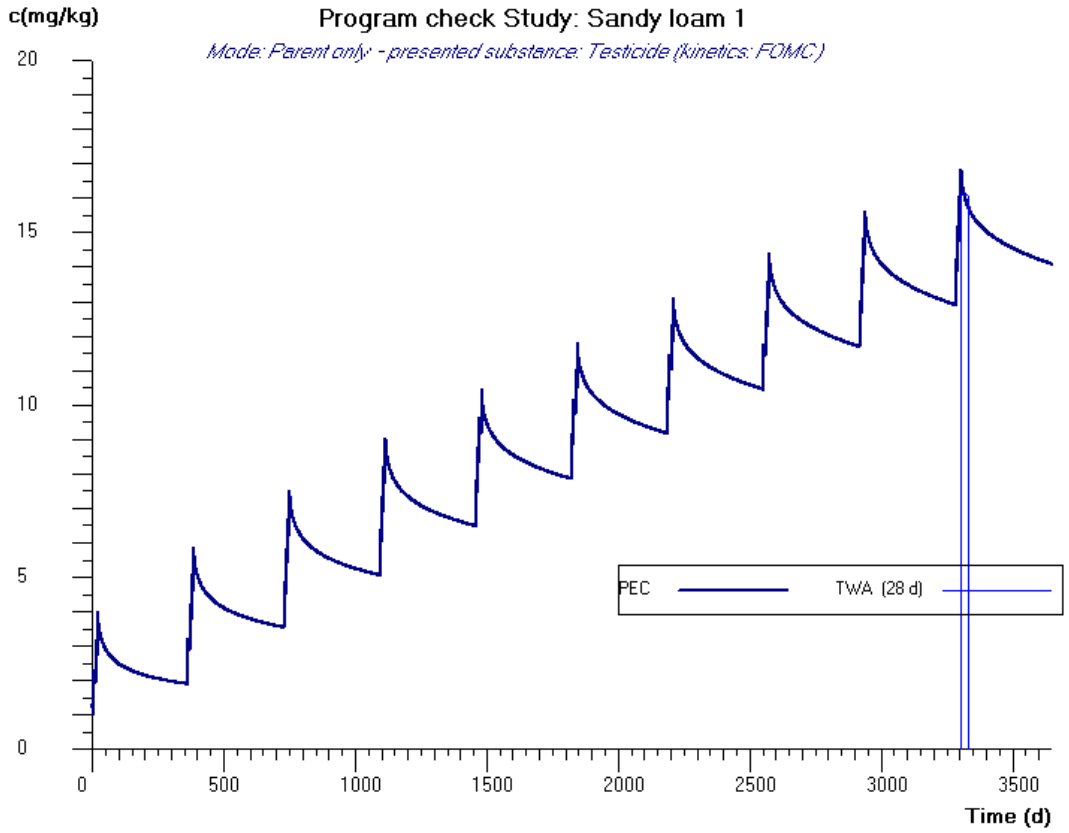


Figure 10: FOMC-model (10*4 applications, α=0.2, ß=2), separating of residues switched on

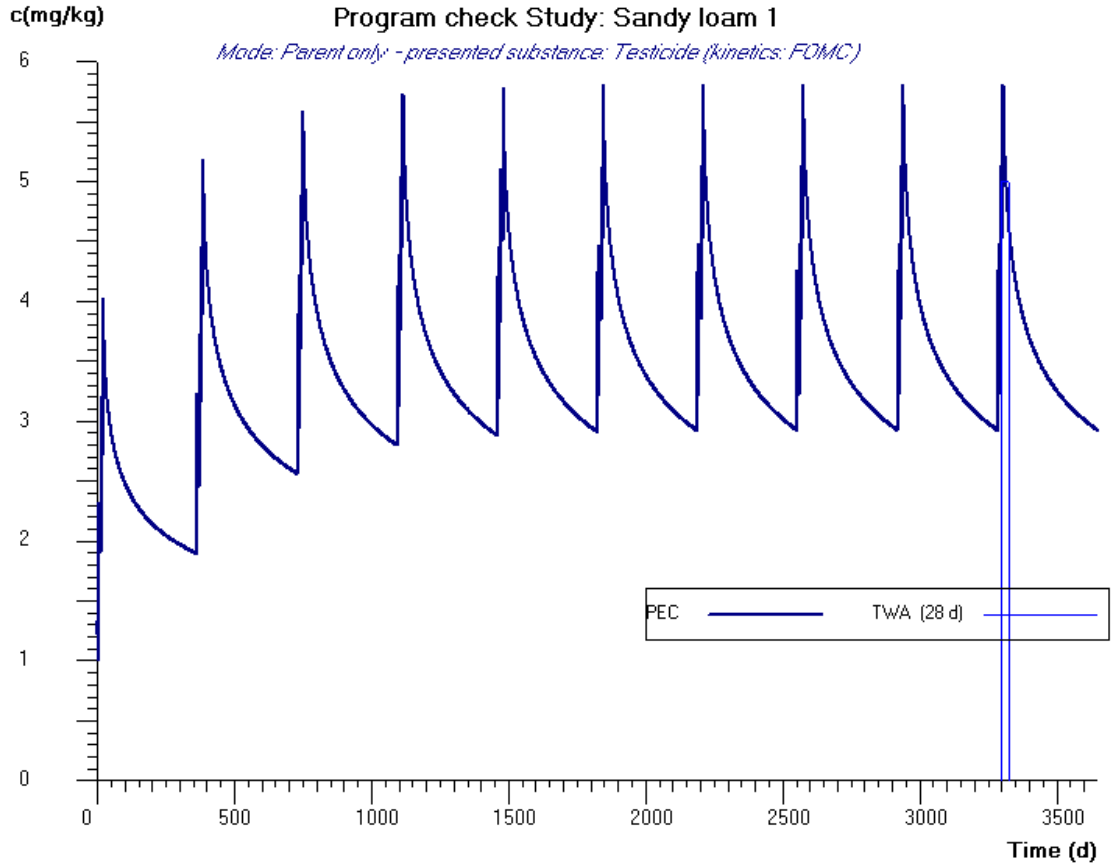


Figure 11: FOMC-model (10*4 applications, α=0.2, ß=2), separating of residues within a year

Of course, the differences between the three options are highly influenced by the fitting parameters used in the calculation.
As already mentioned, if single first order or DFOP kinetics are selected, there is no difference between these options.

The time dependent concentrations for metabolites are calculated similarly as for the parent compound. Instead of a series of applications the daily formation is considered as the base for soil concentrations. The formation is calculated considering the ratio of the molecular masses and the formation rate according to the equations presented in chapter 3.3.2 to chapter 3.3.4.
The degradation of metabolites follows in principle the same equation as explained for parent compounds earlier in this chapter. However, in contrast to parent compounds there are no counters defined when new pesticide amounts arrive after applications. These counters influence the rate of degradation when the kinetics follow the HS- or the FOMC-model. Consequently, these two kinetics are generally not available for metabolites.

For risk assessment purposes some simulation days after the maximum soil concentration are highlighted due to regular comparisons with eco-toxicity data. ESCAPE considers two different lists of dates as summarised in Table 1. The times listed in this table are also the base for all time weighted average concentrations calculated by ESCAPE (see the next chapter). It is possible to change the lists by modifying the file “ESCAPE.ini”.

Table 1: Series of special times used by ESCAPE to calculate PEC_{act} and PEC_{TWA}

EU-regulation	BBA-regulation (Germany)
1 d	30 d
2 d	60 d
4 d	90 d
7 d	120 d
14 d	150 d
21 d	180 d
28 d	210 d
42 d	240 d
50 d	300 d
100 d	330 d
	360 d

3.4.3. Time weighted average (TWA) concentrations

In addition to maximum soil concentrations also time weighted average concentrations ($PEC_{TWA)}$ are important endpoints for comparisons with results of eco-toxicity. ESCAPE uses two different lists for the duration of time weighted average concentrations (see Table 1). These type of concentrations are calculated based on a moving time frame assuring that always the worst case PEC_{TWA} is found for a given time duration.

Generally, all time weighted average concentrations are calculated by ESCAPE within a two-steps-procedure:
In the first step the integral of actual soil concentrations (cumulative concentrations) for parent compounds and metabolites is calculated according to equation *(23)*.

$$C_{cum,\,j} = \sum_{j=0}^{n} C_j \qquad (23)$$

$C_{cum,j}$: cumulative soil concentration at time j (mg/kg)

C_j: actual soil concentration at time j (mg/kg)

j: current simulation day

n: total number of simulation days

Based on the cumulative concentrations a search for the worst case time frame is performed for each TWA in the second step according to the following two equations:

$$PEC_{TWA,\,j} = \frac{C_{cum,\,(j\,+\,dtwa)} - C_{cum,\,j}}{d_{twa}} \qquad (24)$$

$$PEC_{TWA} = \text{Maximum(all } PEC_{TWA,j}) \qquad (25)$$

PEC_{TWA}: Time weighted average concentration (mg/kg)

$PEC_{TWA,j}$: Time weighted average concentration beginning at time j (mg/kg)

$C_{cum,j}$: Cumulative concentration at time j (mg/kg)

$C_{cum,+dtwa}$: Cumulative concentration at time $j + d_{twa}$ (mg/kg)

d_{twa}: duration of the time weighted average concentration (mg/kg)

3.4.4. Background concentrations

Background concentrations are concentrations after many years with pesticide applications. ESCAPE considers the plateau bottom (just before a new application is performed) as background load. In contrast to annual concentrations the tillage depth is used to define the depth of the soil compartment for background concentrations.

To estimate the background concentrations calculations are always performed over ten years.

Dependent on the degradation parameters the final plateau might not be reached within this period. Therefore, ESCAPE performs an additional estimation about the maximum plateau concentration obtained after infinite years of applications.

For this estimation the last three maximum annual soil concentrations are considered (maximums in the years 8, 9 and 10). The derivative of the parabola through these three

maximums is calculated and based on this function the final maximum plateau after many years is estimated. The final bottom plateau is then calculated by abstracting the maximum concentration in the first year.

3.4.5. Annual concentrations considering accumulation

ESCAPE uses the background concentration and the time dependent concentrations in the first year for the calculation of annual concentrations including accumulation (PEC_{accum}) according to the following equation.

$$PEC_{accum} = C_{background} + PEC_{year1} \qquad (26)$$

PEC_{accum}: Time dependent concentration including accumulation (mg/kg)

PEC_{year1}: Time dependent concentration in the first year (mg/kg)

$C_{background}$: background concentration related to tillage depth (mg/kg)

3.5. Calculation of pore water concentrations

For the calculation of pore water concentrations it is assumed that there is equilibrium between soil water and soil matrix for all compounds.
Based on this assumption the pore water concentrations are calculated using following equation:

$$C_{PW} = \frac{C_T}{\frac{\Theta}{\rho} + \frac{C_{org}\ K_d}{}} \qquad (27)$$

C_{PW}: pore water concentration (mg/L)
C_T: total content in soil (mg/kg)
C_{org}: organic carbon content in soil (%)
K_d: sorption constant (L/kg)
ρ: soil density (kg/m³)
Θ: actual soil moisture (m³/m³)

3.6. Consideration of scenario soil profiles and weather files

ESCAPE is able to calculate soil concentrations based on pre-defined weather and soil scenarios. As no special scenarios has been defined in the field of persistence in soil so far, the nine FOCUS groundwater standard scenarios have been implemented in this version of ESCAPE.

All scenarios are based on a combination of the first horizon of the FOCUS-soil scenario and a single weather year (same location) that has been selected based on cold, normal, warm weather conditions. A summary of the annual temperatures at the locations and the respective years selected for ESCAPE is given in Table 2.

Table 2: Selected weather year at the FOCUS locations

Year	Château-dun	Hamburg	Jokioinen	Krems-münster	Oke-hampton	Piacenza	Porto	Sevilla	Thiva
1	12.41	10.26	5.83	9.89	11.56	13.57	16.56^{o}	19.35	15.64*
2	12.52	10.43^{o}	5.86	8.99	11.64	14.26	15.41	18.67	16.49$^{\#}$
3	11.24	9.80	6.32^{o}	8.74	10.56	14.16	14.94	18.00	15.69
4	11.55	10.29	6.31	9.90	11.62	15.68^{o}	14.88	18.94	16.39
5	10.88	9.17	3.68	9.30	10.78	14.83	15.51	18.46	16.80
6	12.72^{o}	10.27	4.93	11.03^{o}	11.91^{o}	15.63	15.31	19.81^{o}	17.52^{o}
7	11.35	10.20	5.71	9.54	10.83	14.61	14.75*	17.22*	17.13
8	11.80	9.30	2.84	9.27	10.67	13.76	15.23	17.81	16.12
9	11.34$^{\#}$	9.54	3.57	9.77	10.57	13.52	15.44	17.64	16.65
10	10.74	8.53	3.11	8.49	9.95	13.22	15.41	17.72	16.09
11	10.98	7.67*	3.68	8.91	9.74	13.65	15.42$^{\#}$	18.27$^{\#}$	16.73
12	10.72	8.92	3.76	8.11*	10.38	14.48	14.96	18.06	16.05
13	11.57	8.61	3.85$^{\#}$	8.72	10.65$^{\#}$	13.57	16.05	18.51	16.60
14	12.26	9.29$^{\#}$	4.93	8.93$^{\#}$	11.04	14.99	15.40	18.09	16.46
15	11.95	9.57	5.10	9.30	10.84	14.77	15.61	18.85	16.76
16	11.33	8.84	5.04	8.25	10.46	12.94	15.72	18.00	16.28
17	10.47*	8.46	2.46	8.31	9.72*	12.79*	15.78	18.40	17.11
18	10.66	9.03	3.31	8.65	9.86	13.32	15.71	17.91	16.46
19	10.66	8.45	2.26*	8.79	10.14	14.94	16.03	19.47	16.58
20	12.06	9.80	4.18	9.42	11.06	13.95$^{\#}$	15.77	18.35	17.16

(* considered as cold year, $^{\#}$ considered as normal year, ^{o} considered as warm year)

4. Working with ESCAPE

4.1. Installing ESCAPE

Perform following steps for the installation of ESCAPE:

1. Call ESCAPE_setup.exe
2. Select a directory and start unzipping the files into a temp-folder
3. After unzipping close ESCAPE_setup.zip
4. call setup.exe in the folder where the files were unzipped
5. ESCAPE may be un-installed using first the standard MS-Windows un-install tools provided in the “Control Panel” under “Add/Remove Programs”.

After successful installation the program logo appears as shown in the next figure.

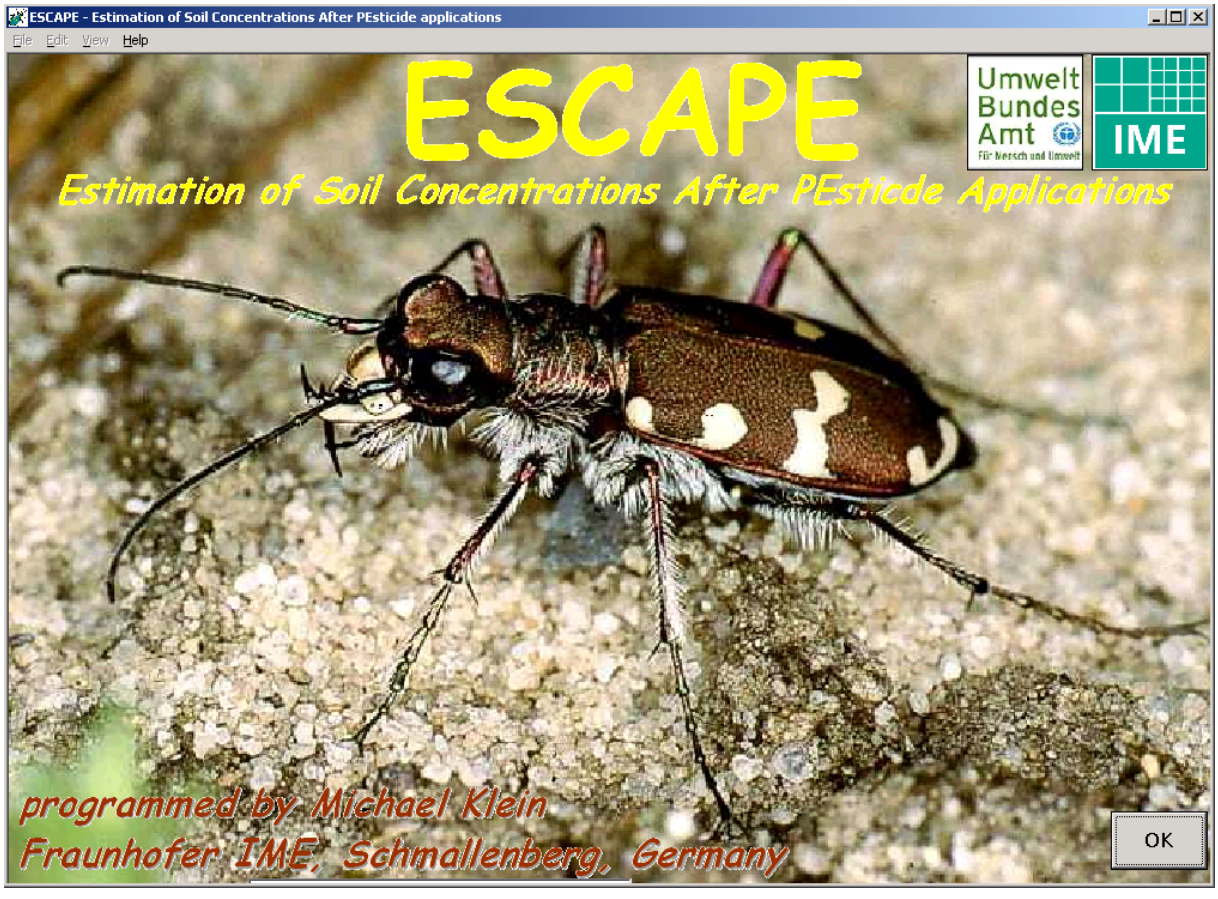


Figure 12: ESCAPE Intro-screen

After pressing the button “OK” the main form of ESCAPE is loaded.
ESCAPE will automatically estimate soil concentrations based on the information found in the file “Programcheck.txt” (saved in the subdirectory: “input”)
In white input fields results of ESCAPE are always directly updated when an input parameter was changed. Fields with yellow background colour are updated until the input was finished (by pressing “ENTER” or moving to another field). All input data are presented on the main form and can be modified directly. Also part of the results is always presented immediately on the screen (e.g. diagram and/or tables showing the time dependent concentrations in soil) However, a full report, with all input data listed and with more detailed output is only created after a click at the report-button.

4.2. Calculation modes considered by ESCAPE

ESCAPE can be used in four different calculation modes:

- parent compound only
- parent compound and a single metabolite
- parent compound and two metabolites formed in parallel
- parent compound and two metabolites formed in a sequence

The tabs on the main form can be used to switch between the four modes (see the red frame in Figure 13). The number of input parameters on the right part of the main form is influenced by the selection of the calculation mode.
When the calculation mode has been modified ESCAPE tries to perform a new simulation using the current set of input parameters and creates new diagrams automatically (if possible).

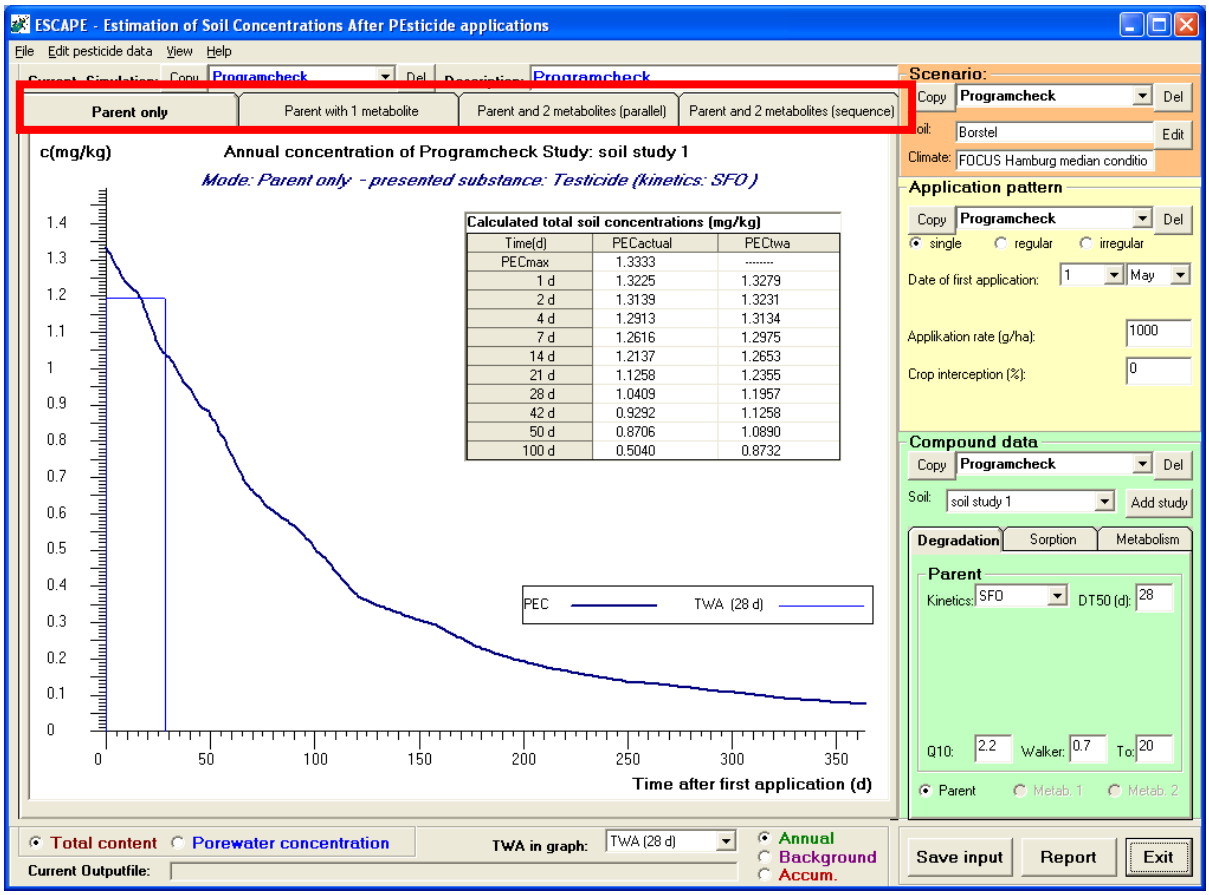


Figure 13: ESCAPE: Main form: Four different calculation modes

4.3. Editing input parameters

Important input parameters can be directly defined or modified at the right hand side of the main form (see Figure 14).

Input parameters are grouped into different blocks according to their meaning namely:

- scenario parameters
- parameters describing the application pattern of the product
- parameters describing the degradation kinetics of the parent and metabolites and additional parameters defining the metabolism scheme (if metabolites are to be simulated)

In order to make editing of input data more user friendly necessary input fields are displayed dependent on the selected calculation mode.

If valid input data have been entered ESCAPE is automatically updating all soil concentrations if the background colour of the field is white. Input data from fields with yellow background colours are only updated after the enter key was pressed. If the current data is not valid a small message will inform the user about the wrong input.

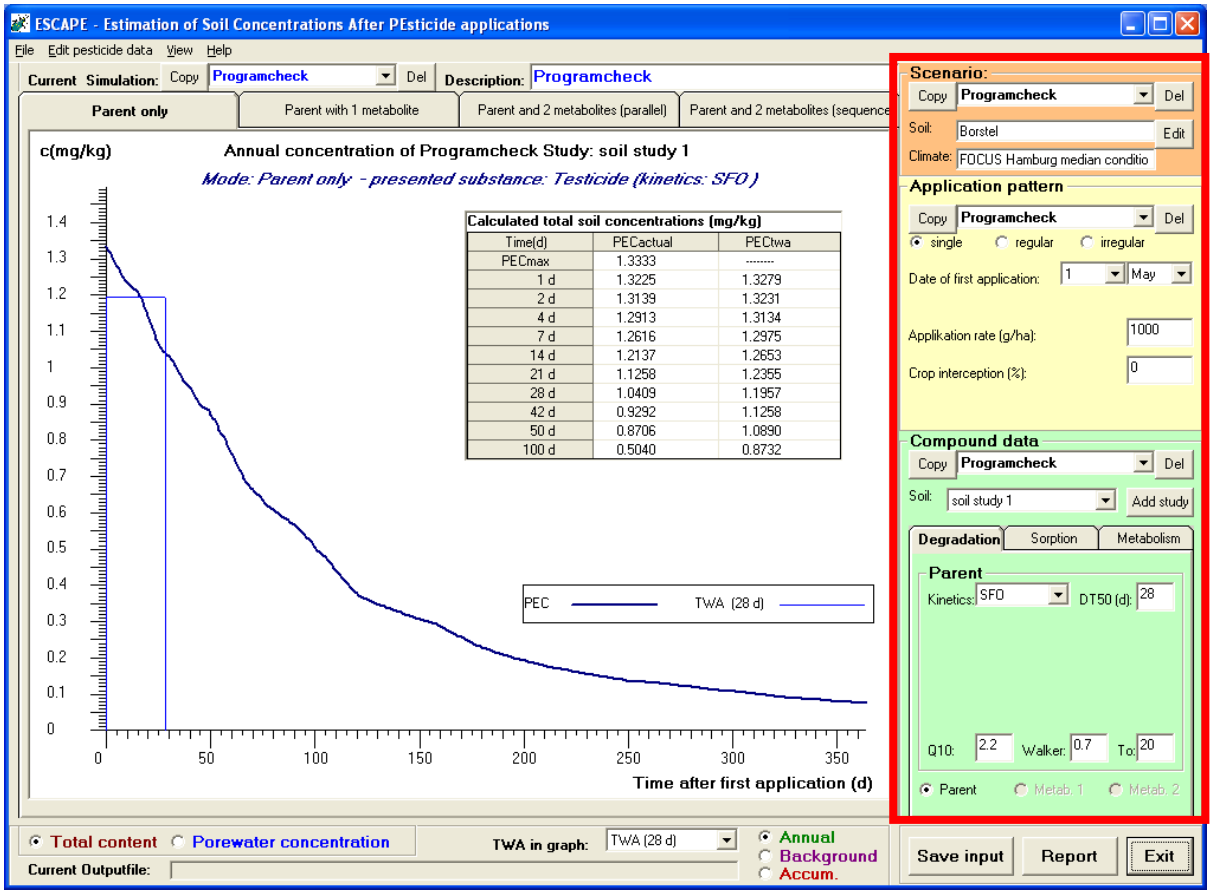


Figure 14: ESCAPE: Main form: Editing input parameters

4.3.1. Scenario parameters

Scenario parameter can be divided into soil related and climate related parameters. Scenario parameter are not frequently modified. Therefore there are not presented on the main form. However, a special window is loaded when the button “Edit” in the brown scenario frame on the main form is pressed (see Figure 14 and Figure 15).

