Version: 2.0
Date: April 11th, 2011

# PELMO - Parameterisation for the FOCUS Groundwater Scenarios

## About this document

The report on which this document is based is that of the FOCUS Groundwater Scenarios workgroup, which is an official guidance document in the context of 91/414/EEC [full citation is 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]. This document does not replace the official FOCUS report. However, a need was identified to maintain the parameterisation of the models for the FOCUS groundwater scenarios in an up-to-date version controlled document, as changes become necessary. That is the purpose of this document.

# Summary of changes made since the official FOCUS Groundwater Scenarios Report (SANCO/321/2000 rev.2).

## *New in Version 1.0*

Compared to the original report changes has been made in

- Figure C.4 Running PELMO simulations using WPELMO.EXE
- Parameterisation description, section on “soil scenario files”
- Parameterisation description, section on “substance files”

The changes were necessary to keep the parameterisation document up-to-date with the current model version.

The only other changes in this version compared with the original report are editorial ones.

## *New in Version 2.0*

Compared to the original report and version 1 extensive changes have been made to fulfil the requirements of FOCUS (2009): “Assessing Potential for Movement of Active Substances and their Metabolites to Ground Water in the EU” Report of the FOCUS Ground Water Work Group, EC Document Reference Sanco/13144/2010 version 1, 604 pp.
That includes

- new shell description
- new scenario parameterisation
- new input file description

# 1. Summary

This manual describes version 4.0 of the computer program PELMO which stands for "Pesticide Leaching Model". Previous versions have been developed and described by Klein (1995) and Jene (1998). PELMO is based originally on the PRZM 1 model of US-EPA (Carsel 1984), but it was independently developed since 1989.
PELMO estimates the vertical transport of pesticides in the unsaturated soil system within and below the plant root zone. The equations which describe transport and transformation of pesticides in PELMO have been selected on the basis of the test studies that are available for these substances. For example, all input data on sorption and degradation of pesticides required for PELMO simulations are readily available because they are requested by the authorities within the registration procedure and published in registration reports. It is recommended to use only (these) parameter sets and parameterisation procedures as agreed with regulatory authorities, when simulations are performed to realistically assess the leaching potential of substances used in current agricultural practice. Information on the validation status of prior PELMO versions with lysimeter studies and groundwater monitoring are available e.g. from Hardy et al 2008, Jene et al. 1998, Jene et al. 1999, Klein et al. 1997, Trevisan et al. 2003.
PELMO considers various environmentally relevant processes (run-off, erosion, plant uptake, sorption, leaching, degradation in soil and on plants, and volatilisation of pesticides). However, the model has been mainly used to estimate the leaching potential in the regulatory context mentioned above (described in more detail at e.g. FOCUS 2000, 2002, 2009, Michalski et al. 2004, website of Federal Office for Consumer Protection BVL[1]).

[1] http://www.bvl.bund.de/DE/04_Pflanzenschutzmittel/03_Antragsteller/04_Zulassungsverfahren/07_Naturhaushalt/psm_naturhaush_node.html

**Table 1.1 Summary of the processes in PELMO**

| Process | Approach |
|---|---|
| water movement | capacity-based water flow (tipping bucket approach) using a daily time step for all hydrological processes<br>A two-parameter linear response model with a threshold to simulate macro pore flow (not parameterised for FOCUS simulations) |
| substance movement | convection dispersion equation |
| crop simulation | changing root zone during growing season, changing foliage (areal extent) during growing season, crop interception of water*, crop interception of substances*, foliar washoff*, foliar degradation* |
| degradation in soil | first order degradation rate, correction of rate constant with depth, soil moisture and soil temperatures |
| substance sorption to soil | Kd, Koc, Freundlich equation for equilibrium sorption<br>kinetic sorption following the Streck approach (which is equivalent to the realisation in FOCUS PEARL ) to describe increase of sorption with time |
| substance volatilisation (from soil) | simple model using Fick's and Henry's law |
| substance fate on plant surfaces | volatilisation from leaves*, penetration into leaves*, wash-off* and photo-transformation* |
| runoff* | Soil Conservation Service curve number technique |
| preferential flow* | simple threshold model assuming perfect mixing with the resident water in a shallow surface layer of soil* |
| soil erosion* | Modified Universal Soil Loss Equation |
| soil temperature | an empirical model that uses air temperatures |
| plant uptake | simple model based on soil concentrations and a plant uptake factor |
| substance applications | applications may be foliar sprays, applied to the soil surface, or incorporated into the soil; for soil incorporated applications a variety of soil distributions can be specified |
| metabolism | a sophisticated scheme with up to 8 metabolites (A -> B as well as A -> B -> C) may be simulated simultaneously with the parent |

* = turned off for the FOCUS scenarios

# 2. Description of the PELMO shell

## 2.1. Introduction

The PELMO version that was used for the implementation of the FOCUS-scenarios was developed in 2009 (PELMO 4). It was necessary to change the format of the scenario and pesticide data files and the handling of leap years slightly because of the needs of the FOCUS-scenarios.
Also the shell had to be changed to fulfil the requirements of FOCUS (2009).

