

# User manual for Nordic PECsoil calculator

(Version 1.3 from April 2018)

## How to start?

Double-check the PC system settings as indicated on the starting page of the PECsoil-calculator. The decimal separator should be '.' and not ','. Otherwise, the PECsoil-calculator will not work properly. This can for instance be done by changing the language settings of your PC to "English". The tool works with MS Office 2013 and later versions. Please save a local copy on your computer before running the calculations.

To start the program, press the button "Initialize or Reset the Calculator". A tool window (given below) will open to enter the input data required for the PECsoil calculations.

## The main page

The screenshot shows the main interface of the Nordic PECsoil calculator. At the top, there is a menu bar with buttons: Calculate, Change input, Screenshot, Save Chemical, Save Chemical As, Delete Chemical, End, and Reset. Below this is a 'Parent' dropdown menu set to 'default'. The main area is divided into several sections:

- Applications:** A table with columns for Appl. No., rate (g/ha), interception (%), and interval/ days until following application. It contains two rows of data.
- Application Frequency:** Radio buttons for 'appl. every year', 'appl. every second year', and 'appl. every third year'.
- Temperature Scenario:** Radio buttons for 'constant temperature' and 'temperature scenario'. The 'temperature scenario' is selected, showing 'Finland (1979-1998)' and a date of '105 (Apr 15)'. There are also input fields for soil depth and soil density.
- Degradation kinetics:** Radio buttons for 'field data (non-norm.; no temp. correction)' and 'normalised lab or field data:'. The 'normalised lab or field data' is selected, with a 'reference temperature (°C)' of 20. There are also input fields for DT50 and DT50 (lab/field; norm.).
- Soil Temperature:** Radio buttons for 'Constant Soil Temperature' and 'Soil Temperature Scenario'. The 'Constant Soil Temperature' is selected, showing 'after last appl. max.' and 'TWA (21 days) TWA (7 days)'. The 'Soil Temperature Scenario' is also shown with similar options.
- PECmax (1st year) and PECacc (after 20 years):** Sections for calculating maximum and accumulated concentrations, with similar input fields and options for soil temperature scenarios.

There are also several 'Note' boxes providing guidance on consulting the Northern Zone Guidance Document and individual Member States for application intervals.

On this main page of the Nordic PECsoil calculator, all input values are given (i.e. information on the application rate, crop interception, DT50, molecular weight of the compound, etc). The output will be presented after running the calculations (press button "Calculate"). Additionally, the metabolites can be calculated and their results are presented, when clicking on the button "Metabolites". Further information on the underlying equations are presented on the sheet opening when clicking on the button "Info".

As the format of the main page may differ depending on operating system, individual PC system settings and screen sizes and numbers, bars for scrolling are introduced so that it will always be possible to see the whole PECsoil calculator.

## The different buttons

| Button           | Function   |
|------------------|--|
| Initialize       | This will open a new sheet ("main page") where you can enter the input data for the PECsoil calculations.  |
| Calculate        | This button starts the PECsoil calculation and provides PECmax (1 <sup>st</sup> year), PECacc (after 20 years), as well as graphical output. Press it, when all input data are correctly entered.  |
| Change input     | Use this button to enter new input data for additional PECsoil-calculations.   |
| Screenshot       | This button produces a screenshot of the Nordic PECsoil-calculator that can be pasted into the registration report submitted for Northern Zone registration.   |
| End              | This button closes the main page of the Nordic PECsoil-calculator with all input and output data. To close the entire PECsoil-calculator, close Excel as usual.  |
| Save Chemical    | Saves the current input data for the Parent substance that had been chosen from the list of parent substances saved.   |
| Save Chemical As | Saves the current input data under a new "parent substance name".  |
| Delete Chemical  | Deletes the chemical (parent substance), which is currently displayed from the list of saved substances.   |
| Reset            | This button only works while you are adding new input data. It will change the inputs back to the values that were listed when you pressed "change input" the last time, i.e. the data that were saved in an internal data base for the parent substance you are currently working with. |
| Parent           | Data sheet for input and output data (+ graphics) for the parent substance. [see further below, regarding DT50]  |
| Metabolites      | Data sheet for input and output data (+ graphics) for the metabolites [see further below, regarding DT50 and other input-parameters needed]  |
| Info             | Data sheet with background information and, where relevant, implemented equations on DT50, kinetics, metabolites and temperature curves.   |

## Which Input data should be used and how?

### *Applications*

Up to 10 applications can be simulated. For each application, the rate [g/ha], the crop interception [%] and, in case of multiple applications, the interval in [days] until the following application should be given. The crop interception values should follow the guidance as indicated in the Northern Zone Guidance Document relevant at the time of application. The effective soil application rate is then internally calculated. Please note that, if no interception shall be accounted for, the user should enter '0' [%] interception. If the field is empty, an error will occur. The date of the first application needs to be entered, when the variable temperature scenario is used (see below). If multiple applications are intended, the dates for the following applications are internally calculated by the model based on the users input of the interval/days until the following application.