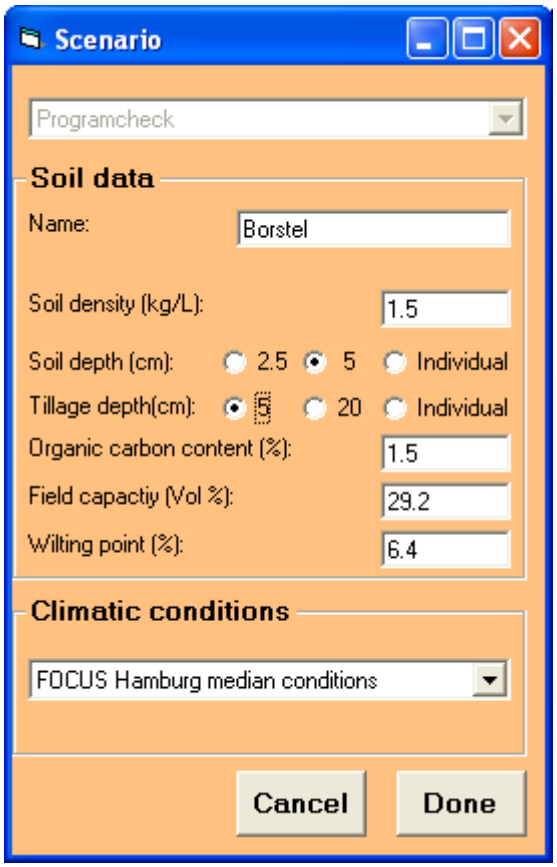


Figure 15: ESCAPE: Editing scenario parameters

There are six different soil parameters that are used to estimate soil concentrations. First, the soil density (kg/L), the normal “ecologically relevant” soil depth (cm), and the tillage depth (cm). Whereas the soil density has to be explicitly typed by the user, a selection have to be made out of three options for the soil and the tillage depth. For the soil depth either radio buttons for 2.5 cm and 5 cm or individual soil depths can be considered. For the tillage depth (used for background concentrations) either radio buttons for 5 cm (pasture) and 20 cm (agriculture field) or individual tillage depths can be selected. If individual depths are selected a list box will appear to select the favoured value.

To calculate pore water concentrations the organic carbon content in soil is needed. The other two soil parameters, field capacity and wilting point, are used to estimate dynamic soil moistures dependent on the weather conditions. A suitable weather can be attached to the soil profile, which itself cannot be modified in the shell. However, weather files are in ASCII-data in the same format as PELMO weather files [FOCUS 2000].

4.3.2. Application related parameters

In total seven different parameter define the application pattern summarised in a yellow frame (if coloured frames are switched on, see preferences).

Application mode

First, the user has to decide between three different application models (“single applications”, “regular application” or “irregular application”). Dependent on the application selected u different further input parameters appear on the form.
“Single application” means one application per season, “regular application” means a series of application within a year with constant rates, constant crop interception and constant intervals between two simulations. Finally, “irregular applications” means a series of applications (within a year) with different rates, different crop interception and/or different intervals between these applications.

Application date (g/ha):

If single or regular applications have been selected the user has to type the date if the first application. The date is important only if degradation rates are corrected using temperature and soil moisture, because then time dependent concentrations are dependent whether substances are applied are in spring or autumn.

Application rate (g/ha):

If single or regular applications have been selected the user has to type the respective application rate, here.

Crop interception (%):

If single or regular applications have been selected the user has to type the respective crop interception here.

Number of applications per year:

If regular or irregular applications have been selected the user has to type the number of simulations per year using the list box. If single applications are selected this field dos not appear on the form. If the application shall be repeated annually the check box “Repeat applications per year” has to be used.

Application table

The application table only appears on the form if “irregular applications” have been selected. The user has to type the explicit application dates, rates and crop interception for each application here. All input must be related to the first year. In the following years the application pattern may be repeated dependent on the check box “Repeat applications per year”.

4.3.3. Compound specific parameters

The compound specific parameters are organised on three green file cards.

File card ‘Degradation’: Degradation kinetics related parameters

The degradation of the parent compounds or metabolites can be characterised based on eleven different input parameters.

Soil:

For up to six soil studies degradation models for parent compounds or metabolites can be defined. This field is to characterise a certain study by comment. If more soil studies shall be be considered by ESCAPE the “add”-button has to be used. If the name of a study should be modified the user has to press the control-key and to click at the list box at the same time. The colour of the box changes from white to yellow and a new text can be entered as long as the colour remains yellow.

Compound:

At the bottom of the file card the substance to which all degradation data is related to can be selected. Dependent on the calculation mode compounds may be deactivated.

Kinetics:

ESCAPE considers in total 4 different degradation kinetics SFO: (S*ingle First Order),* HS (*Hockey Stick)*, DFOP: (*Double First Order in Parallel) and* FOMC: F*irst Order Multi Compartment)* which are explained in detail in chapter 3.1. For each soil study the suitable degradation model can be selected for the activated compound. However, only for parent compounds all four models are available. For metabolites only the SFO- or the DFOP kinetics can be used because the other models are not conceptually correct for a metabolite that is gradually formed over a period of time (see chapter 3.1). Dependent on the selection different parameters appear on the form.

$DT50$ (d):

If the SFO-model has been selected there is only one parameter to characterise the degradation, the first order DT50, which has to be entered here.

DFOP-$DT50_1$ (d):

If the DFOP-model has been selected the first 1st order DT50 has to be selected here.

DFOP-$DT50_2$ (d):

If the DFOP-model has been selected the second 1st order DT50 has to be selected here.

DFOP-parameter g (-):

If the DFOP-model has been selected the parameter g which describes the fraction of the compound that degrades according to the first DT50 has to be entered here. Values for g are only accepted in the range of 0 to 1.

FOMC-parameter α:

If the FOMC model has been selected the parameter α: has to be selected here.

HS-rate constant β:

If the HS-model has been selected the parameter β has to be selected here.

HS-$DT50_1$ (d):

If the HS-model has been selected the first 1st order DT50 has to be selected here.

HS-$DT50_1$ (d) (1/d):

If the HS-model has been selected the second 1st order DT50 has to be selected here.

HS-parameter Tb (-):

If the HS-model has been selected the parameter Tb has to be entered which describes the breakpoint where the degradation switches from the first to the second DT50.

File card 'Sorption': Sorption related parameters

Name of the compounds:
In these (at maximum) three fields the names of the parent compound and the metabolite(s) can be specified by the user. The names will later appear in the report of ESCAPE.

KOC (L/kg):
There is currently a single sorption parameter that can be entered here for all compounds simulated, the sorption constant related to the organic carbon content. The parameter is used to calculate time dependent pore water concentrations in soil.

File card 'Metabolism': Parameters related to the metabolism scheme
If not only the parent compound but also metabolites are considered for a simulation the metabolism scheme can be entered in the third green file card (if coloured frames are switched on, see preferences).
As explained earlier in chapter 3.2 ESCAPE is able to consider a maximum two metabolites (formed in parallel or in a sequence). The metabolism scheme can be characterised by in total eight parameters:

Name of the compounds:
In these three fields the names of the parent compound and the metabolite(s) can be specified by the user. The names will later appear in the report of ESCAPE.

Molecular mass (g/mol):
For the formation of metabolites the user has to enter the molecular masses of all compounds considered for the simulation here.

Formation rate (%):
For the correct calculation of metabolite concentration in soil the user has to enter the formation rates for all metabolites here. The formation fraction is not the same as the maximum formation during the study. If the formation fraction is not known enter "100" as an worst case estimate.

4.3.4. Problem characterisation

Each combination of input data (scenario, application pattern, compound data) is called a 'simulation' and are saved in a special data base. The user may attach a description to this simulation which will later appear in the output documentation. The description is localised on top-right of the main form (see Figure 16). This description has a slight write protection which can be removed if the user presses the control-key when he clicks at the form. The field background colour will turn into yellow and can be edited now.

The list box in the top-left part of the form is to select pre-defined simulations. Simulation records can be copied or removed using the respective buttons close to that list box.

More option for the editing simulation records are available via the menu bar (File – Load Simulation).

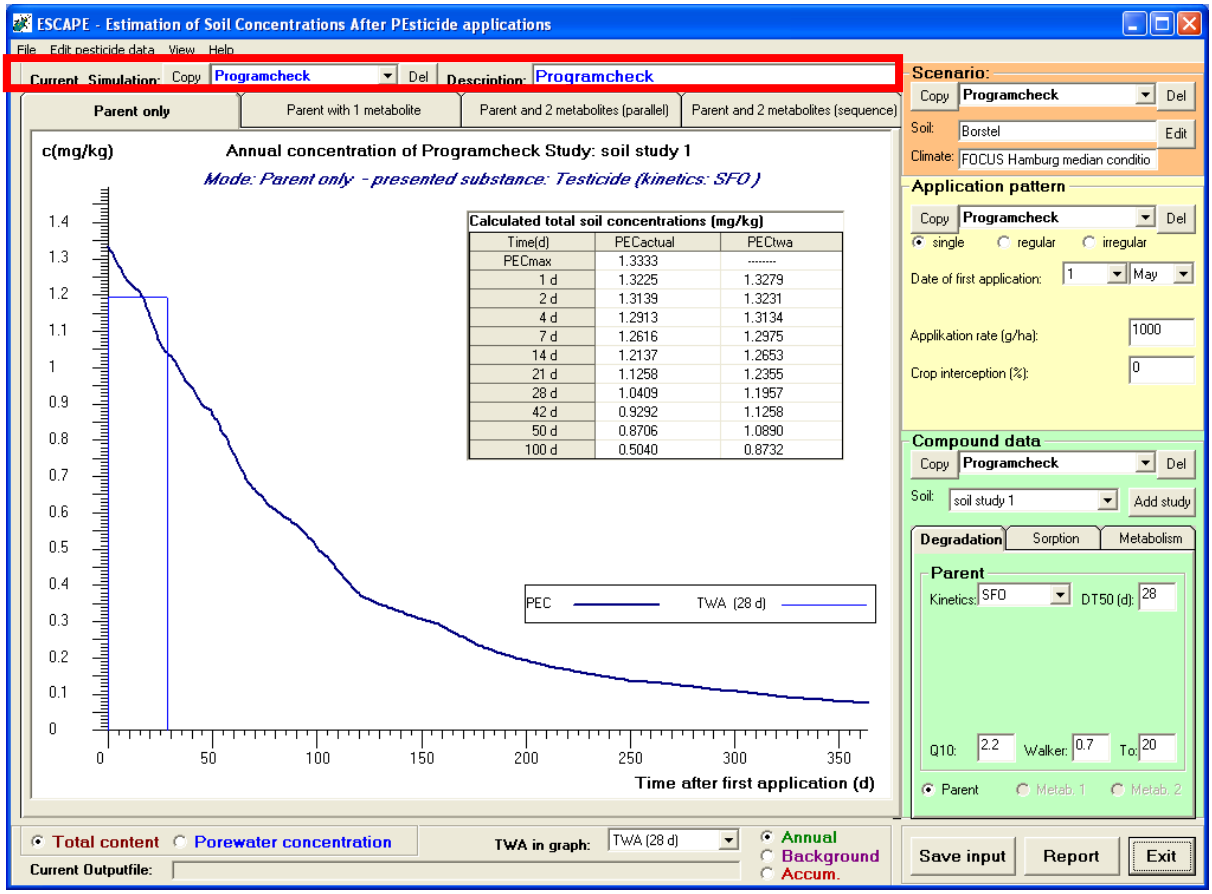


Figure 16: ESCAPE: Main form: Description of the problem

4.4. Combining input data for a simulation

4.5. Command buttons

There are three buttons on the left bottom part of the main form that can be used for most important commands when working with ESCAPE (see Figure 17).

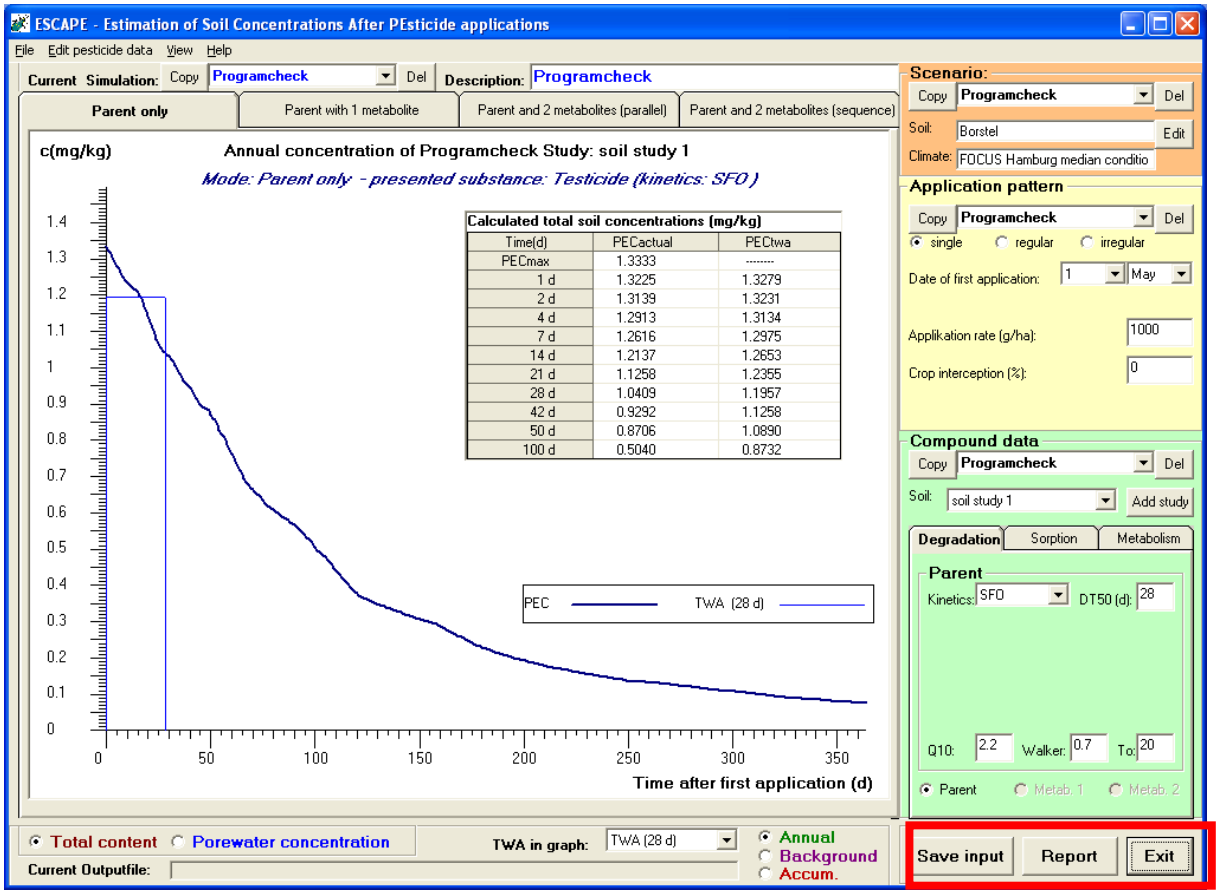


Figure 17: ESCAPE: Main form: Command buttons

<u>Save input:</u>

If the current parameter setting should be saved on the computer the fastest method would be that button. It will save all input under the current names.

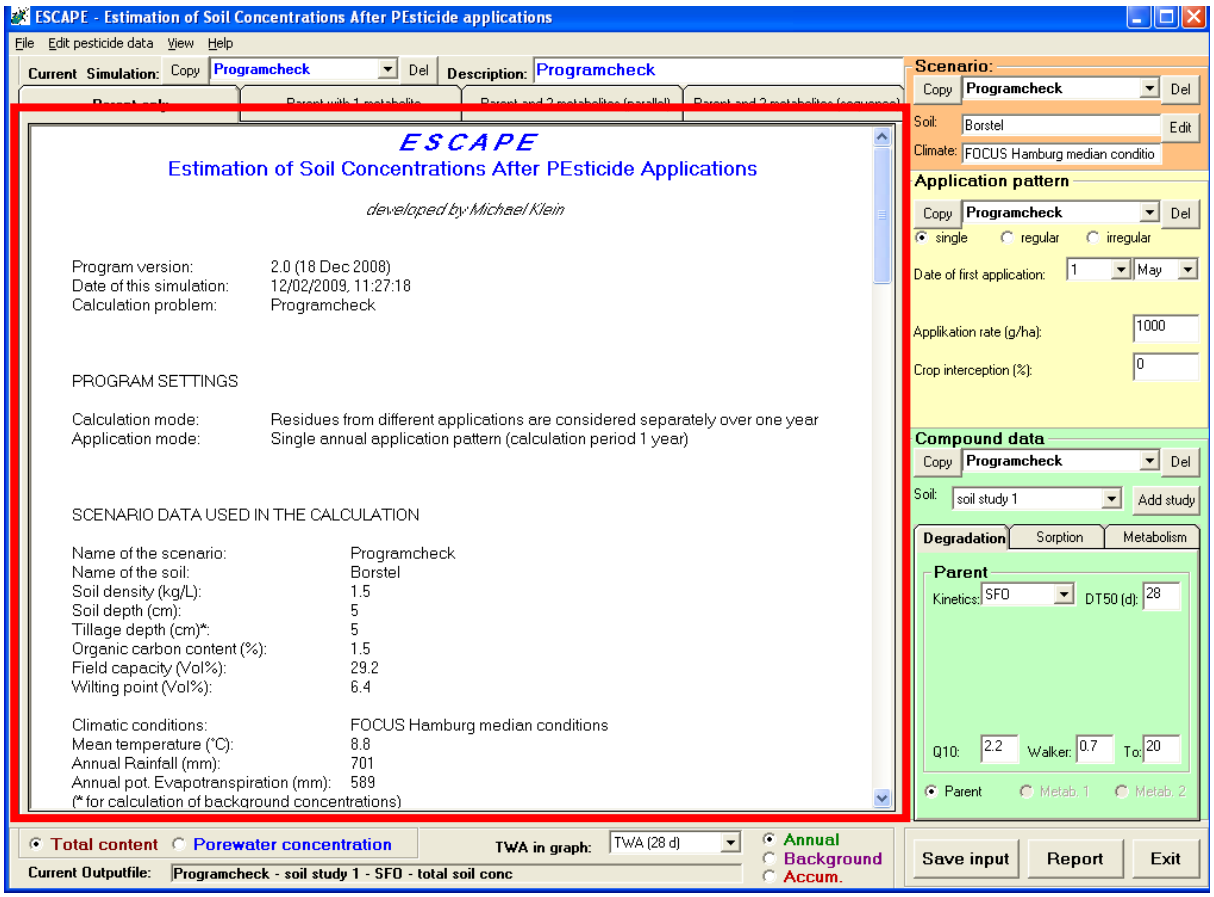


Figure 18: ESCAPE: displaying the report file

Creating reports:

A click at this button generates an output file presenting all results of the simulation, the current input data setting and the actual diagram shown on the screen. The file will be written in RTF-format and directly saved in the ESCAPE-output-folder. The name of the file can be customised using the menu bar (edit – preferences). The actual name is echoed at the bottom of the main form (current output file)

When a report is created it is also displayed at the main form (see Figure 18). It is possible to do some limited text processing (scrolling with cursor keys, copying into the clipboard with “ctrl C”). After a double click at the report the standard diagram sheet returns on top of the screen and the report disappears.

Dependent on whether ESCAPES provides information about an individual study or collects summary information about more than one soil study the report file looks differentially. The menu items “View – Summary” or “View – Individual studies” can be used to switch between these two modes. Via the menu bar (File menu) reports can be also printed.

Exit:

This button will terminate the program.

4.6. Direct endpoint selection

The radio buttons in the left bottom part of the form can be used to switch between total content in soil and pore water concentrations (see the rectangle in Figure 19). The graphs are re-constructed instantaneously because calculations are always performed for both endpoints independent on the actual settings.

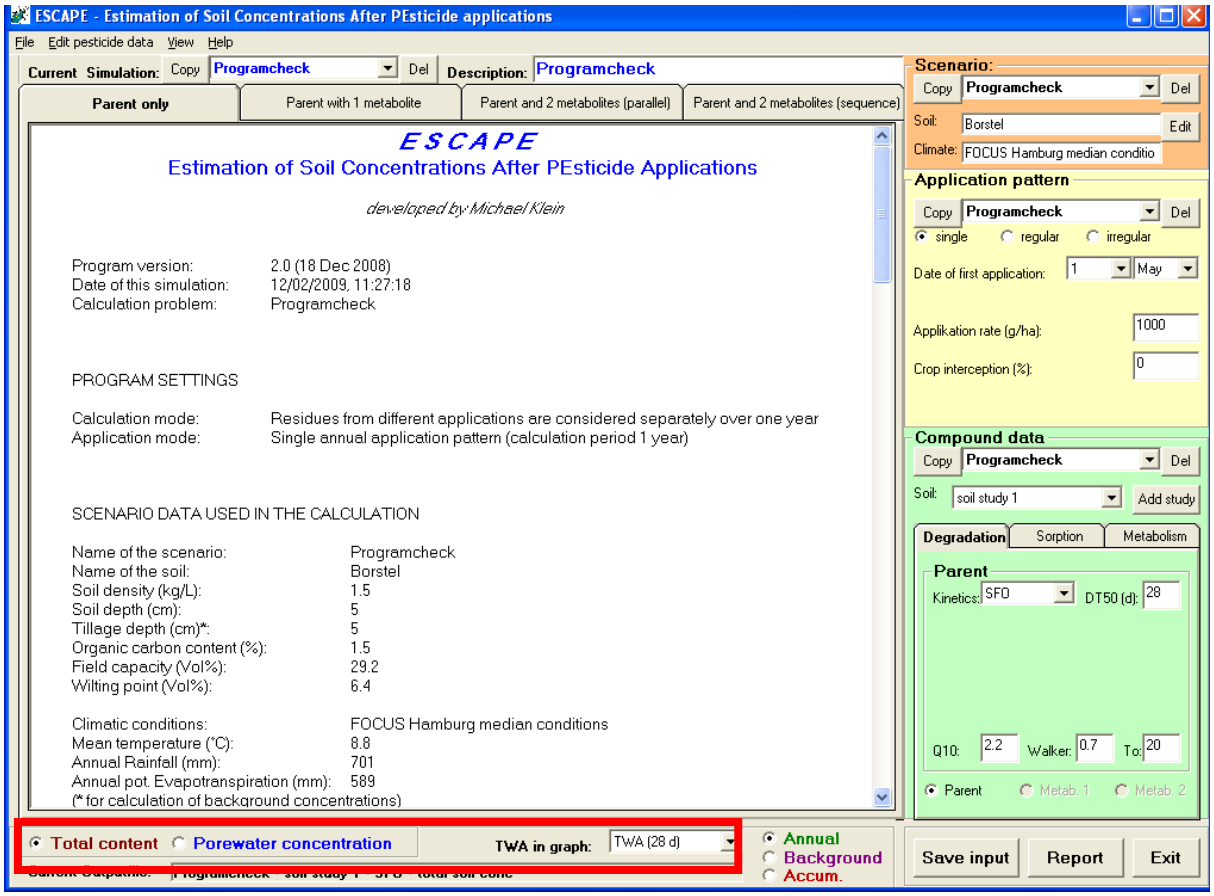


Figure 19: ESCAPE: Selecting endpoints on the main fram

4.7. The menu bar

The menu bar on top of the main form (see Figure 20) provides the user with all possible commands when working with ESCAPE.

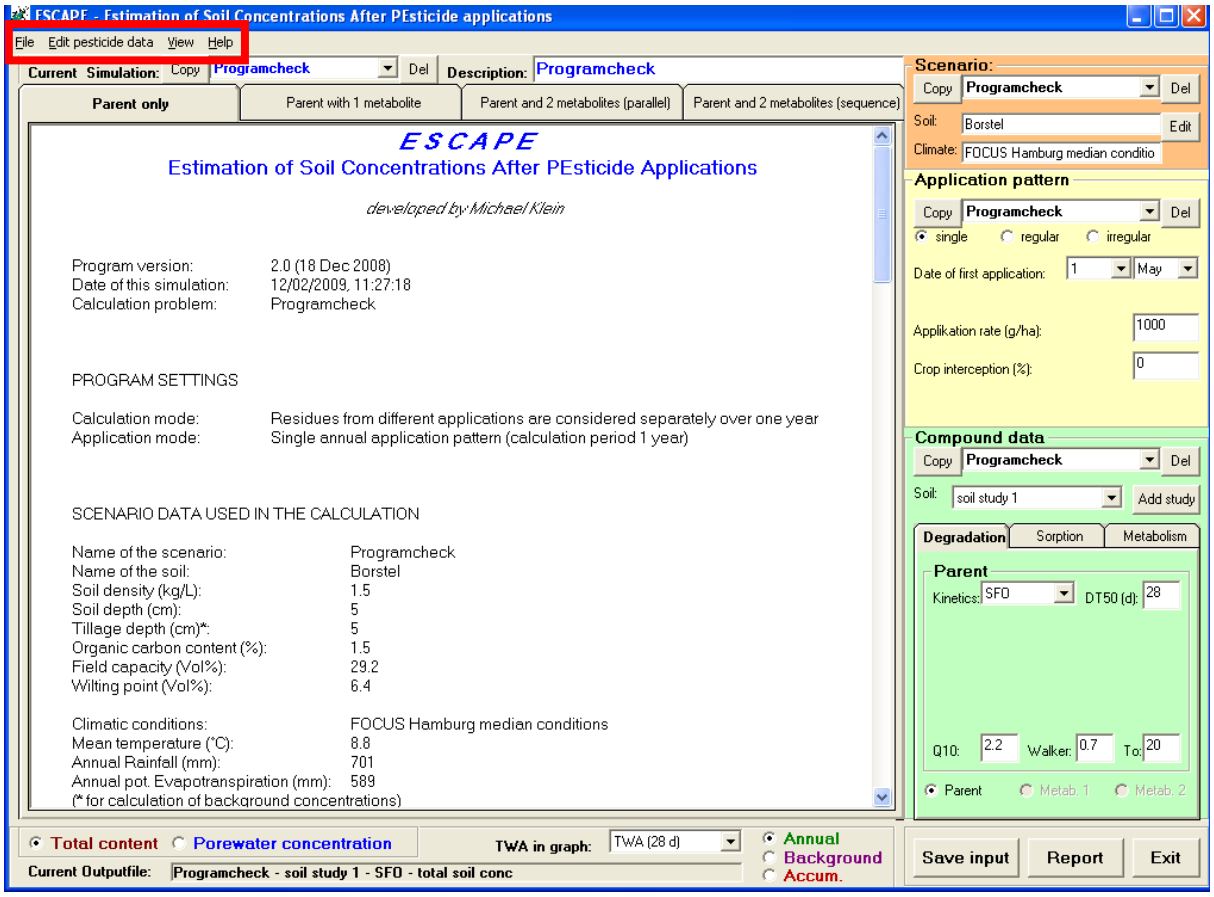


Figure 20: ESCAPE: Working with the menu bar

File – New Pesticide Record:

This command can be used to load a new set of standard input data into ESCAPE. The necessary information on the standard pesticide data is saved in the text file "do not delete this file.chn" The name of the new record will be "new compound1". If the record is already existing the numbering will be incremented.