PELMO.EXE runs under Microsoft DOS. However, to make editing and creating of PELMO input files easier in a Microsoft Windows environment, a shell called WPELMO.EXE was built around PELMO.EXE.

## 2.2. File handling

The information necessary to run PELMO.EXE is divided in a number of input data files. The shell WPELMO.EXE allows creating or editing of these files by the user. For each simulation a single substance data file (extension: PSM), a single scenario data file (extension: SZE) and a number of climate data files (extension: CLI) are necessary. For FOCUS-tier 1 -simulations only the substance data file has to be created by the user himself; the scenario and climate data files are already defined and should not be modified.

Before the user starts a PELMO simulation the scenario (location and crop, possibly irrigation) and the substance data file has to be set. The required scenario and climate input data files (*.cli and *.sze) are automatically selected by the shell and written into a small ASCII file called PELMO.INP. This file will be read by the simulation program PELMO.EXE (see Figure C.1).

The file HAUDE.DAT contains the monthly Haude-factors. This information is not used for FOCUS-simulations. However, the file must be in the FOCUS-directory of PELMO.

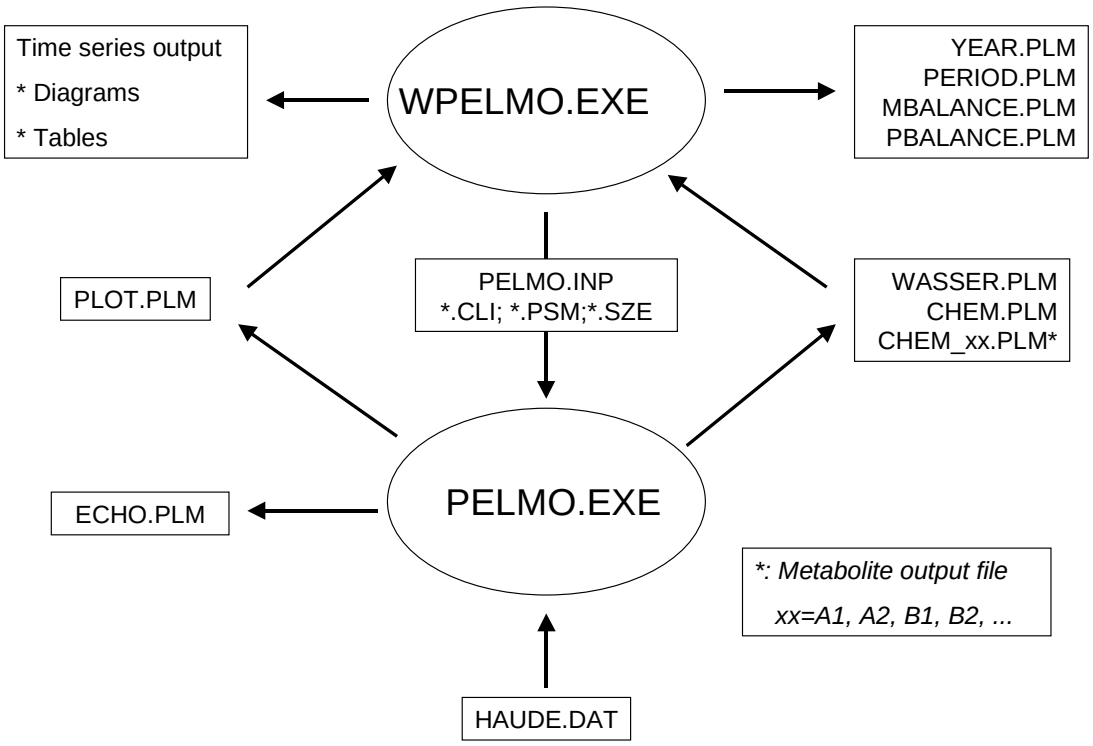


**Figure 1: File handling between the simulation program PELMO.EXE and the shell WPELMO.EXE**

Before the user starts a PELMO simulation the scenario (location and crop, possibly irrigation) and the pesticide data file has to be set. The required scenario and climate input data files (*.cli and *.sze) are automatically selected by the shell and written into a small ASCII file called PELMO.INP. This file will be read by the simulation program PELMO.EXE (see the figure).
The file HAUDE.DAT contains the monthly Haude-factors. This information is not used for FOCUS-simulations. However, the file must be present in the FOCUS-directory of PELMO.