The PECsoil-calculator is able to perform calculations for applications every year, every second year and every third year. Information on whether this might be used to refine the risk assessment for soil living organisms can be obtained from the relevant Northern Zone Guidance Document or from the different MS directly.

### *Constant or Variable Temperature Scenario – Temperature, Soil depth & Soil density*

The Nordic PECsoil-calculator can calculate PECsoil values based on a constant (average) temperature or based on variable temperature scenarios. For applications in the Northern Zone, only the use of the variable temperature scenario with the Finnish scenario for Jokioinen (Finland, 1979-1998), which is pre-implemented into the PECsoil calculator, is accepted.

#### *Temperature*

For the variable temperature scenario, different scenarios could in principle be implemented. However, for the Northern Zone, only the Finnish scenario for Jokioinen, which is pre-implemented into the PECsoil calculator, is accepted. The date of the first application need to be given as Julian Day Number. The program automatically generates the corresponding date of the year, which can be used as a control.

For the constant temperature scenario, the temperatures for a single season should be given (default in the Northern Zone: 10 °C). For the long-term plateau calculation, the average temperature over the whole year should be used for the baseline year 1-19 (default in the Northern Zone: 6 °C), while for the last year an average temperature for the growing season can be used (same as for single season; default in Northern Zone: 10 °C). Additionally, the soil depth [in cm], for which the PECsoil calculation should be performed needs to be provided, as described below.

#### *Soil depth*

The soil depth [in cm], for which the PECsoil calculation should be performed need to be given for single season, baseline plateau and last year plateau. Single season only needs to be given separately for the constant temperature; in the case of the variable temperature scenario, for the PECmax (1<sup>st</sup> year) calculation, the same depth is used as given for the last year in the plateau calculation. In both cases, the soil depth for the single season and the last year (plateau) should be identical. In the Northern Zone, the default is 5 cm soil depth. This should be used for single season, baseline and last year plateau.

*Refinement option:* If required and justified by common tillage practice in the crop concerned, a depth of 20 cm can be used as refinement option for PECacc. In this case, the depth of for the baseline calculation should be set to 20cm, whereas the depth for the last year still needs to be set to the default soil depth of 5 cm.

Please note that PECsoil is calculated and shown for both scenarios (constant and variable temperature). As the user only enters the soil depth for one of them, the display might show different depths for the two scenarios. Nevertheless, internally the same depth is used for the calculations. This allows a proper graphical comparison.

#### *Soil (bulk) density*

The default soil bulk density is 1.5 g/cm<sup>3</sup>.

#### *Application Date*

The date of the first application should be given in Julian Day Numbers (also called 'day of year'). Choose a date appropriate for PECsoil calculations of the intended use. The date as 'Month Day' is automatically filled in. This input is only relevant for the variable temperature scenario.

For parent substance:

*Molecular weight*

The molecular weight should be given in g/mol. This is only needed for the calculation of PECsoil for metabolites.

*DT50*

The user might choose between using non-normalised field DT50 or normalised lab-or field DT50s. The corresponding box for the DT50 values needs to be filled in (see figures below). Otherwise, a warning message will be displayed. When field degradation data are used, this need to be DegT50-values. Please refer to the Northern Zone Guidance Document for further information on the requirements for the DT50s.

Both SFO kinetics and DFOP kinetics can be used, depending on the best-fit kinetics for the worst-case DT50 used for PECsoil calculations. FOMC kinetics are not implemented, as no temperature correction can be applied, and it is neither recommended for multiple applications nor for plateau calculations. If the worst-case DT50 is derived with FOMC kinetics, the user should calculate the pseudo-SFO DT50 by FOMC (DT90)/3.32 and enter the DT50 into the SFO-box.

Degradation kinetics; worst-case DT50:

field data (non-norm.; no temp. correction)

normalised lab or field data:  
reference temperature (°C)

SFO

DT50 (field; non-norm.)

DT50 (lab/field; norm.)

DFOP

k1

k2

g

Figure 1. The intention is to use non-normalised field degradation data derived with SFO kinetics. The DT50 (field; non-normalised) should, therefore, be filled in; as visualized in this figure.

Degradation kinetics; worst-case DT50:

field data (non-norm.; no temp. correction)

normalised lab or field data:  
reference temperature (°C)

SFO

DT50 (field; non-norm.)

DT50 (lab/field; norm.)