File – New Application Record:

This command can be used to load a new set of standard input data into ESCAPE. The necessary information on the standard application data is saved in the text file "do not delete this file.apn". The name of the new record will be "new application pattern 1". If the record is already existing the numbering will be incremented.

File – New Scenario:

This command can be used to load a new set of standard input data into ESCAPE. The necessary information on the standard application data is saved in the text file "do not delete this file.scn". The name of the new record will be "new scenario". If the record is already existing the numbering will be incremented.

File – Load Simulation:

This command is to load a special form the “simulation organiser” which allows to edit ESCAPE input data records and simulation collections. It is however, not absolutely necessary to use this form as the main form has in principle the same functionality as the simulation organiser.

Each combination of input data (scenario, application pattern, compound data) is called a ‘simulation’ and are saved in a special data base. The top list box is to switch between simulations currently saved in the system. A simulation description which will appear in the output documentation is shown below that list box and can be modified here.

Simulation records can be also removed renamed or copied using the respective buttons attached to the list box.

In addition the description each simulation record contains the names of the scenario, application pattern and compound record.

Also these data can be manipulated in a similar way as simulation records using the respective buttons attached to the list boxes. If different input data records have been selected by the user and the simulation organiser is closed (Button: ‘Done”) the new collection is automatically saved in the current simulation record.

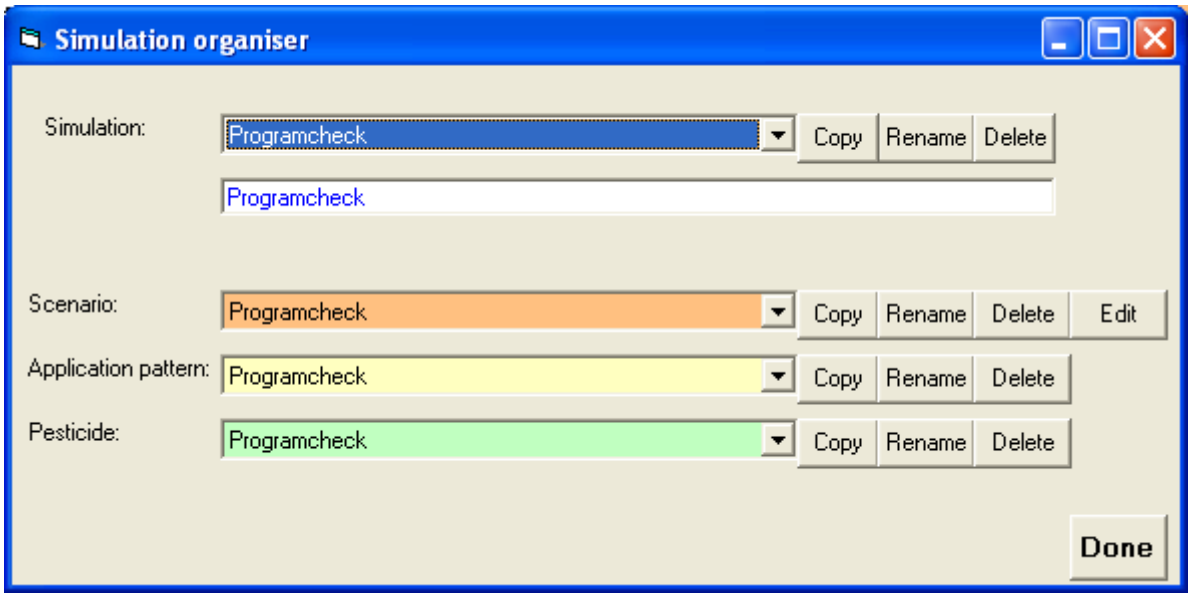


Figure 21: ESCAPE: Editing input data sets

File – Print:

If a report file was generated this command calls the standard windows printer routines. After selecting the desired printer the actual report will be printed. If no report was generated so far the option is disabled.

File – Save All input data

This command will save all input under the current name (given at the bottom of the main form). Instead of using the menu bar a fast possibility of saving the current settings would be the use the button “save input”.

File – Save as:

This command will save all input under a new name. A window is loaded as shown in **Fehler! Verweisquelle konnte nicht gefunden werden.** to define the new name.

File - Exit:

This command will terminate the program. A fast alternative would be the button “exit” at the main form.

Edit pesticide data – Add study:

Use this command if an additional soil study should be considered for ESCAPE. The name of the new soil study can be typed in the yellow field which appears on the right part of the main form (frame: degradation kinetics parameters). Up to six soil studies per data set can be considered for a simulation with ESCAPE. Another possibility of adding soil studies is the button “add study” (frame “degradation kinetics parameters”)

Edit – Delete study:

Use this button if the soil study selected currently in the degradation kinetics frame on the right part of the main form should be deleted.

Note that the last soil study in the data set cannot be removed, but only modified by the user.

Edit – Preferences

Use this command to modify the preferences of ESCAPE. The different model switches can be modified in a special form that will appear on the screen (see Figure 22).

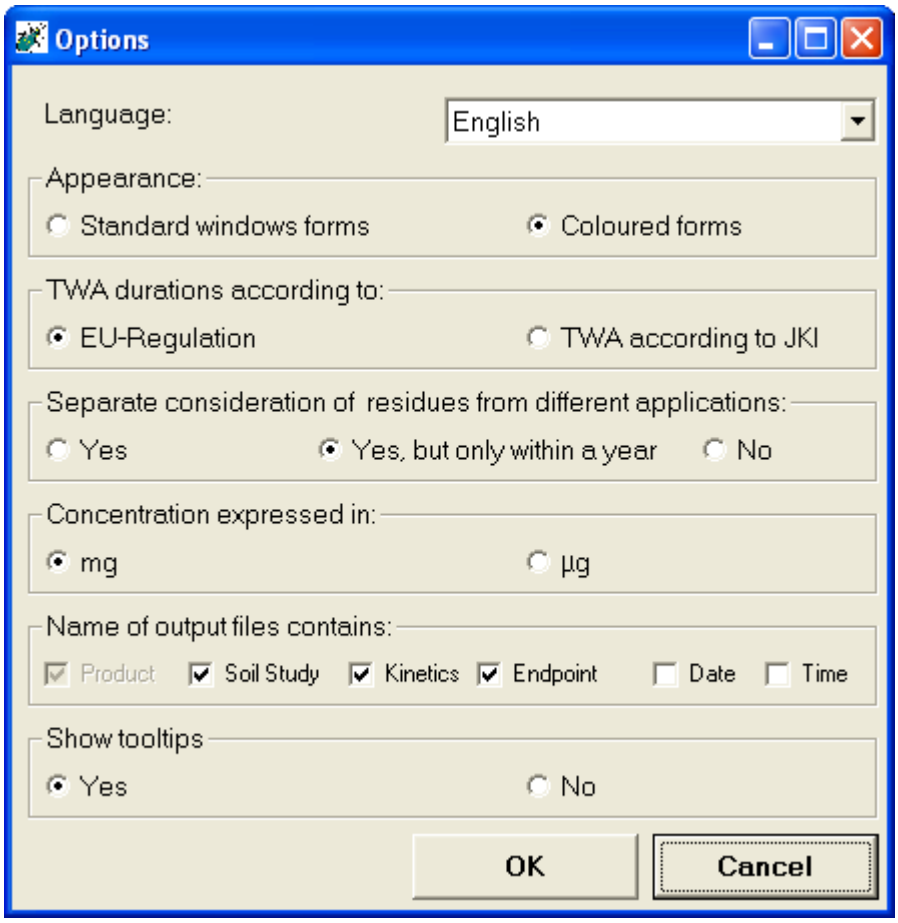


Figure 22: ESCAPE: Modifying preferences

There are presently seven different options that can be modified by the user:

Language:

The user can select the language of the model shell here.

Note, in the current version only English is available.

Appearance

In addition to the windows standard system palette ESCAPE is able to highlight the different forms on the screen using background colours. The user can switch on or off this feature here.

TWA-duration scheme:

The user can decide which list of TWA-duration should be considered for the simulation. The two lists are shown in Table 1 on page 29 in this document.

Separate consideration of residues from different applications:
As explained earlier in chapter 3.4.2 on page 25 ESCAPE has implemented three different procedures of handling residues coming from different applications. The desired calculation can be selected, here. It will be saved also in the input data set and documented in the program report.

Concentrations expressed in mg/kg or µg/kg
ESCAPE can express the soil concentration either in mg/kg or in µg/kg. The user can select the suitable unit for the specific problem here. The selection will be saved also in the input data set.

Naming of output files
The user can customise the names of the ESCAPE report files here to make archiving of results more user friendly.
Note, that in the ESCAPE summary mode the check box “Soil study” will not be taken into consideration.

Tooltips
When working with the model it is possible to fade in a small context sensitive user help. These tooltips can be switched off or on here.

<u>View – Individual studies</u>
The fate of a pesticides and/or its main metabolites can be simulated in up to six soil studies. To visualise the results ESCAPE provides output in two different modes. In its mode “View – Individual studies” only the results of a one of the soil studies in the input data set (the soil study that is selected in the “degradation kinetics frame”) is presented in the output (diagrams, report file, tables).

<u>View – Summary</u>
The fate of a pesticides and/or its main metabolites can be simulated in up to six soil studies. To visualise the results ESCAPE provides output in two different modes. In its mode “View – Summary” results of all soil studies in the input data set are presented in summaries (diagrams, report file, tables).

View - Report:

This menu item generates an output file including all results of the simulation, the current input data setting and the actual diagram on the screen. The file will be written in RTF-format and saved in the ESCAPE-output-folder. The name of the file can be customised using the menu item “Edit – Preferences”. The name selected for the data set is echoed at the bottom of the main form (current output file). At the same time the report is also displayed at the main form (see Figure 18). It is possible to do some limited processing (scrolling with cursor keys, copying into the clipboard with “ctrl C”). After a double click at the report the standard diagram sheet returns on top of the screen.

Dependent on whether ESCAPES provides information about an individual study or collects summary information the report file looks differentially. The menu items “View – Summary” or “View – Individual studies” can be used to switch between these two modes.

Instead of using the menu bar the user could also use the “report”-button on the right-bottom part of the main form.

Report can be printed using the command “File – Print” in the menu bar.

Help – About:

Some information about the current model version is faded in after selecting the menu item “Help – About” as shown in Figure 23.

Figure 23: ESCAPE: Saving input files

4.8. Manipulating the central diagram sheet

Dependent on the current input data set much information about soil concentrations might be available after an ESCAPE simulation. This information cannot be presented in a single figure. Therefore, the central part of ESCAPE (the diagram, see Figure 24) can be interactively changed to make available all important aspects of a certain simulation and customise the presentation of results. The various user options are presented in the following:

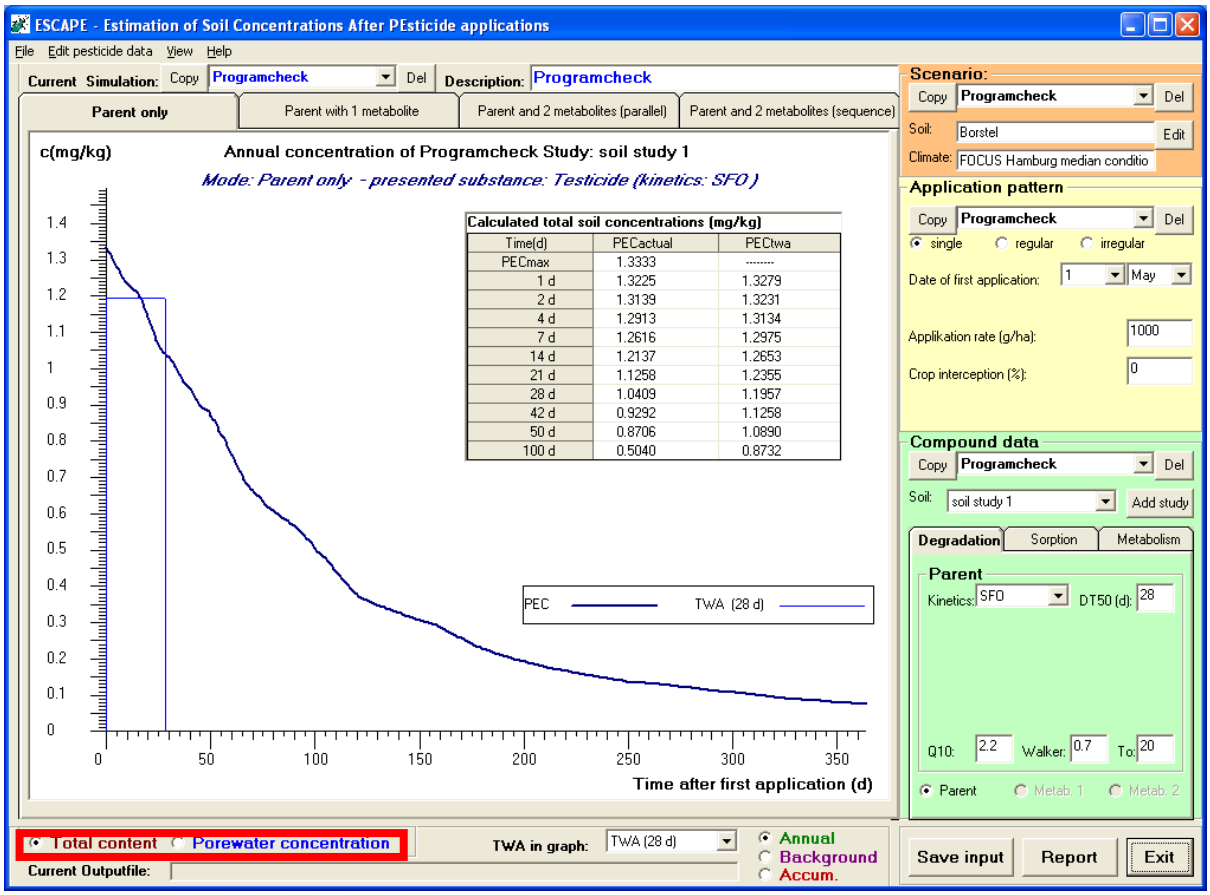


Figure 24: ESCAPE: The central diagram: selecting pore water or total concentrations

4.8.1. Selecting total content or pore water concentration

The radio buttons in the left bottom part of the form can be used to switch between total content in soil and pore water concentrations (see the rectangle in Figure 24). The graphs are re-constructed instantaneously because calculations are always performed for both endpoints independent on the actual settings.

4.8.2. Moving/Removing of the legend

A left mouse click at the legend turns its background colour to blue and the legend can be moved as long as the left mouse button is pressed. A double click (or a click at the legend when the ctrl-key is pressed) will remove it completely from the screen.

By clicking at the diagram together with the ctrl-key pressed will set the legend to its original position (and it becomes visible again).

4.8.3. Moving/Removing of the concentration table

A left mouse click at the title of the concentration table turns its background colour to blue and the table can be moved as long as the left mouse button is pressed. A double click (or a

click at the title when the ctrl-key is pressed) will remove the table completely from the screen.
By clicking at the diagram together with the ctrl-key pressed will set the table to its original position (and it becomes visible again).

4.8.4. Manual changing of the time axis

A right mouse click at the diagram opens a small form to manually set the minimum and maximum times displayed in the diagram. This option only influence the current figure and does not change any setting of additional diagrams prepared in the background.

4.8.5. Changing the duration of the TWA-frame

During the simulation the PEC_{TWA} is internally calculated for many time frames as explained earlier in this document in chapter 3.4.3 on page 29. The worst case time frame found is always displayed in the diagram. However, time weighted average concentrations are available for a list of time durations and dependent on the actual duration different starting and ending days for the time frame are PEC_{TWA} are achieved.
The duration presented in the diagram can be modified using the list box “TWA in diagram” at the bottom of the form.

4.8.6. Selecting the PEC-type in the graph

ESCAPE is always calculating the soil concentrations over a period of ten years repeating the annual application pattern. Depending on the selection of the radio buttons in the right bottom part of the window (see Figure 25) three different types of diagram can be displayed either the situation in the first year (normal soil depth, “Annual”), or the situation after many years of applications (concentrations based on the tillage depth, “Background”), or the situation after many years of applications (normal soil depth, but adding the background concentration, “Accumulation”).

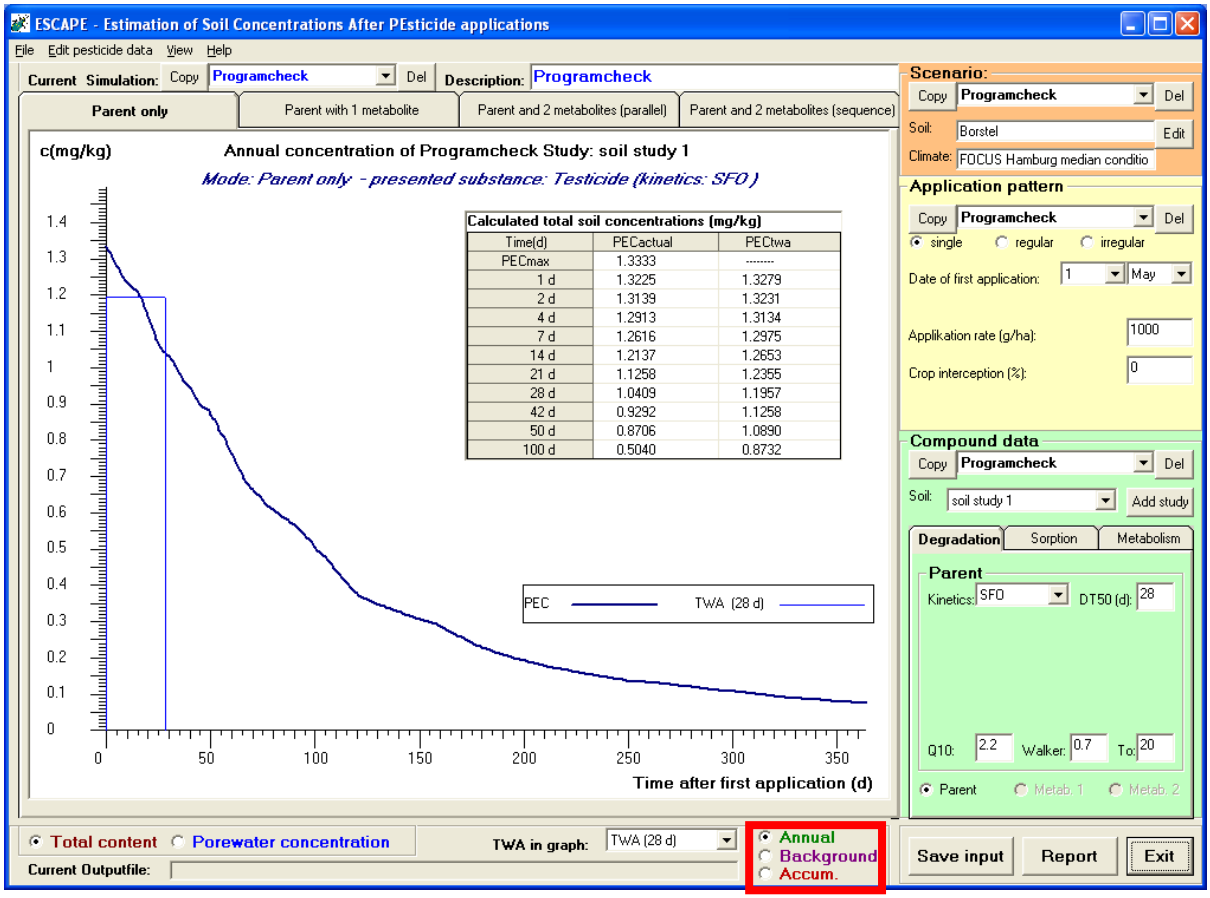


Figure 25: ESCAPE: The central diagram: selecting the PEC-Type in the graph

4.8.7. Scrolling through the list of diagrams prepared in the background

If metabolites have been considered for the simulation more than diagram has been prepared in the background. By clicking with the left mouse button at the diagram figures in the background become available.

If ESCAPE is presenting results from individual studies for each compound a diagram has been prepared. Examples of these diagrams are presented in the next three figures. Figure 26 shows the result for the parent compound which is usually presented in blue colours.

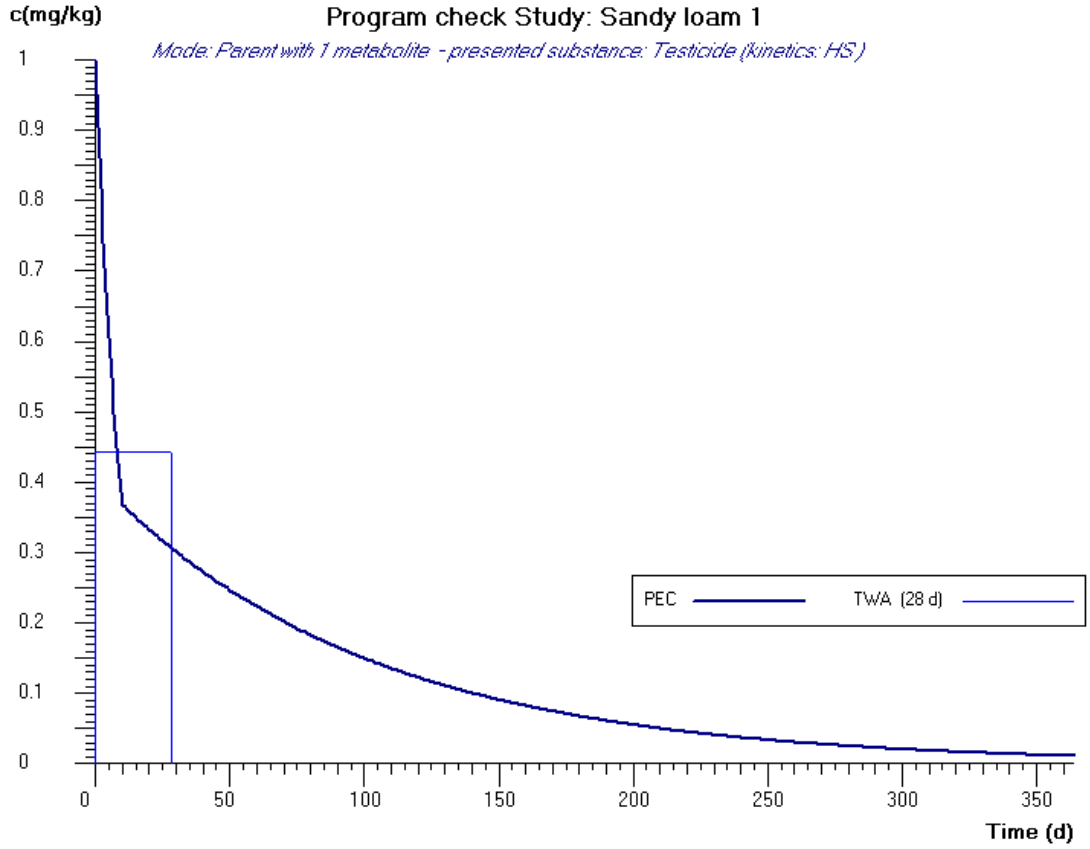


Figure 26: ESCAPE: Graphical results for the parent compound (View - Individual study)

The respective results for the first metabolite is shown in green colours (see Figure 27). Results of the second metabolite will always be shown in red colours.

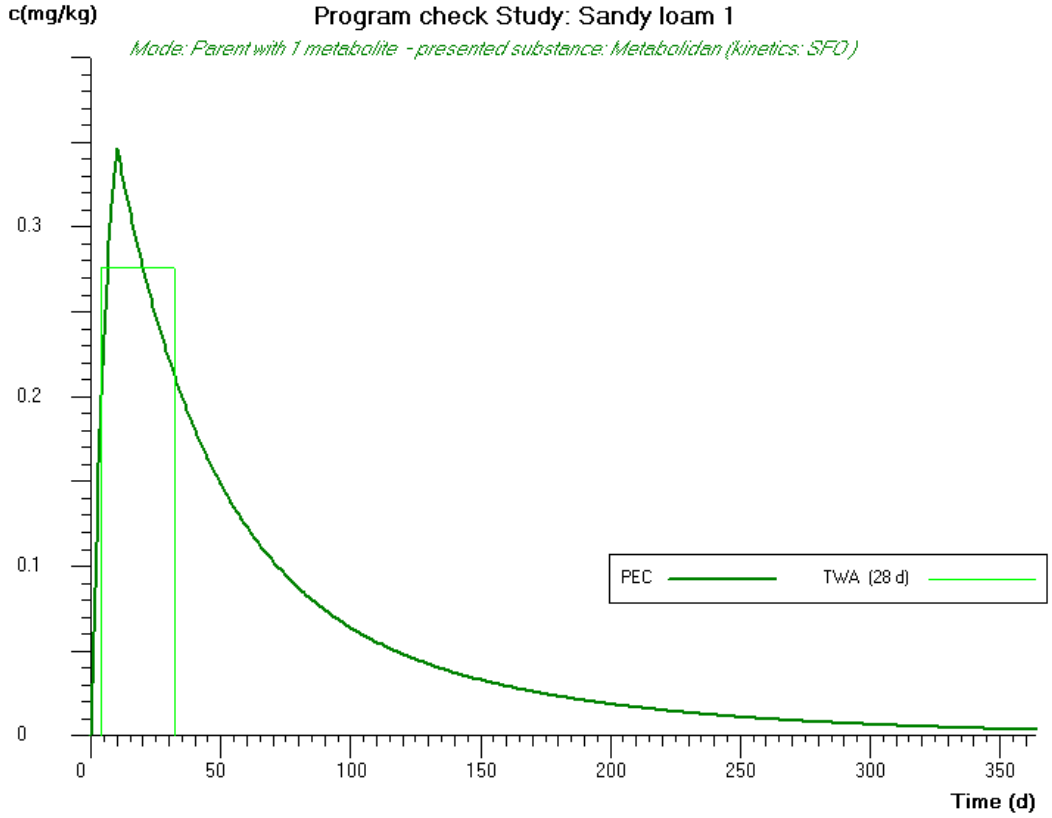


Figure 27: ESCAPE: Graphical results for the first metabolite (View - Individual study)

The final diagram is always a presentation of all compounds involved within one figure as shown in Figure 28.