DFOP

k1

k2

g

Figure 2. The intention is to use normalised lab (or normalised field data), which were derived with SFO kinetics. The “reference temperature” is the temperature to which the data were normalised. In that case, enter the normalised DT50 into the box “DT50 (lab/field; normalised)”. Alternatively, the temperature at which the study was performed can be entered. In that case the originally derived DT50 (before the temperature normalisation) should be entered.

If field-data (non-normalised) are being used, no temperature correction will be performed when calculating the PECsoil for one season and for the 20 year period. Thus, there is no difference in the calculated PECsoil-values obtained for the constant temperature or the variable temperature scenario.

If **DFOP kinetics** were found to give the worst-case DT50 for the PECsoil calculation, the user need to make sure that the entered degradation rate coefficients and reference temperature correspond to each other. For instance, if DFOP kinetics is selected with **lab-data**, the reference temperature should normally be the study temperature. This is because it is usually the pseudo-SFO DT50 derived from

slow-phase rate constant that is normalised to the standard reference temperature of 20 °C and not the degradation rate coefficients k1 and k2. However, kinetic fitting of **field data** is usually performed after a time-step normalisation. This suggests that the derived degradation rate coefficients k1 and k2 shall be used together with the reference temperature of 20 °C.

If, however, a **pseudo SFO-DT50** derived from slow-phase rate constant (DFOP) shall be used, this should be given in the SFO-entry box.

For metabolites:

The metabolites are simulated as if they were applied as parent compound with an application rate of

$$ApplRate (met) = ApplRate (par) * \frac{max. obs. [\%]}{100} * \frac{MW_{met}}{MW_{par}}$$

With

|                |   |
|----------------|---|
| ApplRate (met) | application rate for the metabolite in g/ha   |
| ApplRate (par) | application rate for the parent substance in g/ha, corrected for crop interception. |
| max. obs [%]   | maximum quantity of the metabolite observed in a soil degradation study, in %       |
| MW             | molecular weight in g/mol   |

This calculation is performed internally, the user only needs to provide the input data as listed and described below:

*No of (major) soil metabolites*

Give the number of major soil metabolites, as listed in the definition of residues for the soil compartment in the LoEP of the active substance. Up to 10 different metabolites can be handled simultaneously. The input and output will be displayed (and changed) on different data sheets.

*Metabolite name*

*Enter the name of the metabolite there.*

*Molecular weight*

Should be given in g/mol. Used in the equation presented above.

*Max. obs.*

The maximum quantity of the metabolite observed in a soil degradation study. It should be given in %.

*DT50*

Only SFO kinetics have been implemented for metabolites. Choose between DT50 field (non-normalised), for which temperature correction is not considered, or lab-DT50. The “reference temperature” is the temperature the lab-DT50 was normalised to or at which the study was performed. Make sure that “reference temperature” and DT50 correspond to each other. If normalised field DT50 can be used for the PEC-calculations, these DegT50s should be entered as “lab-DT50”.

## Definitions of the different PECsoil-values that will be calculated

This information is taken from the Northern Zone Guidance Document (v.5.0; April 2016).

|                               |  |
|-------------------------------|--|
| PECmax (1 <sup>st</sup> year) | maximum PECsoil in the first season taking into account all applications. This corresponds to PECini in the Finnish PECsoil calculator.  |
| PECacc (after 20 years)       | highest concentration during a period of 20 years including all applications from the last year  |
| PECplateau                    | PECacc – PECmax. This implies that PECmax corresponds to the contribution of the PECsoil-value from the last year.   |
| PEC <sub>TWA</sub>            | time-weighted average PECsoil. This can be calculated either based on PECmax (1 <sup>st</sup> year) or PECacc (after 20 years). According to the Northern Zone Guidance Document (v.5.0; April 2016), PEC <sub>21d-TWA</sub> should be reported. This is therefore set as default in the Nordic PECsoil-calculator. Other PEC <sub>TWA</sub> might be relevant for some MS and can be calculated (grey numbers). |

The Nordic PECsoil calculator provides PECsoil-values “after last application” and the maximum (“max.”) during the respective time periods (single season, 20 years). Often, the PEC after last application will be identical to the maximum PEC. However, dependent on the DT50, the time interval between applications and the crop cover, there might be a situation where the PEC between applications is higher than after the last application. Both values are reported in order to avoid missing this special situation. The maximum PEC shall be reported in the registration report and shall be used for the ecotoxicological risk assessment.

### Save & Delete Substances

Parameterised substances can be easily saved by clicking on “Save Chemical” or “Save Chemical As”, respectively. When clicking “Save Chemical As”, a new chemical will be added to save the input parameters. Technically, the information is written into the data-sheet “Input Parameter”. On the main page of the PECsoil calculator, the user can choose between the different data sets saved from the drop-down-list for parent substances, and the program will read the information listed in the “Input Parameter” data sheet.