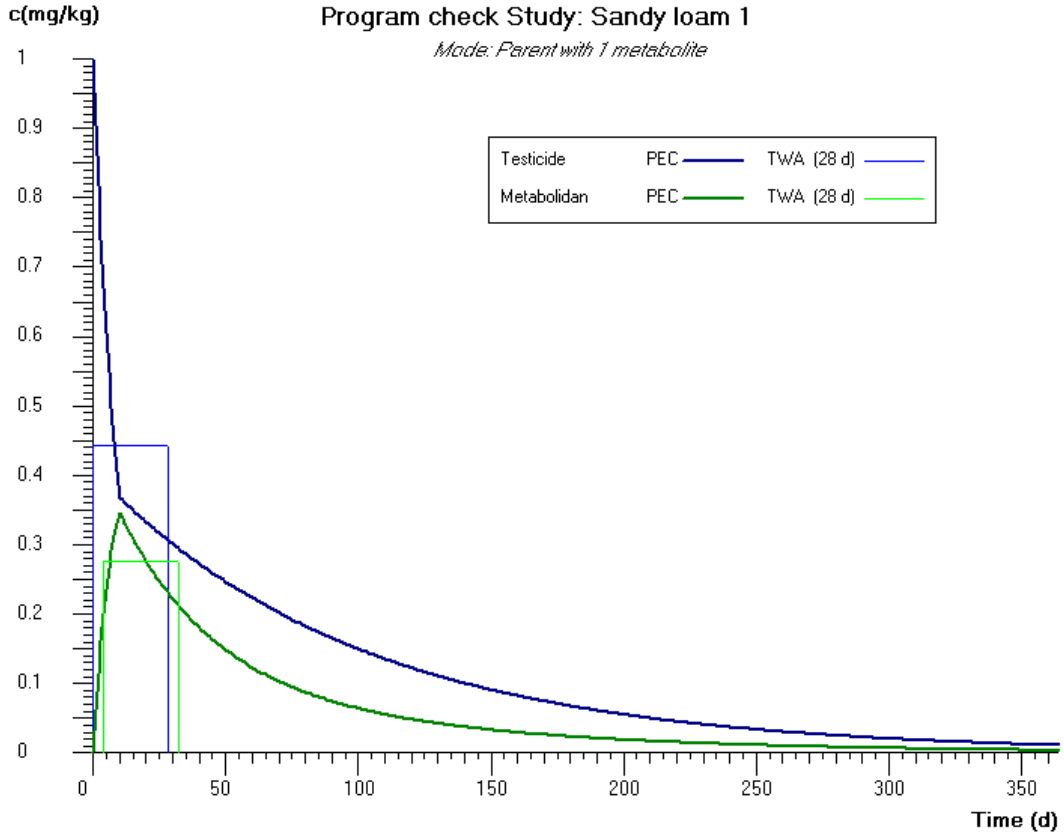


Figure 28: ESCAPE: Graphical results for all compounds (View - Individual study)

The diagram presented in the previous figures were all related to the ESCAPE's "View – Individual study" – mode. However similar diagrams will also be prepared in the "View – Summary" mode of ESCAPE. The respective are shown in the following two figures.
In this mode the blue colour always represent the results of the first, and the green colour the results of the second soil study.
Due to too much complexity there is no diagram available that shows the results of different soil studies **and** different compounds.

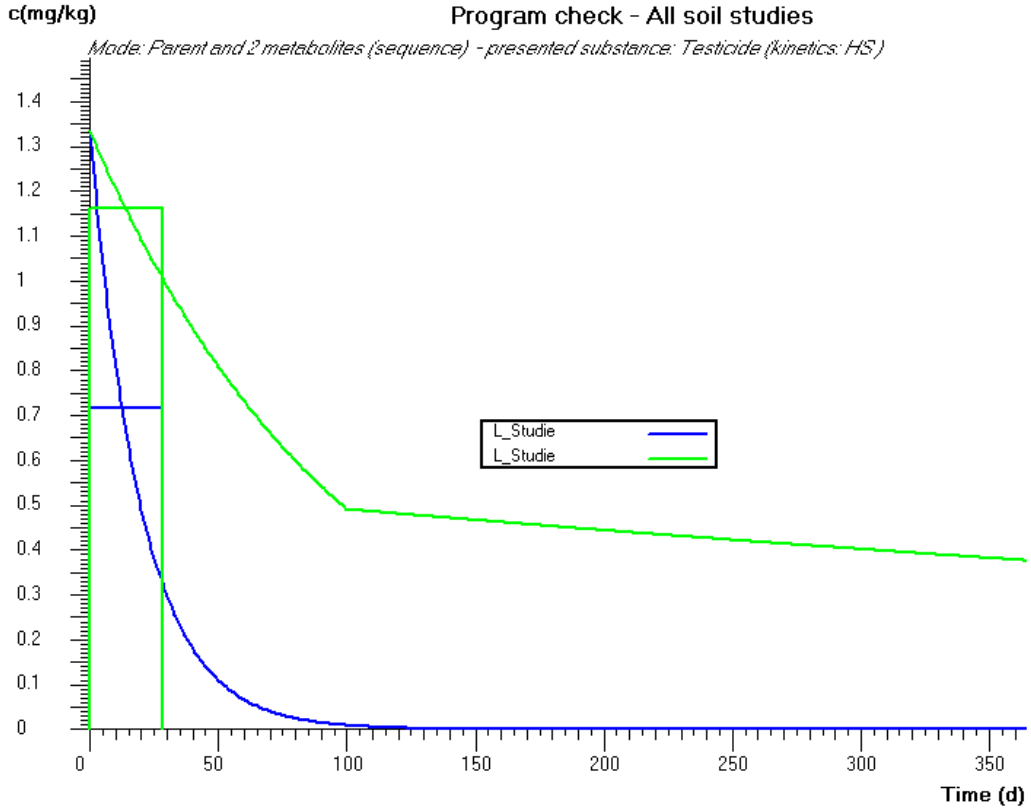


Figure 29: ESCAPE: Graphical results for the parent compound (View - Summary)

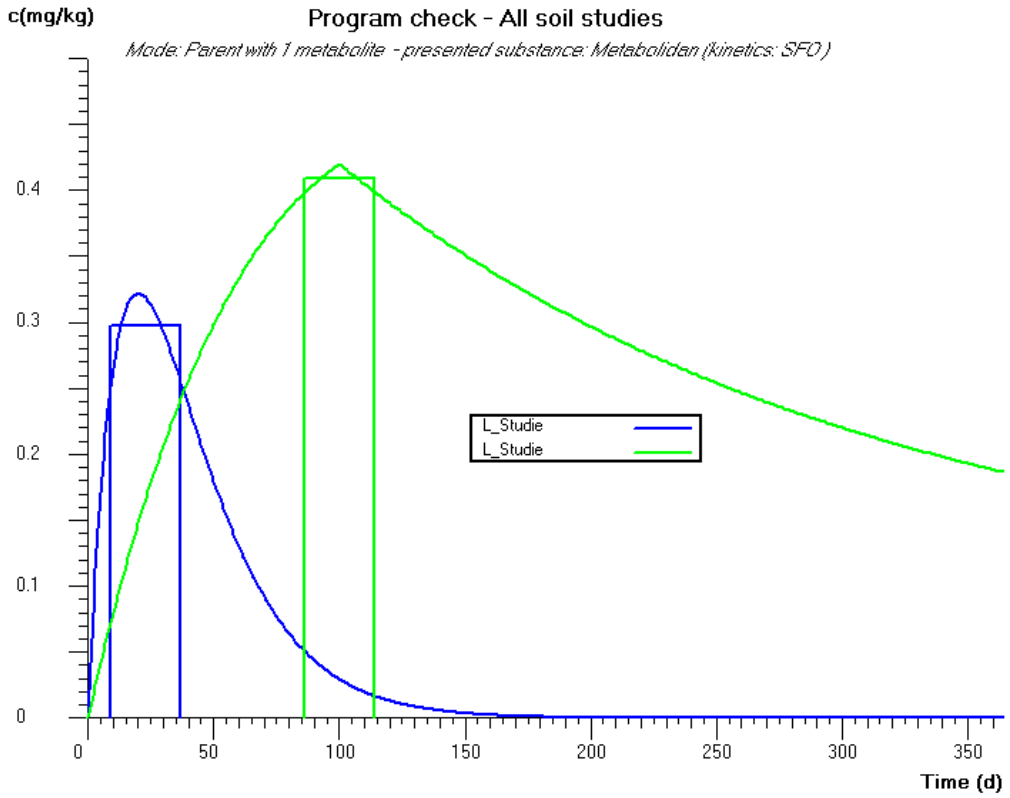


Figure 30: ESCAPE: Graphical results for the first metabolite compound (View - Summary)

5. References

FOCUS (1996). Soil Persistence Models and EU Registration, European Commission Document No. 7617/VI/96. URL: http://europa.eu.int/comm/food/plant/protection/evaluation/focus_en.htm.

FOCUS (2000) “FOCUS groundwater scenarios in the EU review of active substances” Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference Sanco/321/2000 rev.2, 202pp

FOCUS (2006) “Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration” Report of the FOCUS Work Group on Degradation Kinetics, EC Document Reference Sanco/10058/2005 version 2.0, 434 pp

Klein, M. (2008): Calculation of PECsoil including Plateau Concentrations for Pesticides Dependent on FOCUS Degradation Kinetics, FKZ: 360 03 037, Umweltbundesamt, Dessau-Roßlau.

6. Results of test simulations

6.1. Single application, parent compound only, several soil studies

The input parameters for the simulations are summarised in Table 3. TWA times according to EU-guidelines were used for the calculations.

Table 3: Series of special times used by ESCAPE to calculate PEC_{act} and PEC_{TWA}

Parameter	Soil study 1	Soil study 2	Soil study 3	Soil study 4
soil density (kg/L)	1.5			
soil depth (cm)	5			
application rate (g/ha)	1000			
first application date	1 May			
crop interception (%)	0			
Degradation type	SFO	FOMC*	HS*	SFO
SFO DT50 (d)**	28			14
alpha**		0.2		
beta**		0.2		
HS DT50 1 (1/d)**			7	
HS DT50 2 (d)**			70	
HS break point (d)**			10	

(* separate consideration of residues within the year of application only, ** related to standard conditions)

On the following four pages copies of the ESCAPE-report for all four studies are presented summarising the input data and all important results under standard laboratory conditions without considering soil moisture and temperature correction.

E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

12 Feb 2009)

Date of this simulation: 16/02/2009, 10:57:27
Calculation problem: Report example 1

PROGRAM SETTINGS

Calculation mode: Residues from different applications are considered separately over one year
Application mode: Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha): 1000
Crop interception (%): 0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: **soil study 1**

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 1:	Single First order (SFO)
DT50 (d):	28
Rate constant (1/d):	0.0248
Q10-factor:	2.2
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1

Calculations over one year
Maximum annual total soil concentration for Report example 1 over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.3007	1.3170	0	1
2	1.2689	1.3009	0	2
4	1.2076	1.2695	0	4
7	1.1212	1.2243	0	7
14	0.9428	1.1269	0	14
21	0.7928	1.0398	0	21
28	0.6667	0.9618	0	28
42	0.4714	0.8290	0	42
50	0.3867	0.7648	0	50
100	0.1122	0.4933	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 over 5 cm(mg/kg)*: 0.0002**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

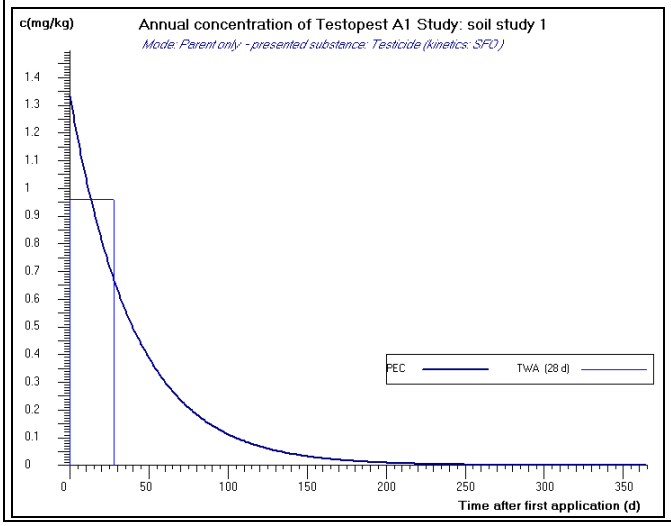
Maximum total soil concentration for Report example 1 over 5 cm considering accumulation* (mg/kg) 1.3335
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.3009	1.3172	0	1
2	1.2691	1.3011	0	2
4	1.2078	1.2697	0	4
7	1.1214	1.2244	0	7
14	0.9430	1.1270	0	14
21	0.7930	1.0400	0	21
28	0.6668	0.9620	0	28
42	0.4716	0.8292	0	42
50	0.3869	0.7650	0	50
100	0.1123	0.4935	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (12 Feb 2009)
Date of this simulation:	16/02/2009, 11:04:11
Calculation problem:	Report example 1

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study:	**soil study 2**
Metabolism scheme:	Parent compound without metabolites
Kinetics for Report example 1:	First Order Multi Compartment (FOMC)
Alpha:	0.2
Beta:	2
Q10-factor:	1
Walker-exponent:	0.0
Ref. temperature (°C):	0.0

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1

Calculations over one year

Maximum annual total soil concentration for Report example 1 over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2295	1.2814	0	1
2	1.1607	1.2383	0	2
4	1.0703	1.1755	0	4
7	0.9870	1.1113	0	7
14	0.8797	1.0193	0	14
21	0.8181	0.9618	0	21
28	0.7757	0.9203	0	28
42	0.7185	0.8618	0	42
50	0.6949	0.8370	0	50
100	0.6073	0.7411	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 over 5 cm(mg/kg)*: 0.7261**

(* estimated to occur after 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

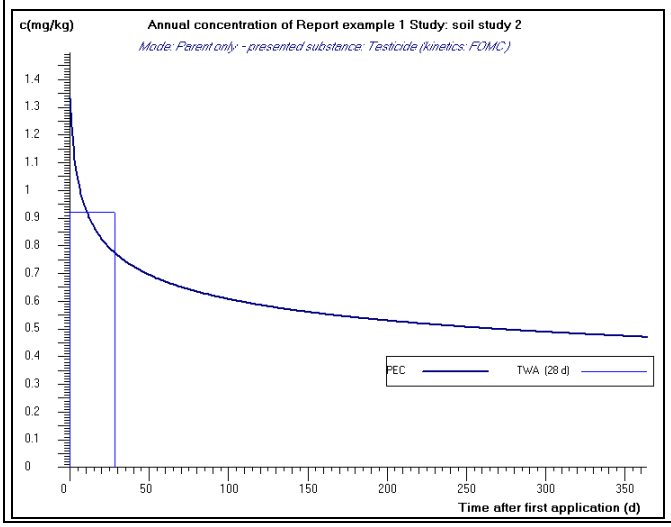
Maximum total soil concentration for Report example 1 over 5 cm considering accumulation* (mg/kg) 2.0594
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.9556	2.0075	0	1
2	1.8868	1.9644	0	2
4	1.7964	1.9016	0	4
7	1.7131	1.8374	0	7
14	1.6058	1.7454	0	14
21	1.5442	1.6879	0	21
28	1.5018	1.6464	0	28
42	1.4446	1.5879	0	42
50	1.4210	1.5631	0	50
100	1.3334	1.4672	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (12 Feb 2009)
Date of this simulation:	16/02/2009, 11:06:49
Calculation problem:	Report example 1

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study:	soil study 3
Metabolism scheme:	Parent compound without metabolites
Kinetics for Report example 1:	Hockey Stick (HS)
DT50 1(d):	7
DT50 2(d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter Tb:	10
Q10-factor:	1
Walker-exponent:	0.0
Ref. temperature (°C):	0.0

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1

Calculations over one year

Maximum annual total soil concentration for Report example 1 over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2076	1.2705	0	1
2	1.0938	1.2106	0	2
4	0.8973	1.1018	0	4
7	0.6667	0.9626	0	7
14	0.4761	0.7437	0	14
21	0.4442	0.6492	0	21
28	0.4145	0.5942	0	28
42	0.3608	0.5251	0	42
50	0.3333	0.4966	0	50
100	0.2032	0.3798	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 over 5 cm(mg/kg)*: 0.0149**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

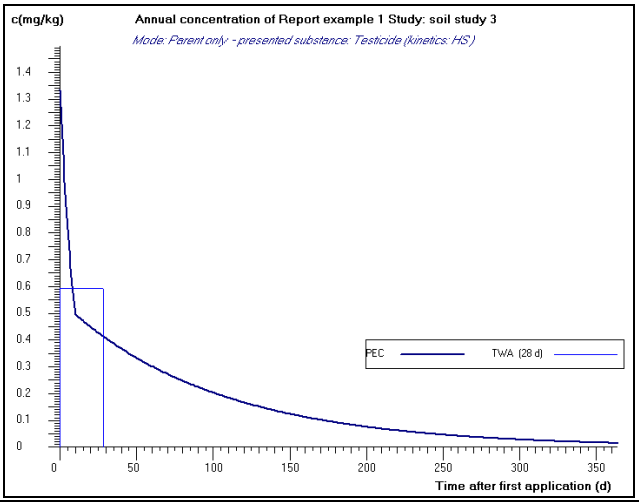
Maximum total soil concentration for Report example 1 over 5 cm considering accumulation* (mg/kg) 1.3482
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2225	1.2854	0	1
2	1.1087	1.2255	0	2
4	0.9122	1.1167	0	4
7	0.6816	0.9775	0	7
14	0.4910	0.7586	0	14
21	0.4591	0.6640	0	21
28	0.4294	0.6091	0	28
42	0.3757	0.5400	0	42
50	0.3482	0.5115	0	50
100	0.2181	0.3946	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (12 Feb 2009)
Date of this simulation:	16/02/2009, 11:07:50
Calculation problem:	Report example 1

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study:	soil study 4
Metabolism scheme:	Parent compound without metabolites
Kinetics for Report example 1:	Single First order (SFO)
DT50 (d):	14
Rate constant (1/d):	0.0495
Q10-factor:	1
Walker-exponent:	0.0
Ref. temperature (°C):	0.0

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1

Calculations over one year

Maximum annual total soil concentration for Report example 1 over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2689	1.3011	0	1
2	1.2076	1.2697	0	2
4	1.0938	1.2099	0	4
7	0.9428	1.1270	0	7
14	0.6667	0.9620	0	14
21	0.4714	0.8292	0	21
28	0.3333	0.7215	0	28
42	0.1667	0.5612	0	42
50	0.1122	0.4934	0	50
100	0.0094	0.2675	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 over 5 cm(mg/kg)*: <0.0001**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

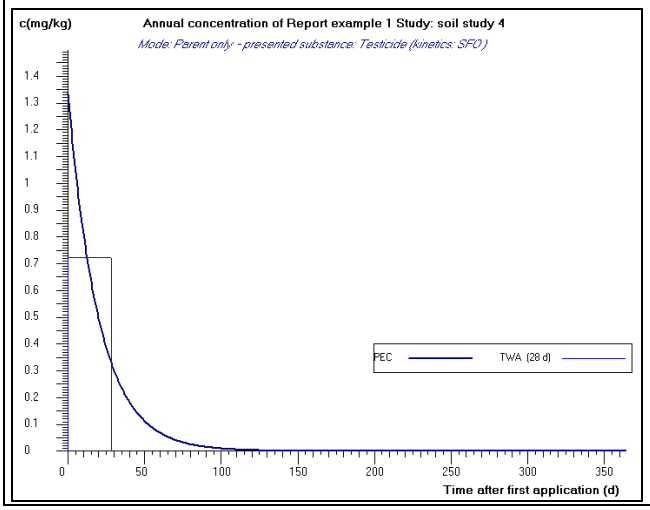
Maximum total soil concentration for Report example 1 over 5 cm considering accumulation* (mg/kg) 1.3333
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2689	1.3011	0	1
2	1.2076	1.2697	0	2
4	1.0938	1.2099	0	4
7	0.9428	1.1270	0	7
14	0.6667	0.9620	0	14
21	0.4714	0.8292	0	21
28	0.3333	0.7215	0	28
42	0.1667	0.5612	0	42
50	0.1122	0.4934	0	50
100	0.0094	0.2675	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



Here, the respective report is shown when ESCAPE is in its summary mode. Results of all four studies are summarised in a single file and the diagram includes results of all studies.

E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (12 Feb 2009)
Date of this simulation:	16/02/2009, 11:09:23
Calculation problem:	Report example 1

SUMMARY REPORT CONSIDERING ALL SOIL STUDIES

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites
Pesticide:	Report example 1

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 1:

Soil study: soil study 1

Single First order (SFO)

DT50 (d):	28
Rate constant (1/d):	0.0248
Q10-factor:	2.2
Walker-exponent:	0.7
TReference (°C):	20

Soil study: soil study 2

First Order Multi Compartment (FOMC)

alpha(i_studie):	0.2
Beta:	2
Q10-factor:	1
Walker-exponent:	0.0
TReference (°C):	0.0

Soil study: soil study 3

Hockey Stick (HS)

DT50 (d):	7
DT50 (d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter Tb (d):	10
Q10-factor:	1
Walker-exponent:	0.0
TReference (°C):	0.0

Soil study: soil study 4

Single First order (SFO)

DT50 (d):	14
Rate constant (1/d):	0.0495
Q10-factor:	1
Walker-exponent:	0.0
TReference (°C):	0.0

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1

Calculations over one year

Maximum annual total soil concentration for Report example 1 over 1.5 cm

soil study 1(mg/kg):	1.3333 occurring on day 0
soil study 2(mg/kg):	1.3333 occurring on day 0
soil study 3(mg/kg):	1.3333 occurring on day 0
soil study 4(mg/kg):	1.3333 occurring on day 0

Calculated PECact* in soil over 1.5 cm for Report example 1(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.3007	1.2295	1.2076	1.2689
2.0000	1.2689	1.1607	1.0938	1.2076
4.0000	1.2076	1.0703	0.8973	1.0938
7.0000	1.1212	0.9870	0.6667	0.9428
14.0000	0.9428	0.8797	0.4761	0.6667
21.0000	0.7928	0.8181	0.4442	0.4714
28.0000	0.6667	0.7757	0.4145	0.3333
42.0000	0.4714	0.7185	0.3608	0.1667
50.0000	0.3867	0.6949	0.3333	0.1122
100.0000	0.1122	0.6073	0.2032	0.0094

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Report example 1(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.3170	1.2814	1.2705	1.3011
2.0000	1.3009	1.2383	1.2106	1.2697
4.0000	1.2695	1.1755	1.1018	1.2099
7.0000	1.2243	1.1113	0.9626	1.1270
14.0000	1.1269	1.0193	0.7437	0.9620
21.0000	1.0398	0.9618	0.6492	0.8292
28.0000	0.9618	0.9203	0.5942	0.7215
42.0000	0.8290	0.8618	0.5251	0.5612
50.0000	0.7648	0.8370	0.4966	0.4934
100.0000	0.4933	0.7411	0.3798	0.2675

Calculation of background concentrations after many years

Final background concentration in total soil for Report example 1 over 5 cm

soil study 1(mg/kg):	0.0002 (estimated to occur within 10 years)
soil study 2(mg/kg):	0.0356 (estimated to occur after 10 years)
soil study 3(mg/kg):	0.0356 (estimated to occur within 10 years)
soil study 4(mg/kg):	<0.0001 (estimated to occur within 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in total soil for Report example 1 over 5 cm considering accumulation*

soil study 1(mg/kg):	1.3335 occurring on day 0
soil study 2(mg/kg):	1.3689 occurring on day 0
soil study 3(mg/kg):	1.3689 occurring on day 0
soil study 4(mg/kg):	1.3333 occurring on day 0

(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Report example 1(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.1123	1.2651	1.2432	1.2689
2.0000	1.3009	1.1963	1.1294	1.2076
4.0000	1.2691	1.1059	0.9328	1.0938
7.0000	1.2078	1.0225	0.7022	0.9428
14.0000	1.1214	0.9153	0.5117	0.6667
21.0000	0.9430	0.8537	0.4798	0.4714
28.0000	0.7930	0.8113	0.4500	0.3333
42.0000	0.6668	0.7541	0.3964	0.1667
50.0000	0.4716	0.7305	0.3689	0.1122
100.0000	0.3869	0.6429	0.2387	0.0094

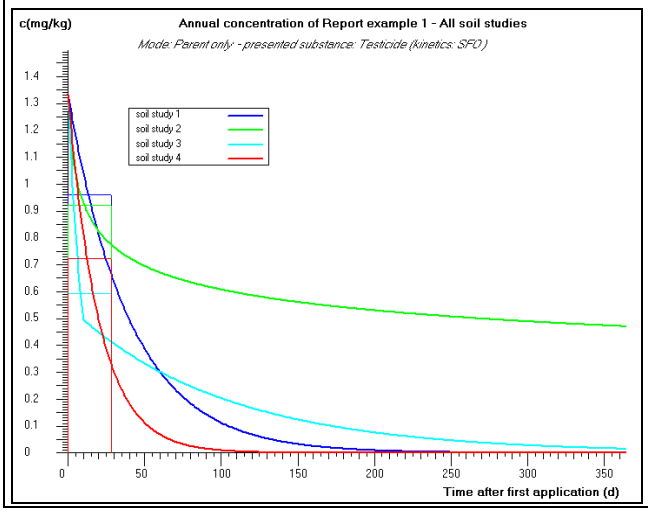
(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 5 cm for Report example 1(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.3172	1.3170	1.3061	1.3011
2.0000	1.3011	1.2738	1.2462	1.2697
4.0000	1.2697	1.2111	1.1374	1.2099
7.0000	1.2244	1.1469	0.9982	1.1270
14.0000	1.1270	1.0549	0.7793	0.9620
21.0000	1.0400	0.9973	0.6847	0.8292
28.0000	0.9620	0.9559	0.6297	0.7215
42.0000	0.8292	0.8974	0.5607	0.5612
50.0000	0.7650	0.8725	0.5322	0.4934
100.0000	0.4935	0.7767	0.4153	0.2675

(* a tillage depth of 5 cm was considered for calculating the background concentration)

GRAPHIC REPRESENTATION OF THE CALCULATION



On the following four pages copies of the ESCAPE-report for the same studies are presented summarising the input data and all important results based on Hamburg climatic conditions and considering soil moisture and temperature correction.

E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (16 Feb 2009)
Date of this simulation:	16/02/2009, 13:49:11
Calculation problem:	Report example 1 Hamburg

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 1

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 1 Hamburg:	Single First order (SFO)
DT50 (d):	28
Rate constant (1/d):	0.0248
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1 Hamburg

Calculations over one year

Maximum annual total soil concentration for Report example 1 Hamburg over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.3246	1.3290	0	1
2	1.3179	1.3251	0	2
4	1.2990	1.3173	0	4
7	1.2751	1.3043	0	7
14	1.2352	1.2779	0	14
21	1.1528	1.2517	0	21
28	1.0723	1.2154	0	28
42	0.9590	1.1490	0	42
50	0.9046	1.1136	0	50
100	0.5325	0.9032	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 Hamburg over 5 cm(mg/kg)*: 0.1183**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

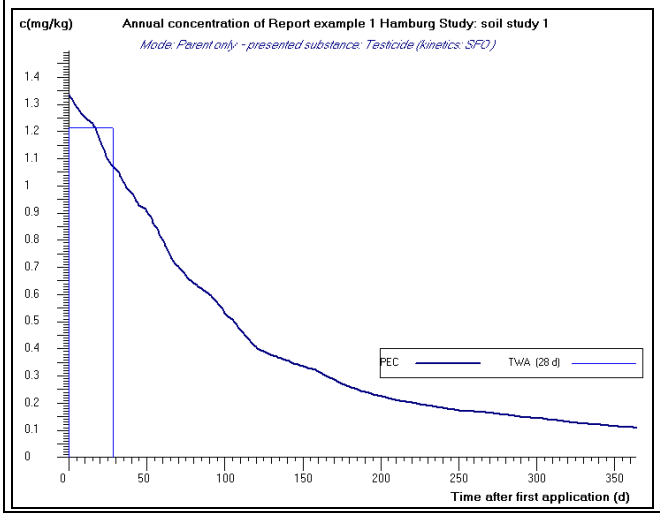
Maximum total soil concentration for Report example 1 Hamburg over 5 cm considering accumulation* (mg/kg)
1.4516
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.4429	1.4473	0	1
2	1.4362	1.4434	0	2
4	1.4173	1.4356	0	4
7	1.3934	1.4226	0	7
14	1.3534	1.3961	0	14
21	1.2710	1.3700	0	21
28	1.1905	1.3336	0	28
42	1.0772	1.2673	0	42
50	1.0229	1.2319	0	50
100	0.6508	1.0214	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (16 Feb 2009)
Date of this simulation:	16/02/2009, 14:00:09
Calculation problem:	Report example 1 Hamburg

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 2

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 1 Hamburg:	First Order Multi Compartment (FOMC)
Alpha:	0.2
Beta:	2
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1 Hamburg

Calculations over one year

Maximum annual total soil concentration for Report example 1 Hamburg over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.3007	1.3170	0	1
2	1.2782	1.3032	0	2
4	1.2251	1.2785	0	4
7	1.1725	1.2438	0	7
14	1.1062	1.1877	0	14
21	1.0136	1.1461	0	21
28	0.9516	1.1036	0	28
42	0.8874	1.0419	0	42
50	0.8624	1.0148	0	50
100	0.7358	0.9004	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 Hamburg over 5 cm(mg/kg)*: 1.1094**

(* estimated to occur after 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

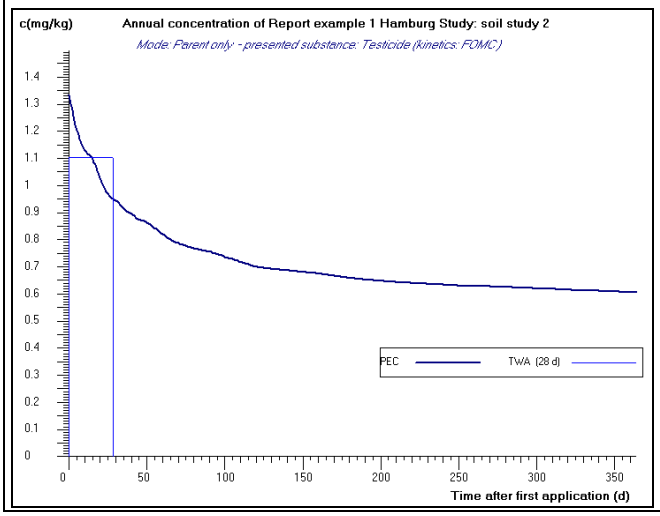
Maximum total soil concentration for Report example 1 Hamburg over 5 cm considering accumulation* (mg/kg)
2.4427
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.4101	2.4264	0	1
2	2.3876	2.4126	0	2
4	2.3345	2.3879	0	4
7	2.2819	2.3532	0	7
14	2.2156	2.2971	0	14
21	2.1230	2.2555	0	21
28	2.0610	2.2130	0	28
42	1.9968	2.1513	0	42
50	1.9718	2.1243	0	50
100	1.8452	2.0098	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (16 Feb 2009)
Date of this simulation:	16/02/2009, 13:58:47
Calculation problem:	Report example 1 Hamburg

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4

Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 3

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 1 Hamburg:	Hockey Stick (HS)
DT50 1(d):	7
DT50 2(d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter Tb:	10
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1 Hamburg

Calculations over one year

Maximum annual total soil concentration for Report example 1 Hamburg over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2989	1.3161	0	1
2	1.2727	1.3010	0	2
4	1.2012	1.2708	0	4
7	1.1152	1.2222	0	7
14	0.9820	1.1288	0	14
21	0.7449	1.0443	0	21
28	0.5577	0.9417	0	28
42	0.4896	0.7973	0	42
50	0.4783	0.7470	0	50
100	0.3870	0.5879	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 Hamburg over 5 cm(mg/kg)*: 0.2414**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

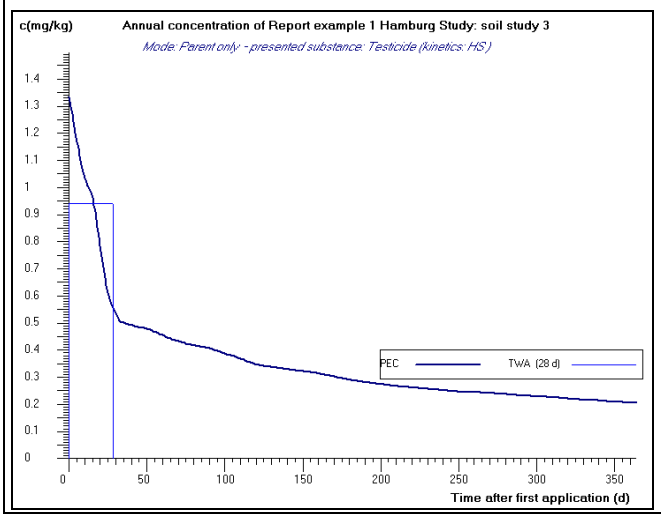
Maximum total soil concentration for Report example 1 Hamburg over 5 cm considering accumulation* (mg/kg)
1.5747
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.5403	1.5575	0	1
2	1.5141	1.5424	0	2
4	1.4426	1.5122	0	4
7	1.3566	1.4636	0	7
14	1.2234	1.3702	0	14
21	0.9863	1.2857	0	21
28	0.7991	1.1831	0	28
42	0.7310	1.0387	0	42
50	0.7197	0.9884	0	50
100	0.6284	0.8293	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version: 2.0 (16 Feb 2009)
Date of this simulation: 16/02/2009, 14:01:20
Calculation problem: Report example 1 Hamburg

PROGRAM SETTINGS

Calculation mode: Residues from different applications are considered separately over one year
Application mode: Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4

Climatic conditions: FOCUS Hamburg median conditions

Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application rate (g/ha): 1000
Crop interception (%): 0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 4

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 1 Hamburg: Single First order (SFO)

DT50 (d):	14
Rate constant (1/d):	0.0495
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 1 Hamburg

Calculations over one year

Maximum annual total soil concentration for Report example 1 Hamburg over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.3160	1.3247	0	1
2	1.3027	1.3170	0	2
4	1.2655	1.3016	0	4
7	1.2194	1.2761	0	7
14	1.1443	1.2254	0	14
21	0.9966	1.1767	0	21
28	0.8623	1.1121	0	28
42	0.6897	1.0000	0	42
50	0.6137	0.9433	0	50
100	0.2127	0.6556	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 1 Hamburg over 5 cm(mg/kg)*: 0.0089**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

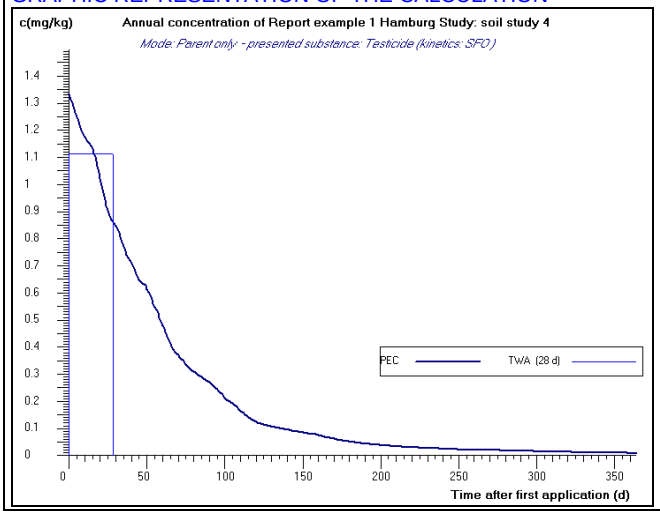
Maximum total soil concentration for Report example 1 Hamburg over 5 cm considering accumulation* (mg/kg)
1.3422
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 1 Hamburg(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.3249	1.3336	0	1
2	1.3116	1.3259	0	2
4	1.2745	1.3105	0	4
7	1.2283	1.2850	0	7
14	1.1532	1.2343	0	14
21	1.0055	1.1857	0	21
28	0.8712	1.1211	0	28
42	0.6986	1.0089	0	42
50	0.6226	0.9522	0	50
100	0.2216	0.6645	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

GRAPHIC REPRESENTATION OF THE CALCULATION



6.2. Regular applications, parent compound only, several soil studies

The input parameters for the simulations are summarised in Table 4. TWA times according to EU-guidelines were used for the calculations.

Table 4: Series of special times used by ESCAPE to calculate PEC_{act} and PEC_{TWA}

Parameter	Soil study 1	Soil study 2	Soil study 3	Soil study 4
soil density (kg/L)	1.5			
soil depth (cm)	5			
first application date	1 May			
application rate (g/ha)	4 * 1000			
crop interception (%)	50			
application interval (d)	14 d			
Degradation type	SFO	FOMC*	HS*	SFO
SFO DT50 (d)**	365			140
alpha**		0.1		
beta		2		
HS DT50 1 (d)**			70	
HS DT50 2 (d)**			700	
HS break point (d)**			20	

(* separate consideration of residues within the year of application only, ** related to standard conditions)

On the following four pages copies of the ESCAPE-report for all four studies are presented summarising the input data and all important results under standard laboratory conditions without considering soil moisture and temperature correction.

E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 11:44:45
Calculation problem:	Report example 2

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 2
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications :	4
1st Application date:	1 May
Application rate (g/ha):	1000
Time between two applications (d):	14
Crop interception (%):	50

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 1

Metabolism scheme:	Parent compound without metabolites
Kinetics for Report example 2:	Single First order (SFO)
DT50 (d):	365
Rate constant (1/d):	0.0019
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 2

Calculations over one year

Maximum annual total soil concentration for Report example 2 over 5 cm(mg/kg): 2.5635 occurring on day 42

Calculated time dependent total soil concentrations over 5 cm for Report example 2 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.5587	2.5611	42	43
2	2.5538	2.5587	42	44
4	2.5441	2.5538	42	46
7	2.5297	2.5466	42	49
14	2.4963	2.5298	42	56
21	2.4633	2.5131	42	63
28	2.4308	2.4966	42	70
42	2.3670	2.4640	42	84
50	2.3313	2.4456	42	92
100	2.1202	2.3359	41	141

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 2 over 5 cm(mg/kg)*: 2.5592**

(* estimated to occur after 11 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

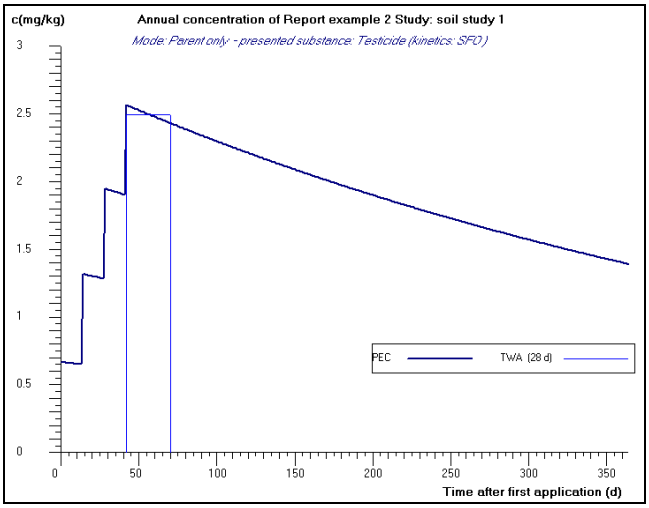
Maximum total soil concentration for Report example 2 over 5 cm considering accumulation* (mg/kg) 5.1227
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 2(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	5.1178	5.1203	42	43
2	5.1130	5.1178	42	44
4	5.1033	5.1130	42	46
7	5.0889	5.1057	42	49
14	5.0555	5.0889	42	56
21	5.0225	5.0723	42	63
28	4.9900	5.0557	42	70
42	4.9262	5.0231	42	84
50	4.8905	5.0048	42	92
100	4.6793	4.8951	41	141

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 11:46:10
Calculation problem:	Report example 2

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 2
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications :	4	
1st Application date:	1 May	
Application rate (g/ha):	1000	
Time between two applications (d):		14
Crop interception (%):	50	

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study:	**soil study 2**
Metabolism scheme:	Parent compound without metabolites
Kinetics for Report example 2:	First Order Multi Compartment (FOMC)
Alpha:	0.1
Beta:	2
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 2

Calculations over one year

Maximum annual total soil concentration for Report example 2 over 5 cm(mg/kg): 2.2061 occurring on day 42

Calculated time dependent total soil concentrations over 5 cm for Report example 2 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.1736	2.1898	42	43
2	2.1497	2.1757	42	44
4	2.1142	2.1534	42	46
7	2.0760	2.1280	42	49
14	2.0155	2.0858	42	56
21	1.9731	2.0550	42	63
28	1.9399	2.0302	42	70
42	1.8890	1.9912	42	84
50	1.8659	1.9731	41	91
100	1.7680	1.8935	41	141

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 2 over 5 cm(mg/kg)*: 2.8582**

(* estimated to occur after 11 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

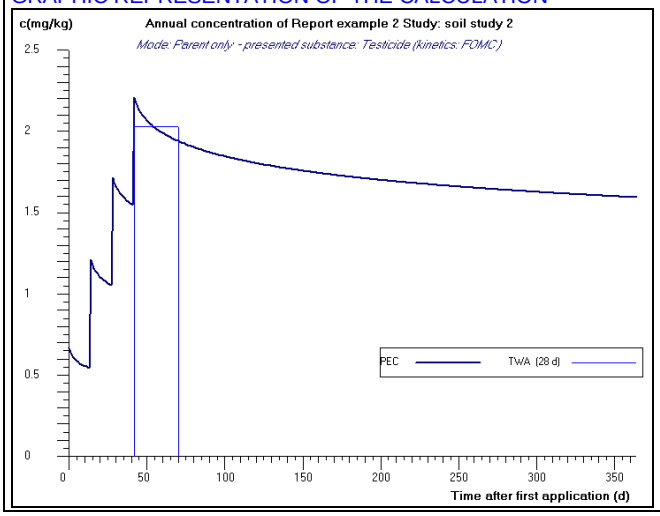
Maximum total soil concentration for Report example 2 over 5 cm considering accumulation* (mg/kg) 5.0643
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 2(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	5.0317	5.0480	42	43
2	5.0078	5.0339	42	44
4	4.9724	5.0116	42	46
7	4.9342	4.9862	42	49
14	4.8737	4.9440	42	56
21	4.8313	4.9132	42	63
28	4.7981	4.8884	42	70
42	4.7472	4.8494	42	84
50	4.7241	4.8313	41	91
100	4.6262	4.7517	41	141

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 11:47:06
Calculation problem:	Report example 2

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 2
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications :	4
1st Application date:	1 May
Application rate (g/ha):	1000
Time between two applications (d):	14
Crop interception (%):	50

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 3

Metabolism scheme:	Parent compound without metabolites
Kinetics for Report example 2:	Hockey Stick (HS)
DT50 1(d):	70
DT50 2(d):	700
Rate constant 1 (1/d):	0.0099
Rate constant 2 (1/d):	0.001
Parameter Tb:	20
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 2

Calculations over one year

Maximum annual total soil concentration for Report example 2 over 5 cm(mg/kg): 2.3247 occurring on day 42

Calculated time dependent total soil concentrations over 5 cm for Report example 2 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.3114	2.3180	42	43
2	2.2981	2.3114	42	44
4	2.2720	2.2982	42	46
7	2.2386	2.2791	42	49
14	2.1858	2.2455	42	56
21	2.1407	2.2173	42	63
28	2.1259	2.1963	42	70
42	2.0966	2.1680	42	84
50	2.0801	2.1552	42	92
100	1.9796	2.0925	41	141

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 2 over 5 cm(mg/kg)*: 3.0362**

(* estimated to occur after 11 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

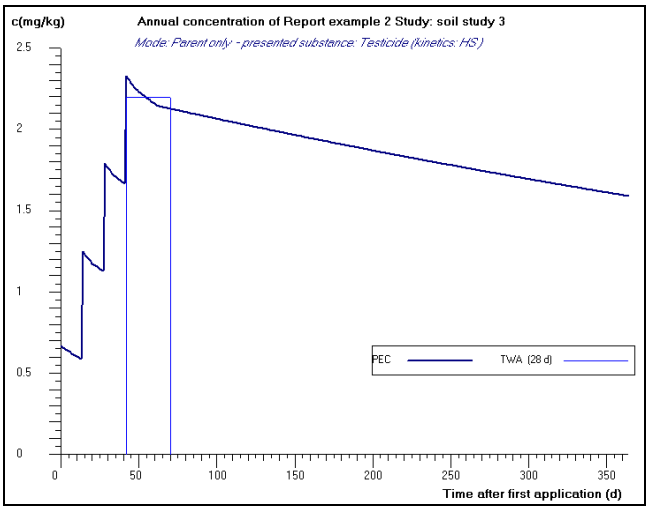
Maximum total soil concentration for Report example 2 over 5 cm considering accumulation* (mg/kg) 5.3609
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 2(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	5.3475	5.3542	42	43
2	5.3343	5.3476	42	44
4	5.3082	5.3344	42	46
7	5.2748	5.3153	42	49
14	5.2220	5.2817	42	56
21	5.1768	5.2535	42	63
28	5.1621	5.2325	42	70
42	5.1328	5.2041	42	84
50	5.1163	5.1914	42	92
100	5.0158	5.1286	41	141

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 11:48:31
Calculation problem:	Report example 2

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 2
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications :	4
1st Application date:	1 May
Application rate (g/ha):	1000
Time between two applications (d):	14
Crop interception (%):	50

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 4

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 2:	Single First order (SFO)
DT50 (d):	140
Rate constant (1/d):	0.005
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 2

Calculations over one year

Maximum annual total soil concentration for Report example 2 over 5 cm(mg/kg): 2.4106 occurring on day 42

Calculated time dependent total soil concentrations over 5 cm for Report example 2 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.3987	2.4046	42	43
2	2.3868	2.3987	42	44
4	2.3633	2.3868	42	46
7	2.3284	2.3693	42	49
14	2.2491	2.3289	42	56
21	2.1725	2.2895	42	63
28	2.0985	2.2509	42	70
42	1.9580	2.1793	41	83
50	1.8819	2.1393	41	91
100	1.4693	1.9444	28	128

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 2 over 5 cm(mg/kg)*: 0.4733**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

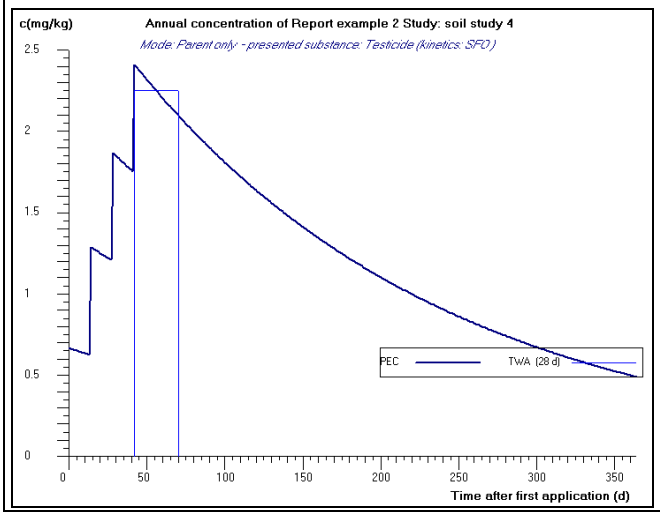
Maximum total soil concentration for Report example 2 over 5 cm considering accumulation* (mg/kg) 2.8839
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 2(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.8720	2.8779	42	43
2	2.8601	2.8720	42	44
4	2.8366	2.8602	42	46
7	2.8018	2.8426	42	49
14	2.7224	2.8022	42	56
21	2.6458	2.7628	42	63
28	2.5718	2.7242	42	70
42	2.4313	2.6526	41	83
50	2.3553	2.6126	41	91
100	1.9426	2.4177	28	128

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



Here, the respective report is shown when ESCAPE is in its summary mode. Results of all four studies are summarised in a single file and the diagram includes results of all studies.

E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 11:51:25
Calculation problem:	Report example 2

SUMMARY REPORT CONSIDERING ALL SOIL STUDIES

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Iteration of annual application pattern over 10 years

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 2
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications :	4
1st Application date:	1 May
Application rate (g/ha):	1000
Time between two applications (d):	14
Crop interception (%):	50

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites
Pesticide:	Report example 2

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 2:

Soil study: soil study 1

Single First order (SFO)

DT50 (d):	365
Rate constant (1/d):	0.0019
Q10-factor:	2.58
Walker-exponent:	0.7
TReference (°C):	20

Soil study:	soil study 2
First Order Multi Compartment (FOMC)	
alpha(i_studie):	0.1
Beta:	2
Q10-factor:	2.58
Walker-exponent:	0.7
TReference (°C):	20
Soil study:	soil study 3
Hockey Stick (HS)	
DT50 (d):	70
DT50 (d):	700
Rate constant 1 (1/d):	0.0099
Rate constant 2 (1/d):	0.001
Parameter Tb (d):	20
Q10-factor:	2.58
Walker-exponent:	0.7
TReference (°C):	20
Soil study:	soil study 4
Single First order (SFO)	
DT50 (d):	140
Rate constant (1/d):	0.005
Q10-factor:	2.58
Walker-exponent:	0.7
TReference (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 2

Calculations over one year

Maximum annual total soil concentration for Report example 2 over 1.5 cm

soil study 1(mg/kg):	2.5635 occurring on day 42
soil study 2(mg/kg):	2.2061 occurring on day 42
soil study 3(mg/kg):	2.3247 occurring on day 42
soil study 4(mg/kg):	2.4106 occurring on day 42

Calculated PECact* in soil over 1.5 cm for Report example 2(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	2.5587	2.1736	2.3114	2.3987
2.0000	2.5538	2.1497	2.2981	2.3868
4.0000	2.5441	2.1142	2.2720	2.3633
7.0000	2.5297	2.0760	2.2386	2.3284
14.0000	2.4963	2.0155	2.1858	2.2491
21.0000	2.4633	1.9731	2.1407	2.1725
28.0000	2.4308	1.9399	2.1259	2.0985
42.0000	2.3670	1.8890	2.0966	1.9580
50.0000	2.3313	1.8659	2.0801	1.8819
100.0000	2.1202	1.7680	1.9796	1.4693

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Report example 2(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	2.5611	2.1898	2.3180	2.4046
2.0000	2.5587	2.1757	2.3114	2.3987
4.0000	2.5538	2.1534	2.2982	2.3868
7.0000	2.5466	2.1280	2.2791	2.3693
14.0000	2.5298	2.0858	2.2455	2.3289
21.0000	2.5131	2.0550	2.2173	2.2895
28.0000	2.4966	2.0302	2.1963	2.2509
42.0000	2.4640	1.9912	2.1680	2.1793
50.0000	2.4456	1.9731	2.1552	2.1393
100.0000	2.3359	1.8935	2.0925	1.9444

Calculation of background concentrations after many years

Final background concentration in total soil for Report example 2 over 5 cm

soil study 1(mg/kg):	2.5592 (estimated to occur after 11 years)
soil study 2(mg/kg):	2.8582 (estimated to occur after 11 years)
soil study 3(mg/kg):	3.0362 (estimated to occur after 11 years)
soil study 4(mg/kg):	0.4733 (estimated to occur within 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in total soil for Report example 2 over 5 cm considering accumulation*

soil study 1(mg/kg):	5.1227 occurring on day 42
soil study 2(mg/kg):	5.0643 occurring on day 42
soil study 3(mg/kg):	5.3609 occurring on day 42
soil study 4(mg/kg):	2.8839 occurring on day 42

(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Report example 2(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	4.6793	5.0317	5.3475	2.8720
2.0000	5.1178	5.0078	5.3343	2.8601
4.0000	5.1130	4.9724	5.3082	2.8366
7.0000	5.1033	4.9342	5.2748	2.8018
14.0000	5.0889	4.8737	5.2220	2.7224
21.0000	5.0555	4.8313	5.1768	2.6458
28.0000	5.0225	4.7981	5.1621	2.5718
42.0000	4.9900	4.7472	5.1328	2.4313
50.0000	4.9262	4.7241	5.1163	2.3553
100.0000	4.8905	4.6262	5.0158	1.9426

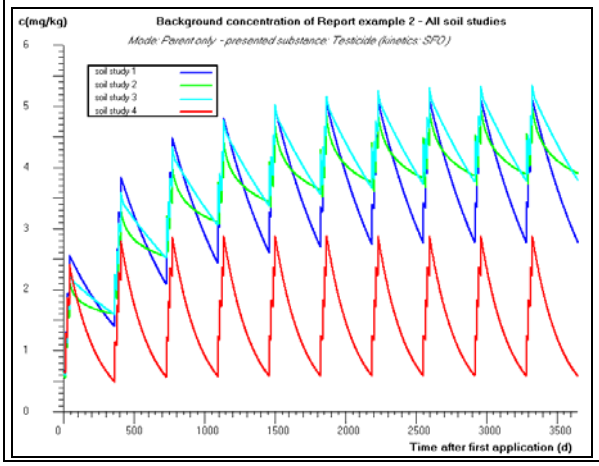
(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 5 cm for Report example 2(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	5.1203	5.0480	5.3542	2.8779
2.0000	5.1178	5.0339	5.3476	2.8720
4.0000	5.1130	5.0116	5.3344	2.8602
7.0000	5.1057	4.9862	5.3153	2.8426
14.0000	5.0889	4.9440	5.2817	2.8022
21.0000	5.0723	4.9132	5.2535	2.7628
28.0000	5.0557	4.8884	5.2325	2.7242
42.0000	5.0231	4.8494	5.2041	2.6526
50.0000	5.0048	4.8313	5.1914	2.6126
100.0000	4.8951	4.7517	5.1286	2.4177

(* a tillage depth of 5 cm was considered for calculating the background concentration)

GRAPHIC REPRESENTATION OF THE CALCULATION



6.3. Irregular applications, parent compound only, several soil studies

The input parameters for the simulations are summarised in Table 5. TWA times according to EU-guidelines were used for the calculations.