To delete previously saved substances, the button “Delete Chemical” can be used. Only the chemical that is currently displayed is deleted from the data-sheet “Input Parameter”. In order to remove the substance from the drop-down-list, the main page needs to be closed (e.g. by using the button “end”) and re-initialized (press “Initialize or Reset the Calculator”)

### Implementation of the PECsoil-calculations

In accordance with FOCUS degradation kinetics guidance (e.g. FOCUS, 2011; p. 366), the degradation is set to zero, if the soil temperature is below 0 °C, independent of whether the DT50 is determined in the field or in the laboratory. This is both implemented for the constant temperature scenario and the variable temperature scenario.

## Temperature correction & Degradation kinetics

### Non-normalised field data:

No temperature correction is performed. The DT50 is used as provided in the main-page interface.

### Normalised lab or field data:

The Arrhenius equation was implemented for temperature correction of degradation rates. The degradation rate is corrected for temperature as follows:

$$k(T) = k(T_{ref}) * \exp\left(\frac{-E_A}{R} * \left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right)$$

With

|                  |   |
|------------------|---|
| k                | degradation rate constant [d <sup>-1</sup> ]  |
| E <sub>A</sub>   | molar activation energy; 65400 J/mol  |
| R                | gas constant; 8.314 J/mol/K   |
| T                | soil temperature [K]<br>The temperature is constant in the case of the “constant temperature scenario” and variable in the “variable temperature scenario” following the temperature curve for Jokioinen. |
| T <sub>ref</sub> | Reference temperature [K], provided as input to the calculator.<br>The reference temperature is usually 20°C, if the DT50 provided is the DT50 normalised to 20 °C.                                       |

The Arrhenius equation was used instead of the Q10 since it is more accurate. The Q10-approach is a simplification of the Arrhenius equation and works well for temperatures around 20°C. At the lower Nordic temperatures the deviations are, however, rather large.

The temperature-corrected degradation rate constant, i.e. k(T) as presented above, is then calculated for each time step t and included in the degradation kinetics calculated for either only a single season or the plateau/accumulation calculation over 20 years.

### SFO degradation kinetics

$$M(t) = M_0 * \exp(-k(T_t) * t)$$

With

|                    |   |
|--------------------|---|
| t                  | time [d]  |
| M(t)               | Total amount of chemical [g/ha] present at time t                                     |
| M <sub>0</sub>     | Total amount of chemical [g/ha] present at time t=0                                   |
| k(T <sub>t</sub> ) | degradation rate constant [d <sup>-1</sup> ] at soil temperature T [K] and time t [d] |

### DFOP degradation kinetics

The soil is sub-divided into two compartments; one describing the fast and one describing the slow degradation phase. In each compartment, degradation follows SFO-kinetics. The fraction of applied pesticide ascribed to the fast and the slow degradation compartment, respectively, is defined by the parameter  $g$ .

$$M(t) = M_0 * (g * \exp(-k_1(T_t) * t) + (1 - g) * \exp(-k_2(T_t) * t))$$

With

|            |  |
|------------|--|
| $t$        | time [d]   |
| $M(t)$     | Total amount of chemical [g/ha] present at time $t$  |
| $M_0$      | Total amount of chemical [g/ha] present at time $t=0$  |
| $g$        | fraction of $M_0$ applied to compartment 1   |
| $k_1(T_t)$ | degradation rate constant [ $d^{-1}$ ] at soil temperature $T$ [K] and time $t$ [d] in compartment 1 (often corresponding to the fast-degradation phase) |
| $k_2(T_t)$ | degradation rate constant [ $d^{-1}$ ] at soil temperature $T$ [K] and time $t$ [d] in compartment 2 (often corresponding to the slow-degradation phase) |

Further explanations and a visual description regarding degradation kinetics is provided on the “main page” of the Nordic PECsoil calculator in the data sheet “Info” under “Kinetic”.

### FOMC degradation kinetics – use pseudo-SFO instead!

FOMC is not implemented (see above). Therefore, a pseudo-SFO approach needs to be used instead of FOMC. This means that DT50 should be calculated as DT90 (FOMC)/3.32 in accordance with common practice for deriving modelling endpoints.

### **Copying into the dRR**

In order to simply copy and paste the relevant information into the dRR, the button “Screenshot” was created. Upon pressing, a screenshot of the currently visible main window of the PECsoil calculator will be pasted into a word-document and saved in the same working directory as that of the PECsoil-calculator. The name of the word-file contains the name of the selected chemical substance as given in the PECsoil calculator window.