Table 5: Series of special times used by ESCAPE to calculate PEC_{act} and PEC_{TWA}

Parameter	Soil study 1	Soil study 2
soil density (kg/L)	1.5	
soil depth (cm)	5	
application rate (g/ha)	500, 750, 600, 1000	
crop interception (%)	0, 25, 50, 90	
application dates(d)	1st May, 10th May, 1st June, 1st July	
Degradation type	SFO	FOMC
SFO DT50 (d)	25	
alpha		1
beta		1

(* separate consideration of residues within the year of application only)

On the following two pages copies of the ESCAPE-report for both soil studies are presented summarising the input data and all important results.

E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 13:51:11
Calculation problem:	Report example 3

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 3
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 1

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 3:	Single First order (SFO)
DT50 (d):	25
Rate constant (1/d):	0.0277
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 3

Calculations over one year

Maximum annual total soil concentration for Report example 3 over 5 cm(mg/kg): 1.2694 occurring on day 9

Calculated time dependent total soil concentrations over 5 cm for Report example 3 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2347	1.2521	9	10
2	1.2010	1.2350	9	11
4	1.1362	1.2017	9	13
7	1.0455	1.1539	9	16
14	0.8611	1.0542	8	22
21	0.7092	0.9710	8	29
28	0.9228	0.9690	9	37
42	0.6259	0.9073	8	50
50	0.5014	0.8578	0	50
100	0.1606	0.6354	0	100

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 3 over 5 cm(mg/kg)*: 0.0001**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

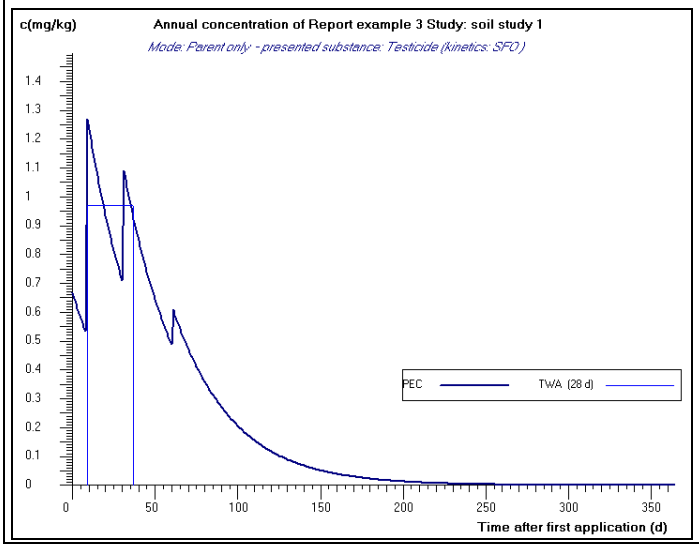
Maximum total soil concentration for Report example 3 over 5 cm considering accumulation* (mg/kg) 1.2695
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 3(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2348	1.2522	9	10
2	1.2011	1.2351	9	11
4	1.1363	1.2018	9	13
7	1.0456	1.1540	9	16
14	0.8612	1.0543	8	22
21	0.7093	0.9711	8	29
28	0.9229	0.9691	9	37
42	0.6260	0.9074	8	50
50	0.5015	0.8579	0	50
100	0.1607	0.6355	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 13:52:37
Calculation problem:	Report example 3

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 3
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Parent compound without metabolites

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 2

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 3:	First Order Multi Compartment (FOMC)
Alpha:	1
Beta:	1
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 3

Calculations over one year

Maximum annual total soil concentration for Report example 3 over 5 cm(mg/kg): 0.8167 occurring on day 9

Calculated time dependent total soil concentrations over 5 cm for Report example 3 after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.4356	0.6261	9	10
2	0.3056	0.5358	8	10
4	0.1976	0.4286	8	12
7	0.1330	0.3250	8	15
14	0.0778	0.2594	0	14
21	0.0556	0.2128	0	21
28	0.1005	0.1777	0	28
42	0.0493	0.1634	0	42
50	0.0396	0.1468	0	50
100	0.0213	0.0945	0	100

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Report example 3 over 5 cm(mg/kg)*: 0.0006**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

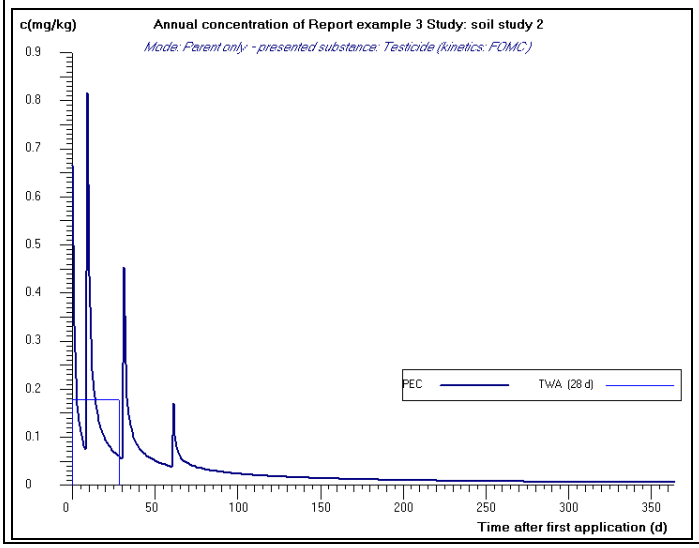
Maximum total soil concentration for Report example 3 over 5 cm considering accumulation* (mg/kg) 0.8172
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Report example 3(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.4362	0.6267	9	10
2	0.3061	0.5363	8	10
4	0.1982	0.4291	8	12
7	0.1335	0.3256	8	15
14	0.0783	0.2600	0	14
21	0.0562	0.2133	0	21
28	0.1011	0.1783	0	28
42	0.0499	0.1639	0	42
50	0.0402	0.1473	0	50
100	0.0218	0.0951	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



Here, the respective report is shown when ESCAPE is in its summary mode. Results of both studies are summarised in a single file and also the diagram includes results of both studies.

E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 14:00:30
Calculation problem:	Report example 3

SUMMARY REPORT CONSIDERING ALL SOIL STUDIES

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 3
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	Laboratory conditions
Mean temperature (°C):	19.5
Annual Rainfall (mm):	18245
Annual pot. Evapotranspiration (mm):	

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites
Pesticide:	Report example 3

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 3:

Soil study: soil study 1

Single First order (SFO)

DT50 (d):	25
Rate constant (1/d):	0.0277
Q10-factor:	2.58
Walker-exponent:	0.7
TReference (°C):	20

Soil study: soil study 2

First Order Multi Compartment (FOMC)
alpha(i_studie): 1
Beta: 1
Q10-factor: 2.58
Walker-exponent: 0.7
TReference (°C): 20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 3

Calculations over one year

Maximum annual total soil concentration for Report example 3 over 1.5 cm
soil study 1(mg/kg): 1.2694 occurring on day 9
soil study 2(mg/kg): 0.8167 occurring on day 9

Calculated PECact* in soil over 1.5 cm for Report example 3(mg/kg)

Time (d)	soil study 1	soil study 2
1.0000	1.2347	0.4356
2.0000	1.2010	0.3056
4.0000	1.1362	0.1976
7.0000	1.0455	0.1330
14.0000	0.8611	0.0778
21.0000	0.7092	0.0556
28.0000	0.9228	0.1005
42.0000	0.6259	0.0493
50.0000	0.5014	0.0396
100.0000	0.1606	0.0213

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Report example 3(mg/kg)

Time (d)	soil study 1	soil study 2
1.0000	1.2521	0.6261
2.0000	1.2350	0.5358
4.0000	1.2017	0.4286
7.0000	1.1539	0.3250
14.0000	1.0542	0.2594
21.0000	0.9710	0.2128
28.0000	0.9690	0.1777
42.0000	0.9073	0.1634
50.0000	0.8578	0.1468
100.0000	0.6354	0.0945

Calculation of background concentrations after many years

Final background concentration in total soil for Report example 3 over 5 cm
soil study 1(mg/kg): 0.0001 (estimated to occur within 10 years)
soil study 2(mg/kg): 0.0006 (estimated to occur within 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in total soil for Report example 3 over 5 cm considering accumulation*
soil study 1(mg/kg): 1.2695 occurring on day 9
soil study 2(mg/kg): 0.8172 occurring on day 9
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Report example 3(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2
1.0000	0.1607	0.4362

2.0000	1.2348	0.3061
4.0000	1.2011	0.1982
7.0000	1.1363	0.1335
14.0000	1.0456	0.0783
21.0000	0.8612	0.0562
28.0000	0.7093	0.1011
42.0000	0.9229	0.0499
50.0000	0.6260	0.0402
100.0000	0.5015	0.0218

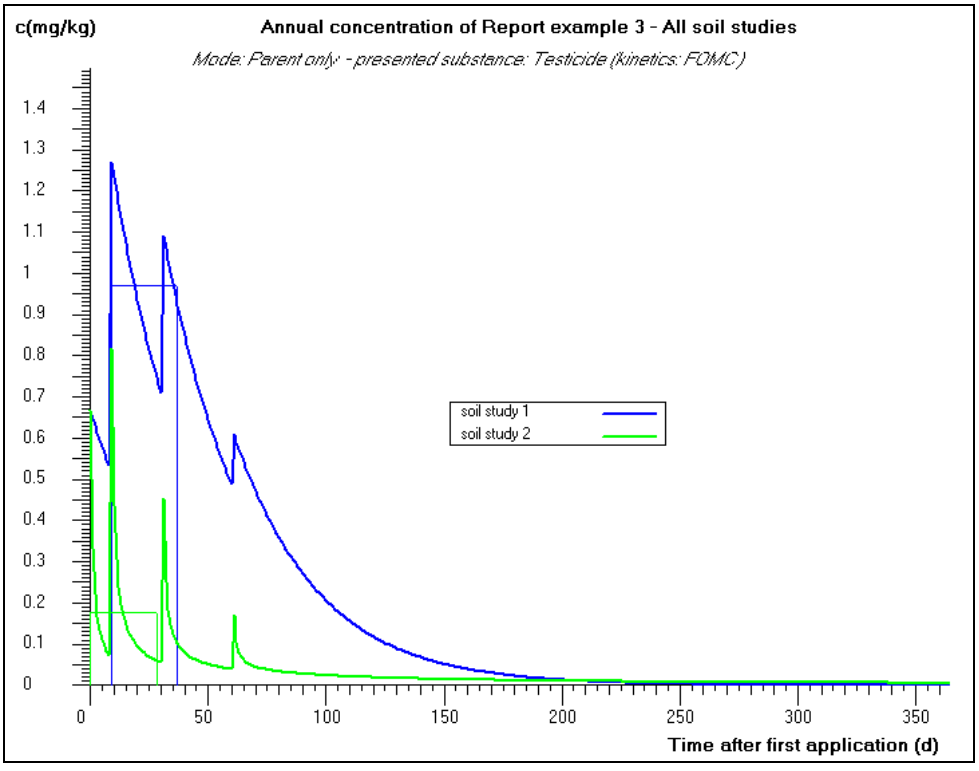
(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 5 cm for Report example 3(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2
1.0000	1.2522	0.6267
2.0000	1.2351	0.5363
4.0000	1.2018	0.4291
7.0000	1.1540	0.3256
14.0000	1.0543	0.2600
21.0000	0.9711	0.2133
28.0000	0.9691	0.1783
42.0000	0.9074	0.1639
50.0000	0.8579	0.1473
100.0000	0.6355	0.0951

(* a tillage depth of 5 cm was considered for calculating the background concentration)

GRAPHIC REPRESENTATION OF THE CALCULATION



On the following pages copies of the ESCAPE-report for the same studies are presented summarising the input data and all important results based on Hamburg climatic conditions and considering soil moisture and temperature correction (again summary mode)

E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 14:16:14
Calculation problem:	Report example 3

SUMMARY REPORT CONSIDERING ALL SOIL STUDIES

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 3
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme:	Parent compound without metabolites
Pesticide:	Report example 3

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Metabolism scheme: Parent compound without metabolites

Kinetics for Report example 3:

Soil study: soil study 1

Single First order (SFO)

DT50 (d):	25
Rate constant (1/d):	0.0277
Q10-factor:	2.58
Walker-exponent:	0.7
TReference (°C):	20

Soil study: soil study 2

First Order Multi Compartment (FOMC)

alpha(i_studie):	1
Beta:	1
Q10-factor:	2.58

Walker-exponent:	0.7
TReference (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Parent compound without metabolites

RESULTS FOR: Report example 3

Calculations over one year

Maximum annual total soil concentration for Report example 3 over 1.5 cm
soil study 1(mg/kg): 1.5296 occurring on day 31
soil study 2(mg/kg): 0.9502 occurring on day 9

Calculated PECact* in soil over 1.5 cm for Report example 3(mg/kg)

Time (d)	soil study 1	soil study 2
1.0000	1.5151	0.8008
2.0000	1.4983	0.7167
4.0000	1.4609	0.6309
7.0000	1.4158	0.4751
14.0000	1.3258	0.2167
21.0000	1.2636	0.1614
28.0000	1.1389	0.2370
42.0000	1.0544	0.1421
50.0000	0.9756	0.1061
100.0000	0.5364	0.0526

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Report example 3(mg/kg)

Time (d)	soil study 1	soil study 2
1.0000	1.5224	0.8755
2.0000	1.5146	0.8172
4.0000	1.4973	0.7451
7.0000	1.4712	0.6768
14.0000	1.4232	0.5193
21.0000	1.3849	0.4736
28.0000	1.3432	0.4058
42.0000	1.3241	0.3618
50.0000	1.3058	0.3301
100.0000	1.1340	0.2146

Calculation of background concentrations after many years

Final background concentration in total soil for Report example 3 over 5 cm
soil study 1(mg/kg): 0.1096 (estimated to occur within 10 years)
soil study 2(mg/kg): 0.0043 (estimated to occur within 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in total soil for Report example 3 over 5 cm considering accumulation*
soil study 1(mg/kg): 1.6392 occurring on day 31
soil study 2(mg/kg): 0.9546 occurring on day 9
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Report example 3(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2
1.0000	0.8123	0.4532
2.0000	1.4761	0.3782
4.0000	1.4696	0.2869
7.0000	1.4610	0.2293
14.0000	1.4369	0.1687
21.0000	1.3186	0.1436
28.0000	1.2473	0.1104

42.0000	1.5370	0.0987
50.0000	1.3813	0.0851
100.0000	1.2485	0.0457

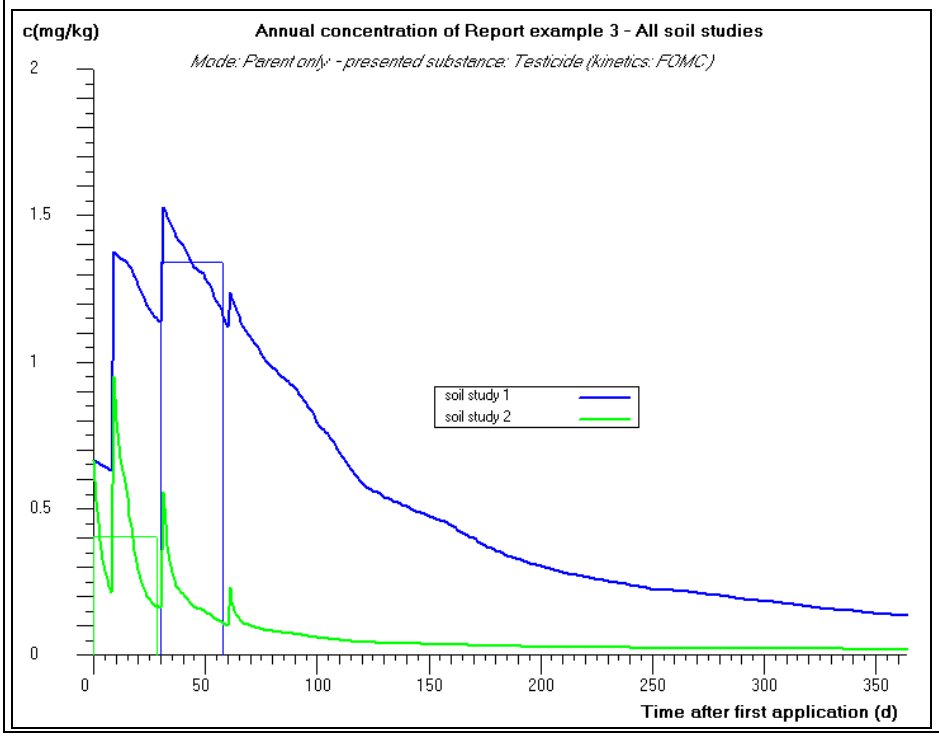
(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 5 cm for Report example 3(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2
1.0000	1.6319	0.8799
2.0000	1.6241	0.8215
4.0000	1.6069	0.7494
7.0000	1.5808	0.6811
14.0000	1.5328	0.5236
21.0000	1.4945	0.4780
28.0000	1.4528	0.4101
42.0000	1.4337	0.3662
50.0000	1.4154	0.3345
100.0000	1.2436	0.2189

(* a tillage depth of 5 cm was considered for calculating the background concentration)

GRAPHIC REPRESENTATION OF THE CALCULATION



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6.4. Single application, parent compound with metabolite, several soil studies

Table 6: Series of special times used by ESCAPE to calculate PEC_{act} and PEC_{TWA}

Parameter	Soil study 1	Soil study 2	Soil study 3	Soil study 4
soil density (kg/L)	1.5			
soil depth (cm)	5			
application rate (g/ha)	1000			
crop interception (%)	0			
parent molecular mass (g/mol)	250			
metabolite molecular mass (g/mol)	200			
metabolite formation fraction (-)	1 (100 %)			
parent degradation data	SFO	FOMC*	HS*	DFOP
SFO DT50 (d)**	7			
alpha**		0.2		
beta**		2		
HS DT501 (d)**			7	
HS DT50 2 (d)**			70	
HS break point (d)**			10	
DFOP DT50 1 (d)**				7
DFOP DT50 2 (d)**				70
parameter g (-)**				0.5
metabolite degradation data	SFO	SFO	SFO	SFO
SFO rate constant (1/d)**	35	350	140	14

(* separate consideration of residues within the year of application only, ** related to standard conditions)

On the following eight pages copies of the ESCAPE-report for all four studies are presented summarising the input data and all important results based on Hamburg climatic conditions and considering soil moisture and temperature correction.

E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 14:39:50
Calculation problem:	Report example 4

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application date:	1 May
Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 1

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	Single First order (SFO)
DT50 (d):	7
Rate constant (1/d):	0.099
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	35
Rate constant (1/d):	0.0198
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual total soil concentration for Testicide over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Testicide after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2989	1.3161	0	1
2	1.2727	1.3010	0	2
4	1.2012	1.2708	0	4
7	1.1152	1.2222	0	7
14	0.9820	1.1288	0	14
21	0.7449	1.0443	0	21
28	0.5577	0.9417	0	28
42	0.3568	0.7790	0	42
50	0.2825	0.7044	0	50
100	0.0339	0.4076	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Testicide over 5 cm(mg/kg)*: 0.0001**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum total soil concentration for Testicide over 5 cm considering accumulation* (mg/kg) 1.3334
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Testicide(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2990	1.3162	0	1
2	1.2727	1.3010	0	2
4	1.2013	1.2709	0	4
7	1.1153	1.2223	0	7
14	0.9820	1.1288	0	14
21	0.7450	1.0444	0	21
28	0.5578	0.9417	0	28
42	0.3568	0.7790	0	42
50	0.2825	0.7045	0	50
100	0.0340	0.4076	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual total soil concentration for Metabolidan over 5 cm(mg/kg): 0.6604 occurring on day 67^
(^ This is 61.91 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.6591	0.6598	67	68
2	0.6541	0.6596	66	68
4	0.6342	0.6581	65	69
7	0.6035	0.6555	62	69
14	0.5443	0.6485	58	72
21	0.4982	0.6399	52	73
28	0.4375	0.6308	46	74
42	0.3734	0.6148	35	77

50	0.3655	0.6069	29	79
100	0.2281	0.5262	18	118

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Metabolidan over 5 cm(mg/kg)*: 0.0875**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

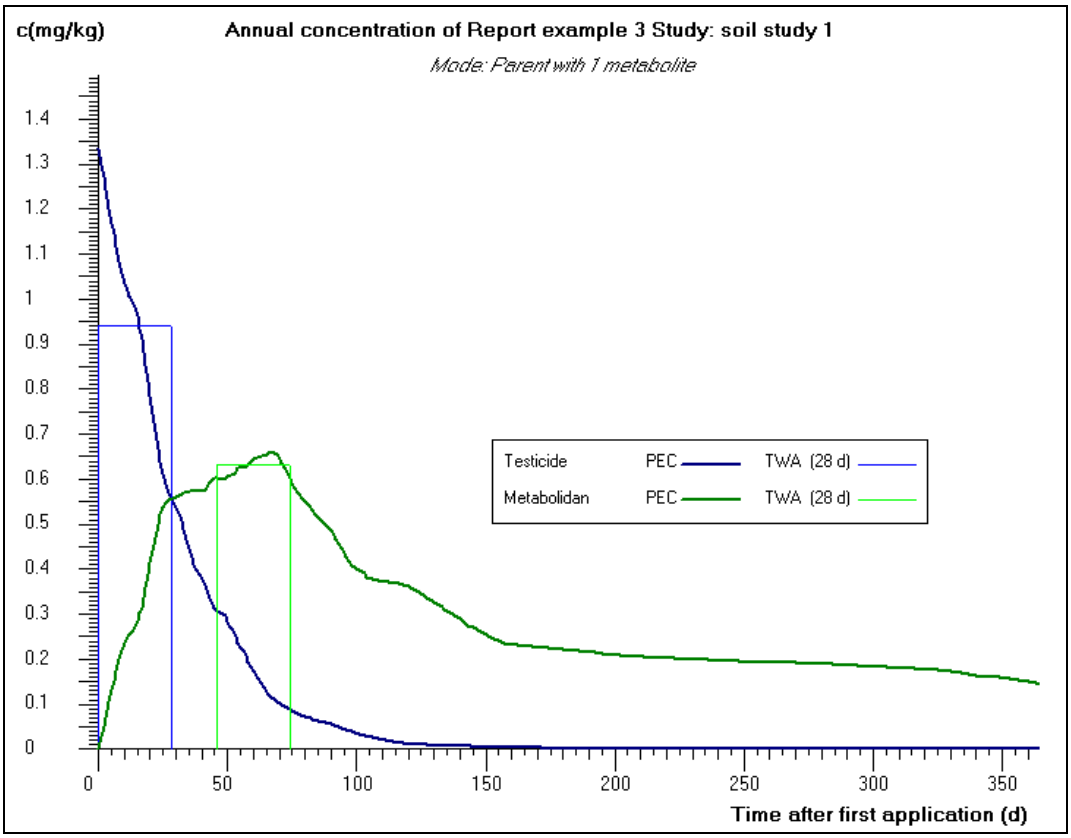
Maximum total soil concentration for Metabolidan over 5 cm considering accumulation* (mg/kg) 0.7479
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.7467	0.7473	67	68
2	0.7416	0.7471	66	68
4	0.7217	0.7457	65	69
7	0.6910	0.7430	62	69
14	0.6318	0.7360	58	72
21	0.5857	0.7274	52	73
28	0.5250	0.7184	46	74
42	0.4610	0.7024	35	77
50	0.4530	0.6944	29	79
100	0.3156	0.6137	18	118

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 14:42:11
Calculation problem:	Report example 4

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Iteration of annual application pattern over 10 years

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application date:	1 May
Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 2

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	First Order Multi Compartment (FOMC)
Alpha:	0.2
Beta:	0.2
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	350
Rate constant (1/d):	0.002
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual total soil concentration for Testicide over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Testicide after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.1268	1.2301	0	1
2	1.0469	1.1585	0	2
4	0.9236	1.0725	0	4
7	0.8409	0.9893	0	7
14	0.7616	0.8899	0	14
21	0.6736	0.8329	0	21
28	0.6227	0.7854	0	28
42	0.5741	0.7227	0	42
50	0.5559	0.6972	0	50
100	0.4687	0.6000	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Testicide over 5 cm(mg/kg)*: 0.5385**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum total soil concentration for Testicide over 5 cm considering accumulation* (mg/kg) 1.8718
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Testicide(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.6653	1.7686	0	1
2	1.5854	1.6970	0	2
4	1.4621	1.6110	0	4
7	1.3794	1.5278	0	7
14	1.3001	1.4284	0	14
21	1.2121	1.3714	0	21
28	1.1612	1.3239	0	28
42	1.1126	1.2612	0	42
50	1.0944	1.2357	0	50
100	1.0072	1.1385	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual total soil concentration for Metabolidan over 5 cm(mg/kg): 0.6291 occurring on day 121^
(^ This is 58.97 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.6289	0.6290	121	122
2	0.6287	0.6290	120	122
4	0.6281	0.6289	119	123
7	0.6271	0.6287	118	125
14	0.6240	0.6280	116	130
21	0.6203	0.6272	113	134
28	0.6171	0.6266	303	331
42	0.6143	0.6266	289	331
50	0.6163	0.6265	282	332
100	0.6224	0.6258	240	340

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Metabolidan over 5 cm(mg/kg)*: 3.9234**

(* estimated to occur after 13 years)
(** according to the estimation 95% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

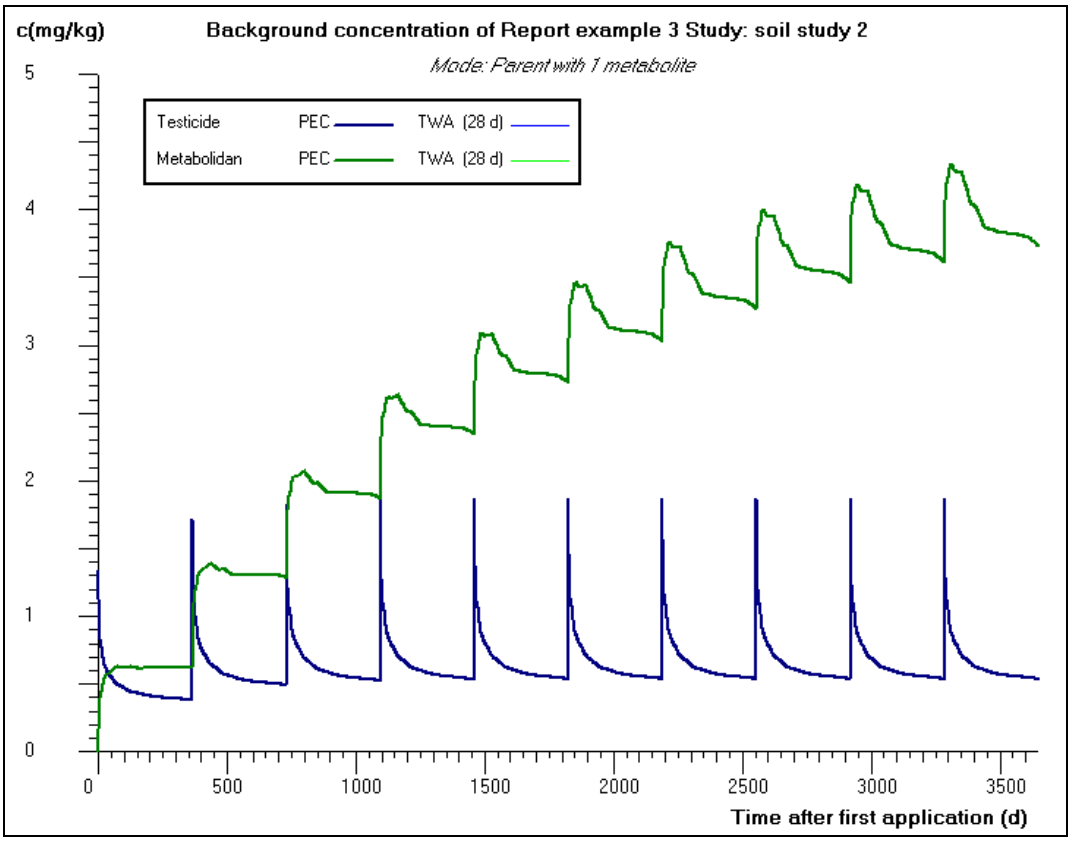
Maximum total soil concentration for Metabolidan over 5 cm considering accumulation* (mg/kg) 4.5524
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	4.5523	4.5524	121	122
2	4.5520	4.5524	120	122
4	4.5515	4.5522	119	123
7	4.5504	4.5520	118	125
14	4.5474	4.5513	116	130
21	4.5437	4.5505	113	134
28	4.5404	4.5500	303	331
42	4.5377	4.5499	289	331
50	4.5397	4.5499	282	332
100	4.5458	4.5491	240	340

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 14:43:55
Calculation problem:	Report example 4

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application date:	1 May
Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 3

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	Hockey Stick (HS)
DT50 1(d):	7
DT50 2(d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter Tb:	10
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	140
Rate constant (1/d):	0.005
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual total soil concentration for Testicide over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Testicide after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2989	1.3161	0	1
2	1.2727	1.3010	0	2
4	1.2012	1.2708	0	4
7	1.1152	1.2222	0	7
14	0.9820	1.1288	0	14
21	0.7449	1.0443	0	21
28	0.5577	0.9417	0	28
42	0.4896	0.7973	0	42
50	0.4783	0.7470	0	50
100	0.3870	0.5879	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Testicide over 5 cm(mg/kg)*: 0.2414**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum total soil concentration for Testicide over 5 cm considering accumulation* (mg/kg) 1.5747
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Testicide(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.5403	1.5575	0	1
2	1.5141	1.5424	0	2
4	1.4426	1.5122	0	4
7	1.3566	1.4636	0	7
14	1.2234	1.3702	0	14
21	0.9863	1.2857	0	21
28	0.7991	1.1831	0	28
42	0.7310	1.0387	0	42
50	0.7197	0.9884	0	50
100	0.6284	0.8293	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual total soil concentration for Metabolidan over 5 cm(mg/kg): 0.6355 occurring on day 32^
(^ This is 59.58 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.6335	0.6345	32	33
2	0.6313	0.6337	67	69
4	0.6267	0.6332	66	70
7	0.6219	0.6321	64	71
14	0.6215	0.6299	59	73
21	0.6213	0.6275	54	75
28	0.6266	0.6258	47	75
42	0.6232	0.6255	31	73
50	0.6096	0.6244	30	80
100	0.5798	0.6072	26	126

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Metabolidan over 5 cm(mg/kg)*: 1.5434**

(* estimated to occur after 11 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

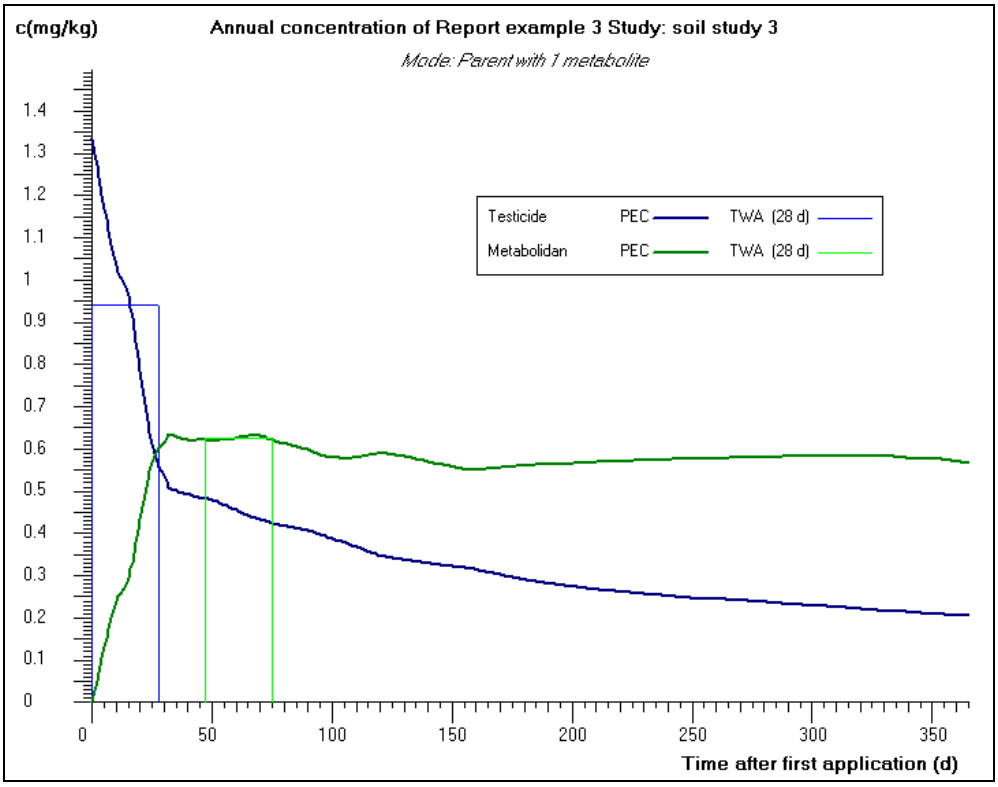
Maximum total soil concentration for Metabolidan over 5 cm considering accumulation* (mg/kg) 2.1789
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.1769	2.1779	32	33
2	2.1747	2.1771	67	69
4	2.1701	2.1766	66	70
7	2.1654	2.1756	64	71
14	2.1650	2.1733	59	73
21	2.1648	2.1710	54	75
28	2.1700	2.1692	47	75
42	2.1666	2.1689	31	73
50	2.1530	2.1678	30	80
100	2.1233	2.1506	26	126

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version: 2.0 (17 Feb 2009)
Date of this simulation: 17/02/2009, 14:45:22

Calculation problem:	Report example 4

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application date:	1 May
Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 4

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	Double First Order in Parallel (DFOP)
DT50 1(d):	7
DT50 2(d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter g:	0.5
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	14
Rate constant (1/d):	0.0495
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual total soil concentration for Testicide over 5 cm(mg/kg): 1.3333 occurring on day 0

Calculated time dependent total soil concentrations over 5 cm for Testicide after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.3144	1.3239	0	1
2	1.2999	1.3155	0	2
4	1.2603	1.2989	0	4
7	1.2125	1.2719	0	7
14	1.1376	1.2198	0	14
21	1.0014	1.1721	0	21
28	0.8899	1.1130	0	28
42	0.7627	1.0169	0	42
50	0.7121	0.9715	0	50
100	0.4788	0.7693	0	100

(* PECact values are related to the time after the first application)

Calculation of background concentrations after many years

Final Background concentration in total soil for Testicide over 5 cm(mg/kg)*: 0.3861**

(* estimated to occur after 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum total soil concentration for Testicide over 5 cm considering accumulation* (mg/kg) 1.7195
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Testicide(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.7005	1.7100	0	1
2	1.6860	1.7016	0	2
4	1.6465	1.6850	0	4
7	1.5986	1.6581	0	7
14	1.5237	1.6059	0	14
21	1.3876	1.5582	0	21
28	1.2760	1.4991	0	28
42	1.1488	1.4030	0	42
50	1.0982	1.3576	0	50
100	0.8649	1.1554	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the first application)

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual total soil concentration for Metabolidan over 5 cm(mg/kg): 0.2782 occurring on day 26^
(^ This is 26.08 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan after one year (mg/kg)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.2742	0.2779	25	26
2	0.2719	0.2770	25	27
4	0.2677	0.2753	24	28
7	0.2558	0.2724	24	31
14	0.2254	0.2634	22	36
21	0.2343	0.2523	21	42
28	0.2427	0.2478	21	49
42	0.2623	0.2469	23	65
50	0.1923	0.2480	21	71
100	0.0980	0.1960	7	107

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in total soil for Metabolidan over 5 cm(mg/kg)*: 0.0925**

(* estimated to occur after 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

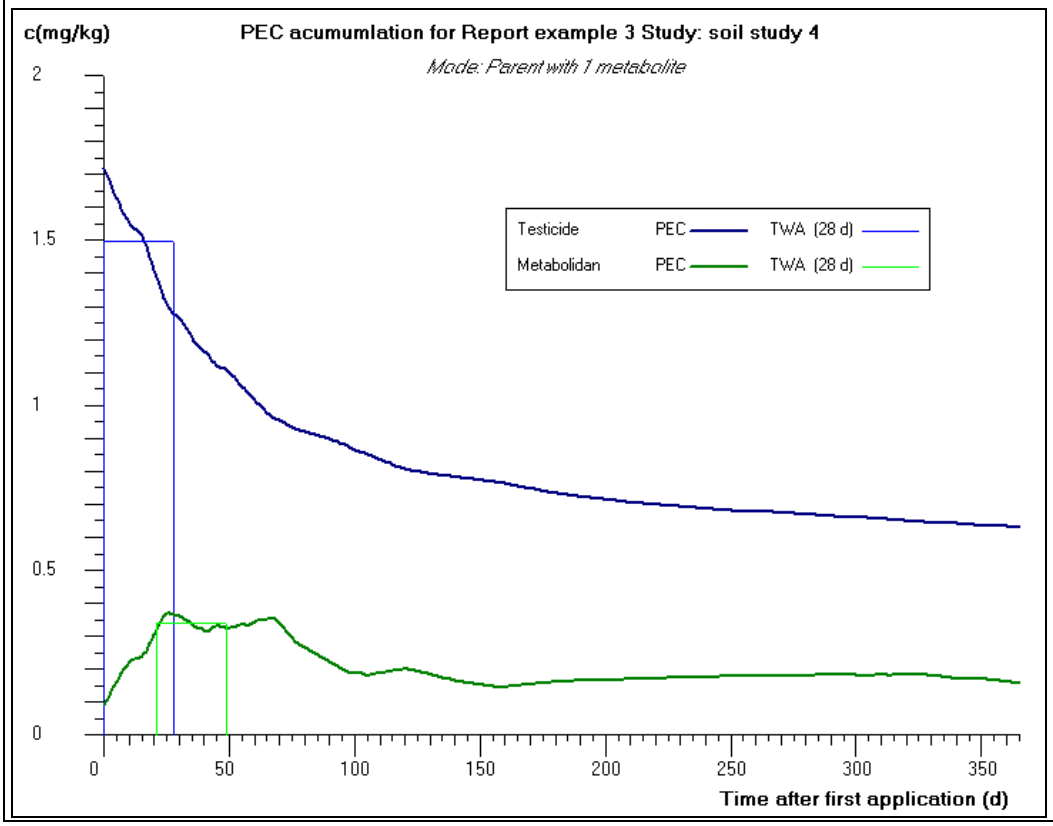
Maximum total soil concentration for Metabolidan over 5 cm considering accumulation* (mg/kg) 0.3707
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent total soil concentrations over 5 cm for Metabolidan(mg/kg) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.3667	0.3704	25	26
2	0.3644	0.3696	25	27
4	0.3602	0.3678	24	28
7	0.3484	0.3650	24	31
14	0.3180	0.3559	22	36
21	0.3269	0.3448	21	42
28	0.3353	0.3403	21	49
42	0.3548	0.3395	23	65
50	0.2848	0.3405	21	71
100	0.1905	0.2885	7	107

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



Here, the respective report is shown when ESCAPE's summary mode was selected. Results of all studies are summarised for the parent compound and the metabolite.

E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 14:48:31
Calculation problem:	Report example 4

SUMMARY REPORT CONSIDERING ALL SOIL STUDIES

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Programcheck
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Application date:	1 May
Application rate (g/ha):	1000
Crop interception (%):	0

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	format_berichtion (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Soil study: soil study 1

Kinetics for Testicide:	Single First order (SFO)
DT50 (d):	7
Rate constant (1/d):	0.099
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

Soil study: soil study 2

Kinetics for Testicide:	First Order Multi Compartment (FOMC)
alpha(i_studie):	0.2
Beta:	0.2
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

Soil study:	soil study 3
Kinetics for Testicide:	Hockey Stick (HS)
DT50 (d):	7
DT50 (d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter Tb (d):	10
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 4
Kinetics for Testicide:	Double First Order in Parallel (DFOP)
DT50 (d):	7
DT50 (d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter g:	0.5
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 1
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	35
Rate constant (1/d):	0.099
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 2
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	350
Rate constant (1/d):	0.005
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 3
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	140
Rate constant (1/d):	0.001
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 4
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	14
Rate constant (1/d):	0.0495
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual total soil concentration for Testicide over 1.5 cm

soil study 1(mg/kg):	1.3333 occurring on day 0
soil study 2(mg/kg):	1.3333 occurring on day 0
soil study 3(mg/kg):	1.3333 occurring on day 0
soil study 4(mg/kg):	1.3333 occurring on day 0

Calculated PECact* in soil over 1.5 cm for Testicide(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.2989	1.1268	1.2989	1.3144
2.0000	1.2727	1.0469	1.2727	1.2999
4.0000	1.2012	0.9236	1.2012	1.2603
7.0000	1.1152	0.8409	1.1152	1.2125
14.0000	0.9820	0.7616	0.9820	1.1376
21.0000	0.7449	0.6736	0.7449	1.0014
28.0000	0.5577	0.6227	0.5577	0.8899
42.0000	0.3568	0.5741	0.4896	0.7627
50.0000	0.2825	0.5559	0.4783	0.7121
100.0000	0.0339	0.4687	0.3870	0.4788

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Testicide(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.3161	1.2301	1.3161	1.3239
2.0000	1.3010	1.1585	1.3010	1.3155
4.0000	1.2708	1.0725	1.2708	1.2989
7.0000	1.2222	0.9893	1.2222	1.2719
14.0000	1.1288	0.8899	1.1288	1.2198
21.0000	1.0443	0.8329	1.0443	1.1721
28.0000	0.9417	0.7854	0.9417	1.1130
42.0000	0.7790	0.7227	0.7973	1.0169
50.0000	0.7044	0.6972	0.7470	0.9715
100.0000	0.4076	0.6000	0.5879	0.7693

Calculation of background concentrations after many years

Final background concentration in total soil for Testicide over 5 cm

soil study 1(mg/kg):	0.0001 (estimated to occur within 10 years)
soil study 2(mg/kg):	0.5385 (estimated to occur within 10 years)
soil study 3(mg/kg):	0.2414 (estimated to occur within 10 years)
soil study 4(mg/kg):	0.3861 (estimated to occur after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in total soil for Testicide over 5 cm considering accumulation*

soil study 1(mg/kg):	1.3334 occurring on day 0
soil study 2(mg/kg):	1.8718 occurring on day 0
soil study 3(mg/kg):	1.5747 occurring on day 0
soil study 4(mg/kg):	1.7195 occurring on day 0

(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Testicide(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.0340	1.6653	1.5403	1.7005
2.0000	1.2990	1.5854	1.5141	1.6860
4.0000	1.2727	1.4621	1.4426	1.6465
7.0000	1.2013	1.3794	1.3566	1.5986
14.0000	1.1153	1.3001	1.2234	1.5237
21.0000	0.9820	1.2121	0.9863	1.3876
28.0000	0.7450	1.1612	0.7991	1.2760
42.0000	0.5578	1.1126	0.7310	1.1488
50.0000	0.3568	1.0944	0.7197	1.0982
100.0000	0.2825	1.0072	0.6284	0.8649

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 5 cm for Testicide(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.3162	1.7686	1.5575	1.7100
2.0000	1.3010	1.6970	1.5424	1.7016
4.0000	1.2709	1.6110	1.5122	1.6850
7.0000	1.2223	1.5278	1.4636	1.6581
14.0000	1.1288	1.4284	1.3702	1.6059

21.0000	1.0444	1.3714	1.2857	1.5582
28.0000	0.9417	1.3239	1.1831	1.4991
42.0000	0.7790	1.2612	1.0387	1.4030
50.0000	0.7045	1.2357	0.9884	1.3576
100.0000	0.4076	1.1385	0.8293	1.1554

(* a tillage depth of 5 cm was considered for calculating the background concentration)

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual total soil concentration for Metabolidan over 1.5 cm
soil study 1(mg/kg): 0.6604 occurring on day 67
soil study 2(mg/kg): 0.6291 occurring on day 121
soil study 3(mg/kg): 0.6355 occurring on day 32
soil study 4(mg/kg): 0.2782 occurring on day 26

Calculated PECact* in soil over 1.5 cm for Metabolidan(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.6591	0.6289	0.6335	0.2742
2.0000	0.6541	0.6287	0.6313	0.2719
4.0000	0.6342	0.6281	0.6267	0.2677
7.0000	0.6035	0.6271	0.6219	0.2558
14.0000	0.5443	0.6240	0.6215	0.2254
21.0000	0.4982	0.6203	0.6213	0.2343
28.0000	0.4375	0.6171	0.6266	0.2427
42.0000	0.3734	0.6143	0.6232	0.2623
50.0000	0.3655	0.6163	0.6096	0.1923
100.0000	0.2281	0.6224	0.5798	0.0980

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Metabolidan(mg/kg)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.6598	0.6290	0.6345	0.2779
2.0000	0.6596	0.6290	0.6337	0.2770
4.0000	0.6581	0.6289	0.6332	0.2753
7.0000	0.6555	0.6287	0.6321	0.2724
14.0000	0.6485	0.6280	0.6299	0.2634
21.0000	0.6399	0.6272	0.6275	0.2523
28.0000	0.6308	0.6266	0.6258	0.2478
42.0000	0.6148	0.6266	0.6255	0.2469
50.0000	0.6069	0.6265	0.6244	0.2480
100.0000	0.5262	0.6258	0.6072	0.1960

Calculation of background concentrations after many years

Final background concentration in total soil for Metabolidan over 5 cm
soil study 1(mg/kg): 0.0875 (estimated to occur within 10 years)
soil study 2(mg/kg): 3.9234 (estimated to occur after 13 years)
soil study 3(mg/kg): 1.5434 (estimated to occur after 11 years)
soil study 4(mg/kg): 0.0925 (estimated to occur after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in total soil for Metabolidan over 5 cm considering accumulation*
soil study 1(mg/kg): 0.7479 occurring on day 67
soil study 2(mg/kg): 4.5524 occurring on day 121
soil study 3(mg/kg): 2.1789 occurring on day 32
soil study 4(mg/kg): 0.3707 occurring on day 26
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Metabolidan(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.4289	4.5511	2.1327	0.3484
2.0000	0.6407	4.5515	2.1319	0.3433

4.0000	0.6434	4.5512	2.1302	0.3323
7.0000	0.6475	4.5505	2.1274	0.3206
14.0000	0.6562	4.5490	2.1194	0.3290
21.0000	0.6606	4.5470	2.1102	0.3313
28.0000	0.6887	4.5437	2.1024	0.3459
42.0000	0.7116	4.5453	2.0955	0.3044
50.0000	0.7467	4.5507	2.0998	0.2556
100.0000	0.6662	4.5388	2.1144	0.1801

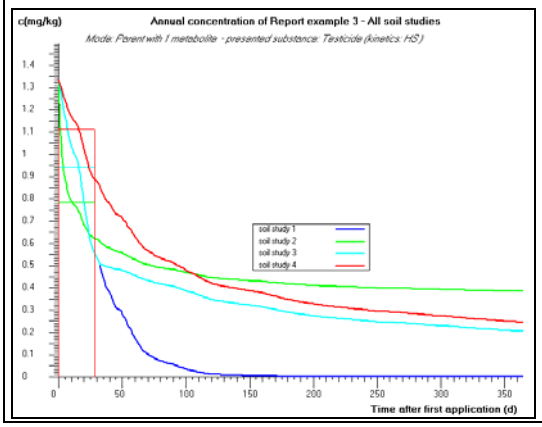
(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

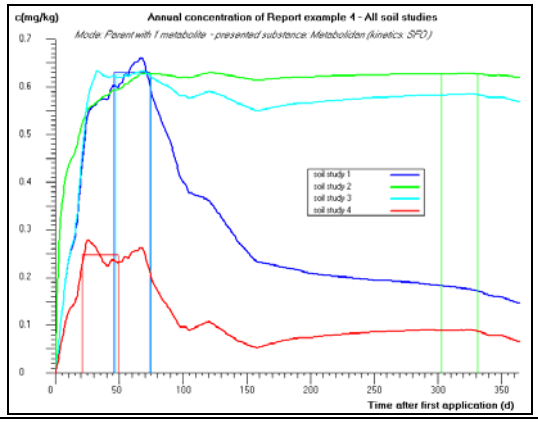
Calculated time weighted average (TWA) concentrations in soil over 5 cm for Metabolidan(mg/kg) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.7473	4.5524	2.1779	0.3704
2.0000	0.7471	4.5524	2.1771	0.3696
4.0000	0.7457	4.5522	2.1766	0.3678
7.0000	0.7430	4.5520	2.1756	0.3650
14.0000	0.7360	4.5513	2.1733	0.3559
21.0000	0.7274	4.5505	2.1710	0.3448
28.0000	0.7184	4.5500	2.1692	0.3403
42.0000	0.7024	4.5499	2.1689	0.3395
50.0000	0.6944	4.5499	2.1678	0.3405
100.0000	0.6137	4.5491	2.1506	0.2885

(* a tillage depth of 5 cm was considered for calculating the background concentration)

GRAPHIC REPRESENTATION OF THE CALCULATION





6.5. Irregular applications, parent compound with metabolite, several soil studies

Table 7: Series of special times used by ESCAPE to calculate PEC_{act} and PEC_{TWA}

Parameter	Soil study 1	Soil study 2	Soil study 3	Soil study 4
soil density (kg/L)	1.5			
soil depth (cm)	5			
application rate (g/ha)	500, 750, 600, 1000			
crop interception (%)	0, 25, 50, 90			
application dates(d)	1st May, 10th May, 1st June, 1st July			
parent molecular mass (g/mol)	250			
metabolite molecular mass (g/mol)	200			
metabolite formation fraction (-)	1 (100 %)			
parent KOC (L/kg)	200	100	300	500
parent degradation data	SFO	FOMC*	HS*	DFOP
SFO DT50 (d)**	70			
alpha**		1		
beta**		1		
HS DT501 (d)**			7	
HS DT50 2 (d)**			70	
HS break point (d)**			5	
DFOP DT50 1 (d)**				7
DFOP DT50 2 (d)**				140
parameter g (-)**				0.5
metabolite KOC (L/kg)	20	10	30	50
metabolite degradation data	SFO	SFO	SFO	SFO
SFO rate constant (1/d)	35	350	140	14

(* separate consideration of residues within the year of application only, ** related to standard conditions)

On the following four pages copies of the ESCAPE-report for all four studies are presented summarising the input data and all important results considering pore water concentrations as endpoint..

E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 16:22:52
Calculation problem:	Report example 5

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 5
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 1

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	Single First order (SFO)
DT50 (d):	70
Rate constant (1/d):	0.0099
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	35
Rate constant (1/d):	0.0198
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual pore water concentration for Testicide over 5 cm(mg/L): 0.5608 occurring on day 31

Calculated time dependent pore water concentrations over 5 cm for Testicide after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.5589	0.5599	31	32
2	0.5567	0.5589	31	33
4	0.5517	0.5566	31	35
7	0.5456	0.5531	31	38
14	0.5220	0.5425	31	45
21	0.5195	0.5362	31	52
28	0.4807	0.5274	30	58
42	0.5129	0.5212	31	73
50	0.4988	0.5186	31	81
100	0.4029	0.4882	9	109

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Testicide over 5 cm(mg/L)*: 0.3532**

(* estimated to occur after 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum pore water concentration for Testicide over 5 cm considering accumulation* (mg/L) 0.9141
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Testicide(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.9122	0.9131	31	32
2	0.9100	0.9121	31	33
4	0.9049	0.9098	31	35
7	0.8988	0.9063	31	38
14	0.8752	0.8958	31	45
21	0.8727	0.8894	31	52
28	0.8340	0.8807	30	58
42	0.8661	0.8745	31	73
50	0.8521	0.8718	31	81
100	0.7561	0.8414	9	109

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual pore water concentration for Metabolidan over 5 cm(mg/L): 1.2833 occurring on day 321^
(^ This is 240.61 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.2522	1.2730	315	316
2	1.2820	1.2730	315	317
4	1.2101	1.2707	314	318
7	1.1045	1.2425	314	321
14	0.8773	1.2345	313	327

21	1.2210	1.2313	304	325
28	1.0896	1.2124	263	291
42	0.8129	1.2033	250	292
50	1.0895	1.1978	243	293
100	0.6800	1.1811	228	328

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Metabolidan over 5 cm(mg/L)*: 1.0048**

(* estimated to occur after 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

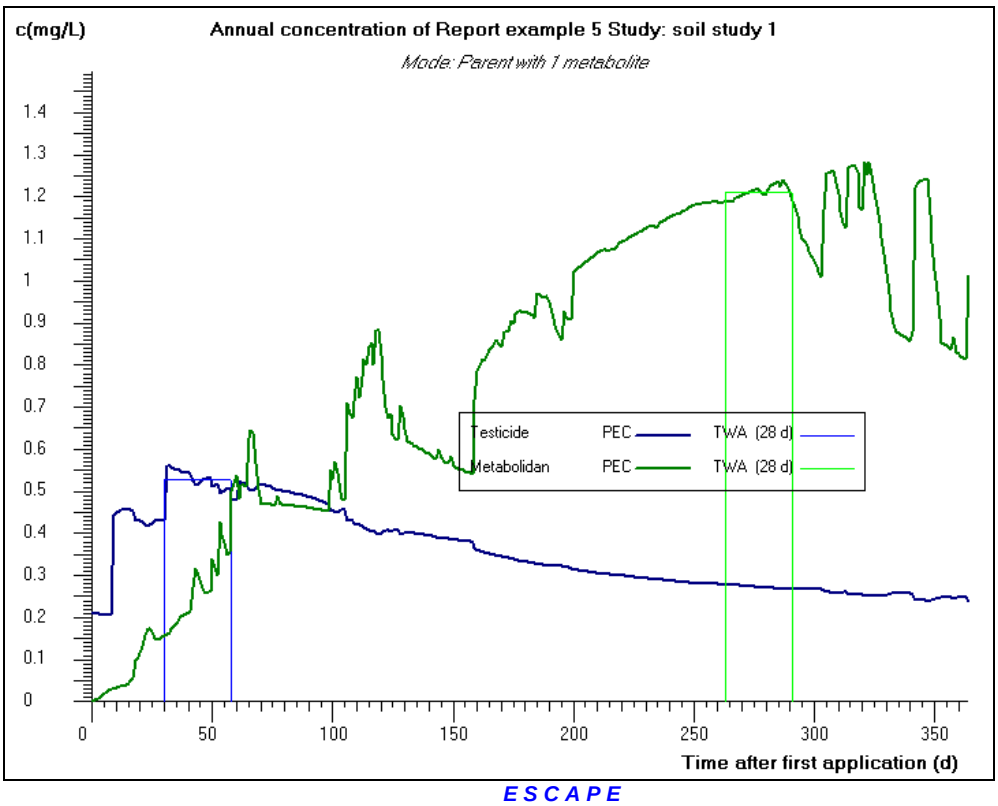
Maximum pore water concentration for Metabolidan over 5 cm considering accumulation* (mg/L) 2.2881
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	2.2570	2.2779	315	316
2	2.2868	2.2778	315	317
4	2.2149	2.2755	314	318
7	2.1094	2.2473	314	321
14	1.8822	2.2393	313	327
21	2.2258	2.2361	304	325
28	2.0944	2.2172	263	291
42	1.8177	2.2081	250	292
50	2.0943	2.2026	243	293
100	1.6848	2.1859	228	328

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 16:24:08
Calculation problem:	Report example 5

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Iteration of annual application pattern over 10 years

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 5
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 2

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	First Order Multi Compartment (FOMC)
Alpha:	1
Beta:	1
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	350
Rate constant (1/d):	0.002
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual pore water concentration for Testicide over 5 cm(mg/L): 0.5748 occurring on day 9

Calculated time dependent pore water concentrations over 5 cm for Testicide after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.4961	0.5354	9	10
2	0.4537	0.5051	9	11
4	0.4089	0.4688	9	13
7	0.3080	0.4268	8	15
14	0.1279	0.3257	8	22
21	0.1046	0.2936	0	21
28	0.1537	0.2512	0	28
42	0.0886	0.2266	0	42
50	0.0626	0.2068	0	50
100	0.0314	0.1344	0	100

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Testicide over 5 cm(mg/L)*: 0.0026**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum pore water concentration for Testicide over 5 cm considering accumulation* (mg/L) 0.5774
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Testicide(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.4987	0.5380	9	10
2	0.4563	0.5078	9	11
4	0.4116	0.4714	9	13
7	0.3106	0.4294	8	15
14	0.1305	0.3283	8	22
21	0.1073	0.2963	0	21
28	0.1563	0.2538	0	28
42	0.0912	0.2292	0	42
50	0.0652	0.2094	0	50
100	0.0340	0.1371	0	100

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual pore water concentration for Metabolidan over 5 cm(mg/L): 7.2742 occurring on day 66^
(^ This is 1363.90 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	6.8370	7.2586	65	66
2	5.4496	7.1571	65	67
4	4.0863	6.8677	112	116
7	4.0780	6.7797	112	119
14	4.0514	6.6780	200	214
21	4.0232	6.6584	219	240
28	3.9833	6.6586	200	228

42	5.9655	6.6567	200	242
50	6.9442	6.6564	200	250
100	6.7322	6.5445	195	295

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Metabolidan over 5 cm(mg/L)*: 27.5037**

(* estimated to occur after 13 years)
(** according to the estimation 95% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

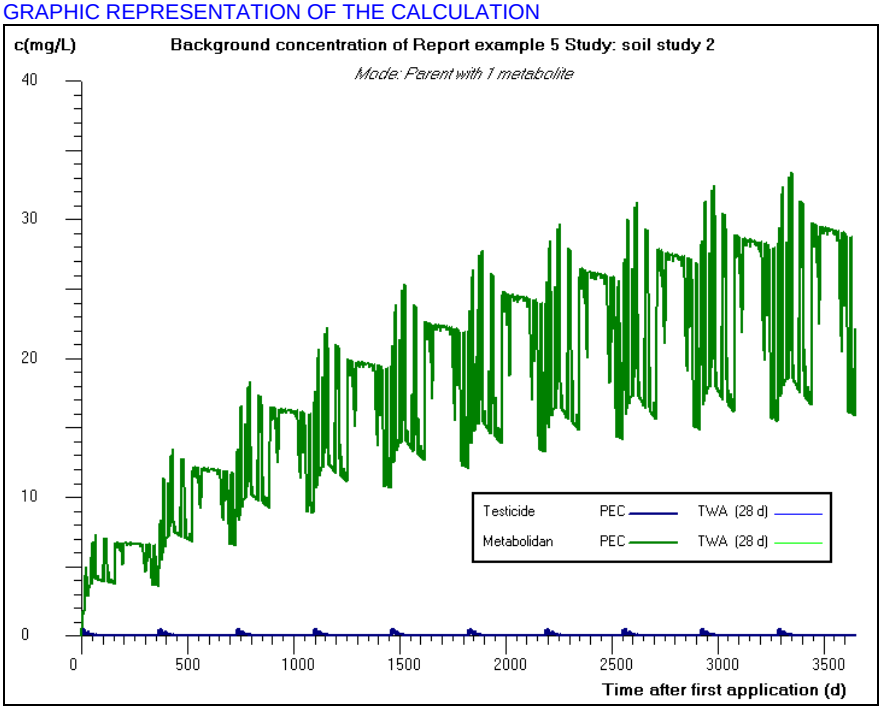
Maximum pore water concentration for Metabolidan over 5 cm considering accumulation* (mg/L) 34.7779
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	34.3407	34.7623	65	66
2	32.9533	34.6608	65	67
4	31.5900	34.3714	112	116
7	31.5817	34.2834	112	119
14	31.5551	34.1817	200	214
21	31.5269	34.1621	219	240
28	31.4870	34.1624	200	228
42	33.4692	34.1604	200	242
50	34.4479	34.1601	200	250
100	34.2359	34.0482	195	295

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E
Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 16:25:17
Calculation problem:	Report example 5

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 5
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 3

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	Hockey Stick (HS)
DT50 1(d):	7
DT50 2(d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter Tb:	5
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	140
Rate constant (1/d):	0.005
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual pore water concentration for Testicide over 5 cm(mg/L): 0.2759 occurring on day 31

Calculated time dependent pore water concentrations over 5 cm for Testicide after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.2723	0.2741	31	32
2	0.2682	0.2722	31	33
4	0.2595	0.2693	9	13
7	0.2495	0.2644	9	16
14	0.2295	0.2506	30	44
21	0.2275	0.2437	30	51
28	0.2133	0.2383	30	58
42	0.2241	0.2345	30	72
50	0.2180	0.2324	30	80
100	0.1760	0.2228	8	108

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Testicide over 5 cm(mg/L)*: 0.1072**

(* estimated to occur within 10 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum pore water concentration for Testicide over 5 cm considering accumulation* (mg/L) 0.3831
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Testicide(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.3795	0.3813	31	32
2	0.3754	0.3794	31	33
4	0.3667	0.3765	9	13
7	0.3567	0.3716	9	16
14	0.3367	0.3578	30	44
21	0.3347	0.3509	30	51
28	0.3205	0.3455	30	58
42	0.3313	0.3417	30	72
50	0.3252	0.3396	30	80
100	0.2832	0.3300	8	108

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual pore water concentration for Metabolidan over 5 cm(mg/L): 1.6462 occurring on day 321^
(^ This is 308.66 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	1.6177	1.6433	346	347
2	1.6438	1.6427	345	347
4	1.5780	1.6416	343	347
7	1.4788	1.6195	342	349
14	1.2584	1.6046	274	288
21	1.6273	1.6026	268	289
28	1.4975	1.5991	262	290

42	1.2418	1.5947	248	290
50	1.5403	1.5916	241	291
100	1.2523	1.5729	226	326

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Metabolidan over 5 cm(mg/L)*: 4.3420**

(* estimated to occur after 11 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

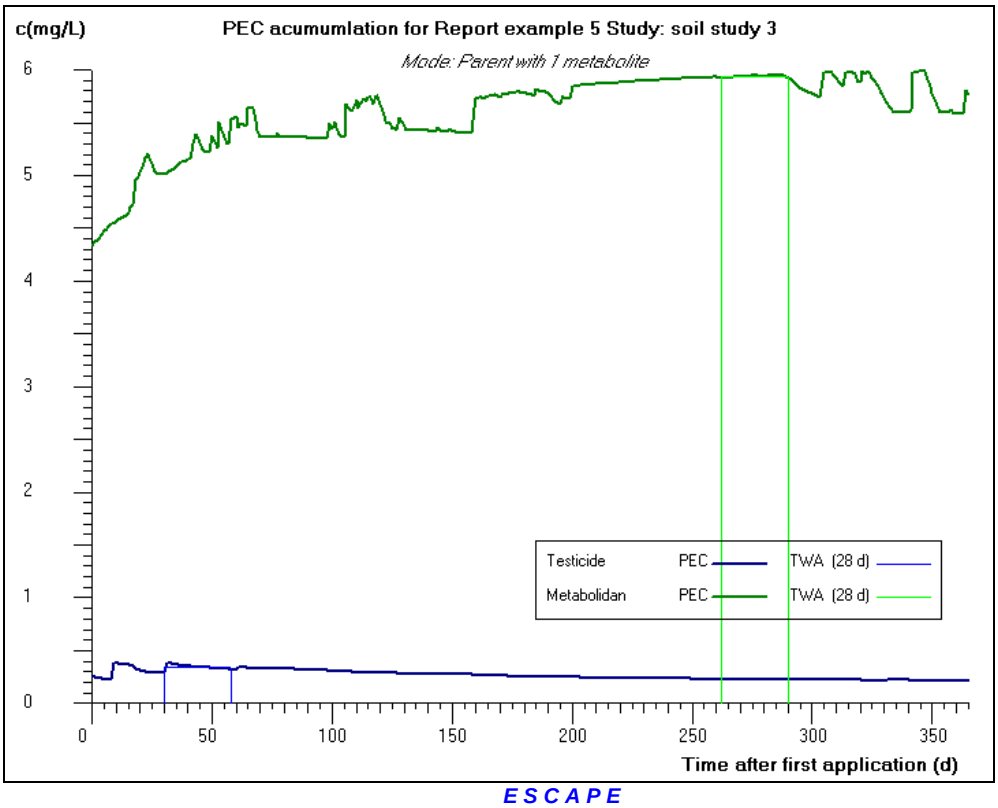
Maximum pore water concentration for Metabolidan over 5 cm considering accumulation* (mg/L) 5.9882
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	5.9597	5.9853	346	347
2	5.9859	5.9847	345	347
4	5.9200	5.9836	343	347
7	5.8209	5.9615	342	349
14	5.6004	5.9467	274	288
21	5.9694	5.9446	268	289
28	5.8395	5.9411	262	290
42	5.5838	5.9367	248	290
50	5.8824	5.9337	241	291
100	5.5944	5.9150	226	326

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version: 2.0 (17 Feb 2009)

Date of this simulation:	17/02/2009, 16:26:34
Calculation problem:	Report example 5

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 5
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	Formation (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Soil study: soil study 4

Metabolism scheme: Active compound and a single metabolite

Kinetics for Testicide:	Double First Order in Parallel (DFOP)
DT50 1(d):	7
DT50 2(d):	140
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.005
Parameter g:	0.5
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	14
Rate constant (1/d):	0.0495
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual pore water concentration for Testicide over 5 cm(mg/L): 0.3109 occurring on day 31

Calculated time dependent pore water concentrations over 5 cm for Testicide after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.3066	0.3088	31	32
2	0.3017	0.3065	31	33
4	0.2912	0.3015	31	35
7	0.2794	0.2943	31	38
14	0.2561	0.2813	30	44
21	0.2445	0.2719	30	51
28	0.2187	0.2626	30	58
42	0.2236	0.2562	9	51
50	0.2134	0.2524	9	59
100	0.1734	0.2320	9	109

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Testicide over 5 cm(mg/L)*: 0.1919**

(* estimated to occur after 11 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

Maximum pore water concentration for Testicide over 5 cm considering accumulation* (mg/L) 0.5028
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Testicide(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.4985	0.5006	31	32
2	0.4936	0.4983	31	33
4	0.4831	0.4934	31	35
7	0.4713	0.4862	31	38
14	0.4480	0.4732	30	44
21	0.4364	0.4638	30	51
28	0.4106	0.4545	30	58
42	0.4155	0.4481	9	51
50	0.4053	0.4443	9	59
100	0.3653	0.4239	9	109

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual pore water concentration for Metabolidan over 5 cm(mg/L): 0.7749 occurring on day 66^
(^ This is 86.41 % of the theoretical maximum concentration of the metabolite)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan after one year (mg/L)

Time(d)	PECact*	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.7734	0.7742	66	67
2	0.7266	0.7706	65	67
4	0.6310	0.7536	64	68
7	0.5684	0.7282	62	69
14	0.4552	0.6944	57	71
21	0.3794	0.6596	52	73
28	0.3030	0.6274	49	77
42	0.2836	0.5803	40	82
50	0.3199	0.5559	33	83

100	0.1612	0.4452	20	120

(* PECact values are related to the time after the maximum concentration)

Calculation of background concentrations after many years

Final Background concentration in pore water for Metabolidan over 5 cm(mg/L)*: 0.1475**

(* estimated to occur after 11 years)
(** according to the estimation 100% of the final plateau was reached after 10 years)

Calculations of concentrations considering accumulation after many years of application

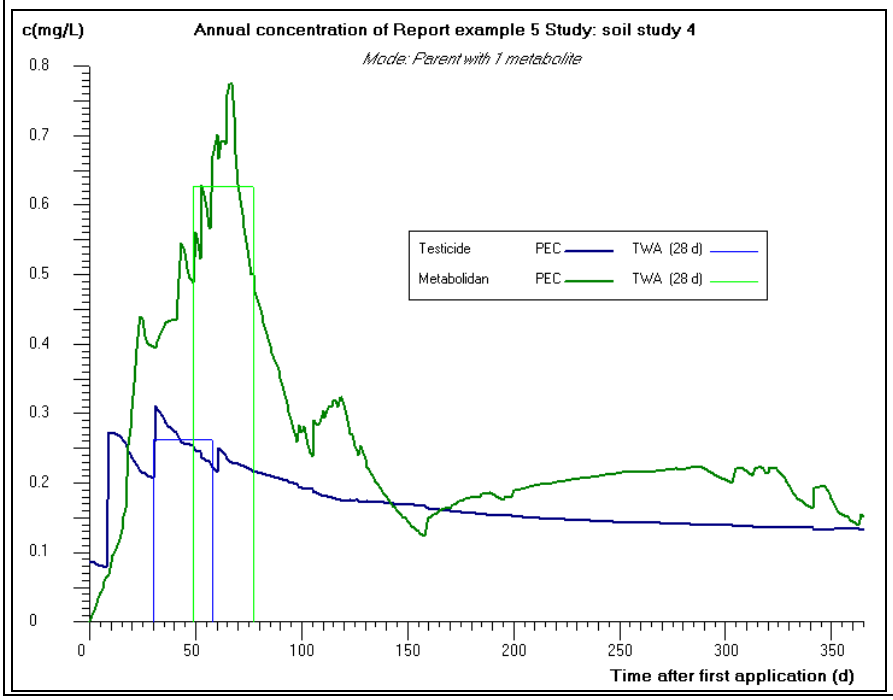
Maximum pore water concentration for Metabolidan over 5 cm considering accumulation* (mg/L) 0.9224
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated time dependent pore water concentrations over 5 cm for Metabolidan(mg/L) considering accumulation*

Time(d)	PECact**	PECtwa	Begin TWAframe(d)	End TWAframe(d)
1	0.9209	0.9217	66	67
2	0.8741	0.9181	65	67
4	0.7785	0.9011	64	68
7	0.7159	0.8757	62	69
14	0.6027	0.8419	57	71
21	0.5269	0.8071	52	73
28	0.4505	0.7749	49	77
42	0.4311	0.7278	40	82
50	0.4674	0.7034	33	83
100	0.3087	0.5927	20	120

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)'

GRAPHIC REPRESENTATION OF THE CALCULATION



Here, the respective report is shown when ESCAPE's summary mode was selected. Results of all four studies are summarised and the diagram shows the time dependent concentrations based on the DT50 and kinetics found in the different soil studies.

E S C A P E

Estimation of Soil Concentrations After PEsticide Applications

developed by Michael Klein

Program version:	2.0 (17 Feb 2009)
Date of this simulation:	17/02/2009, 16:38:53
Calculation problem:	Report example 5

SUMMARY REPORT CONSIDERING ALL SOIL STUDIES

PROGRAM SETTINGS

Calculation mode:	Residues from different applications are considered separately over one year
Application mode:	Single annual application pattern (calculation period 1 year)

SCENARIO DATA USED IN THE CALCULATION

Name of the scenario:	Report example 5
Name of the soil:	Borstel
Soil density (kg/L):	1.5
Soil depth (cm):	5
Tillage depth (cm)*:	5
Organic carbon content (%):	1.5
Field capacity (Vol%):	29.2
Wilting point (Vol%):	6.4
Climatic conditions:	FOCUS Hamburg median conditions
Mean temperature (°C):	8.8
Annual Rainfall (mm):	701
Annual pot. Evapotranspiration (mm):	589

(* for calculation of background concentrations)

APPLICATION PATTERN USED IN THE CALCULATION

Number of Applications : 4

Day	Month	Rate (g/ha)	Interception(%)
01	05	500	0
10	05	750	25
01	06	600	50
01	07	1000	90

COMPOUNDS CONSIDERED IN THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Compound	Molecular mass(g/mol)	format_berichtion (%)
Testicide	250	
Metabolidan	200	100

DEGRADATION KINETICS PARAMETERS CONSIDERED FOR THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

Soil study: soil study 1

Kinetics for Testicide:	Single First order (SFO)
DT50 (d):	70
Rate constant (1/d):	0.0099
Q10-factor:	2.58

Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 2
Kinetics for Testicide:	First Order Multi Compartment (FOMC)
alpha(i_studie):	1
Beta:	1
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 3
Kinetics for Testicide:	Hockey Stick (HS)
DT50 (d):	7
DT50 (d):	70
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.0099
Parameter Tb (d):	5
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 4
Kinetics for Testicide:	Double First Order in Parallel (DFOP)
DT50 (d):	7
DT50 (d):	140
Rate constant 1 (1/d):	0.099
Rate constant 2 (1/d):	0.005
Parameter g:	0.5
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 1
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	35
Rate constant (1/d):	0.0099
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 2
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	350
Rate constant (1/d):	0.005
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 3
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	140
Rate constant (1/d):	0.001
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20
Soil study:	soil study 4
Kinetics for Metabolidan:	Single First order (SFO)
DT50 (d):	14
Rate constant (1/d):	0.0495
Q10-factor:	2.58
Walker-exponent:	0.7
Ref. temperature (°C):	20

RESULTS OF THE CALCULATION

Metabolism scheme: Active compound and a single metabolite

RESULTS FOR: Testicide

Calculations over one year

Maximum annual pore water concentration for Testicide over 1.5 cm
soil study 1(mg/L): 0.5608 occurring on day 31
soil study 2(mg/L): 0.5748 occurring on day 9
soil study 3(mg/L): 0.2759 occurring on day 31
soil study 4(mg/L): 0.3109 occurring on day 31

Calculated PECact* in soil over 1.5 cm for Testicide(mg/L)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.5589	0.4961	0.2723	0.3066
2.0000	0.5567	0.4537	0.2682	0.3017
4.0000	0.5517	0.4089	0.2595	0.2912
7.0000	0.5456	0.3080	0.2495	0.2794
14.0000	0.5220	0.1279	0.2295	0.2561
21.0000	0.5195	0.1046	0.2275	0.2445
28.0000	0.4807	0.1537	0.2133	0.2187
42.0000	0.5129	0.0886	0.2241	0.2236
50.0000	0.4988	0.0626	0.2180	0.2134
100.0000	0.4029	0.0314	0.1760	0.1734

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Testicide(mg/L)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.5599	0.5354	0.2741	0.3088
2.0000	0.5589	0.5051	0.2722	0.3065
4.0000	0.5566	0.4688	0.2693	0.3015
7.0000	0.5531	0.4268	0.2644	0.2943
14.0000	0.5425	0.3257	0.2506	0.2813
21.0000	0.5362	0.2936	0.2437	0.2719
28.0000	0.5274	0.2512	0.2383	0.2626
42.0000	0.5212	0.2266	0.2345	0.2562
50.0000	0.5186	0.2068	0.2324	0.2524
100.0000	0.4882	0.1344	0.2228	0.2320

Calculation of background concentrations after many years

Final background concentration in pore water for Testicide over 5 cm
soil study 1(mg/L): 0.3532 (estimated to occur after 10 years)
soil study 2(mg/L): 0.0026 (estimated to occur within 10 years)
soil study 3(mg/L): 0.1072 (estimated to occur within 10 years)
soil study 4(mg/L): 0.1919 (estimated to occur after 11 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in pore water for Testicide over 5 cm considering accumulation*
soil study 1(mg/L): 0.9141 occurring on day 31
soil study 2(mg/L): 0.5774 occurring on day 9
soil study 3(mg/L): 0.3831 occurring on day 31
soil study 4(mg/L): 0.5028 occurring on day 31
(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Testicide(mg/L) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.7561	0.2936	0.3784	0.4985
2.0000	0.9122	0.2450	0.3758	0.4936
4.0000	0.9100	0.1858	0.3720	0.4831
7.0000	0.9049	0.1485	0.3555	0.4713
14.0000	0.8988	0.1050	0.2934	0.4480
21.0000	0.8752	0.0914	0.2955	0.4364
28.0000	0.8727	0.0652	0.3592	0.4106
42.0000	0.8340	0.0638	0.3334	0.4155
50.0000	0.8661	0.0549	0.3205	0.4053
100.0000	0.8521	0.0294	0.2956	0.3653

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 5 cm for Testicide(mg/L) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	0.9131	0.5380	0.3813	0.5006
2.0000	0.9121	0.5078	0.3794	0.4983
4.0000	0.9098	0.4714	0.3765	0.4934
7.0000	0.9063	0.4294	0.3716	0.4862
14.0000	0.8958	0.3283	0.3578	0.4732
21.0000	0.8894	0.2963	0.3509	0.4638
28.0000	0.8807	0.2538	0.3455	0.4545
42.0000	0.8745	0.2292	0.3417	0.4481
50.0000	0.8718	0.2094	0.3396	0.4443
100.0000	0.8414	0.1371	0.3300	0.4239

(* a tillage depth of 5 cm was considered for calculating the background concentration)

RESULTS FOR: Metabolidan

Calculations over one year

Maximum annual pore water concentration for Metabolidan over 1.5 cm
soil study 1(mg/L): 1.2833 occurring on day 321
soil study 2(mg/L): 7.2742 occurring on day 66
soil study 3(mg/L): 1.6462 occurring on day 321
soil study 4(mg/L): 0.7749 occurring on day 66

Calculated PECact* in soil over 1.5 cm for Metabolidan(mg/L)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.2522	6.8370	1.6177	0.7734
2.0000	1.2820	5.4496	1.6438	0.7266
4.0000	1.2101	4.0863	1.5780	0.6310
7.0000	1.1045	4.0780	1.4788	0.5684
14.0000	0.8773	4.0514	1.2584	0.4552
21.0000	1.2210	4.0232	1.6273	0.3794
28.0000	1.0896	3.9833	1.4975	0.3030
42.0000	0.8129	5.9655	1.2418	0.2836
50.0000	1.0895	6.9442	1.5403	0.3199
100.0000	0.6800	6.7322	1.2523	0.1612

(* PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 1.5 cm for Metabolidan(mg/L)

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.2730	7.2586	1.6433	0.7742
2.0000	1.2730	7.1571	1.6427	0.7706
4.0000	1.2707	6.8677	1.6416	0.7536
7.0000	1.2425	6.7797	1.6195	0.7282
14.0000	1.2345	6.6780	1.6046	0.6944
21.0000	1.2313	6.6584	1.6026	0.6596
28.0000	1.2124	6.6586	1.5991	0.6274
42.0000	1.2033	6.6567	1.5947	0.5803
50.0000	1.1978	6.6564	1.5916	0.5559
100.0000	1.1811	6.5445	1.5729	0.4452

Calculation of background concentrations after many years

Final background concentration in pore water for Metabolidan over 5 cm
soil study 1(mg/L): 1.0048 (estimated to occur after 10 years)
soil study 2(mg/L): 27.5037 (estimated to occur after 13 years)
soil study 3(mg/L): 4.3420 (estimated to occur after 11 years)
soil study 4(mg/L): 0.1475 (estimated to occur after 11 years)

Calculations of concentrations considering accumulation after many years of application

Maximum annual concentration in pore water for Metabolidan over 5 cm considering accumulation*

soil study 1(mg/L):	2.2881 occurring on day 321
soil study 2(mg/L):	34.7779 occurring on day 66
soil study 3(mg/L):	5.9882 occurring on day 321
soil study 4(mg/L):	0.9224 occurring on day 66

(* a tillage depth of 5 cm was considered for calculating the background concentration)

Calculated PECact** in soil over 5 cm for Metabolidan(mg/L) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	1.8494	33.8106	5.6325	0.3679
2.0000	1.6430	34.0567	5.5207	0.3703
4.0000	1.5706	33.4097	5.3705	0.3646
7.0000	1.4752	32.5791	5.3682	0.3544
14.0000	1.4735	31.1796	5.3644	0.3232
21.0000	1.4724	33.9449	5.3596	0.3401
28.0000	1.4679	32.7289	5.3530	0.3313
42.0000	1.4618	31.1304	5.6076	0.2869
50.0000	1.6786	33.1272	5.7431	0.3088
100.0000	1.8579	31.3590	5.7590	0.2272

(* a tillage depth of 5 cm was considered for calculating the background concentration)
(** PECact values are related to the time after the maximum concentration)

Calculated time weighted average (TWA) concentrations in soil over 5 cm for Metabolidan(mg/L) considering accumulation*

Time (d)	soil study 1	soil study 2	soil study 3	soil study 4
1.0000	2.2779	34.7623	5.9853	0.9217
2.0000	2.2778	34.6608	5.9847	0.9181
4.0000	2.2755	34.3714	5.9836	0.9011
7.0000	2.2473	34.2834	5.9615	0.8757
14.0000	2.2393	34.1817	5.9467	0.8419
21.0000	2.2361	34.1621	5.9446	0.8071
28.0000	2.2172	34.1624	5.9411	0.7749
42.0000	2.2081	34.1604	5.9367	0.7278
50.0000	2.2026	34.1601	5.9337	0.7034
100.0000	2.1859	34.0482	5.9150	0.5927

(* a tillage depth of 5 cm was considered for calculating the background concentration)

GRAPHIC REPRESENTATION OF THE CALCULATION