During the simulation PELMO.EXE creates a number of output files:

- ECHO.PLM: echo of all input parameters of the specific simulation
- WASSER.PLM: hydrologic output data (tables)
- CHEM.PLM: pesticide output data (tables)
- CHEM_xx: metabolite output data (tables), xx=A1, A2, B1, B2, ...
- PLOT.PLM: time series output file, used by WPELMO.EXE to create diagrams
- IRR.PLM: time series of daily irrigation. This file was used for internal testing only. The first three column refer to the date (day, month, year), the last column gives the irrigation amount (cm/day)

When a PELMO simulation successfully terminates the annual average concentrations at 1 m depth and at the soil bottom are calculated by WPELMO.EXE based on the results written inti WASSER.PLM (hydrology output), CHEM.PLM (pesticide output) and CHEM_xx (metabolite output). WPELMO also creates the files MBALANCE.PLM and PBALANCE.PLM which contain the total annual mass balances for water (MPBALANCE.PLM) and for the pesticide/metabolites (PBALANCE.PLM).

## 2.3. Creating substance data files for PELMO simulations

After WPELMO has been loaded the form shown in Figure 2 is shown.

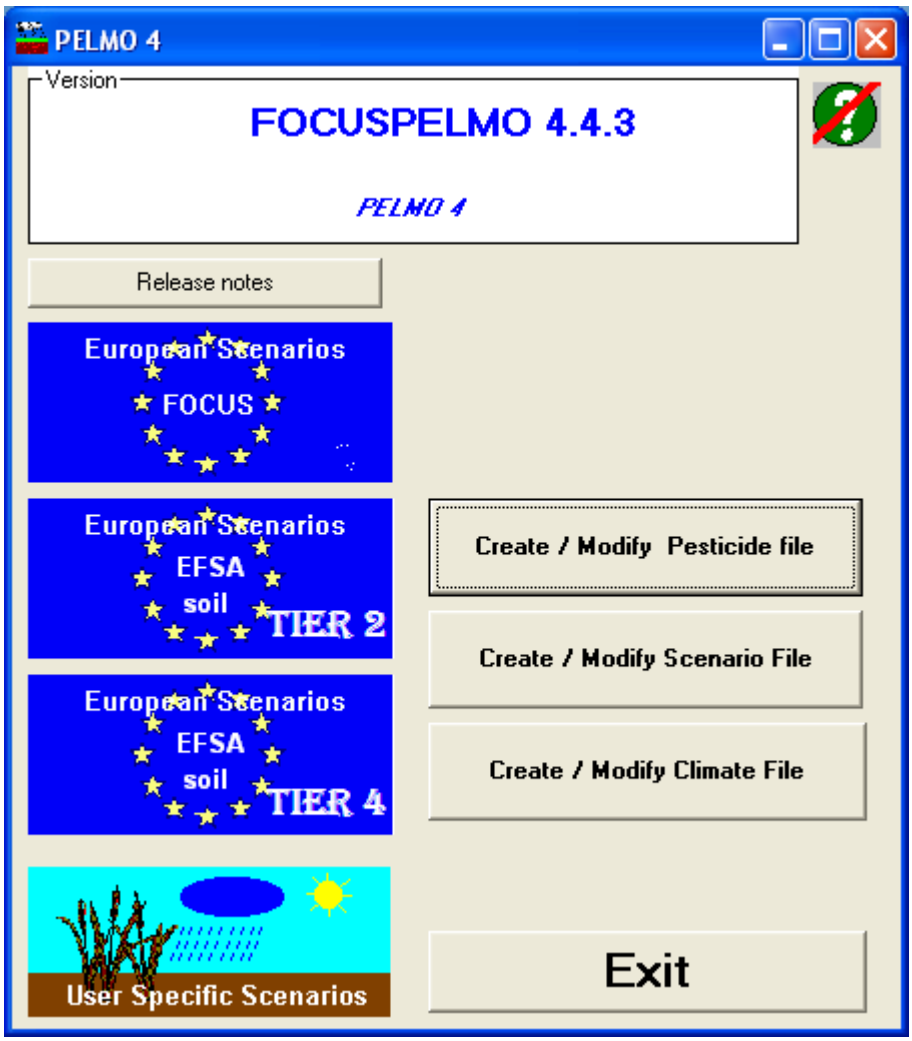


**Figure 2: PELMO 4: Intro screen**

The form objects on the left hand side are used to select input files for simulations the objects on the right hand side can be used to create or modify input files.
When clicking at one of the three blue boxes simulations can be performed considering the FOCUS groundwater or EFSA soil scenarios. These simulations scenarios will be automatically performed according to the respective recommendations. However, as long as the EFSA soil scenarios are not officially released the two EFSA boxes remain disabled.
The forth box can be used to perform individual simulations without the restrictions associated with the predefined scenarios.

To create pesticide data files for PELMO using WPELMO the user has to follow two steps. First the metabolism scheme has to be defined (Figure 3).

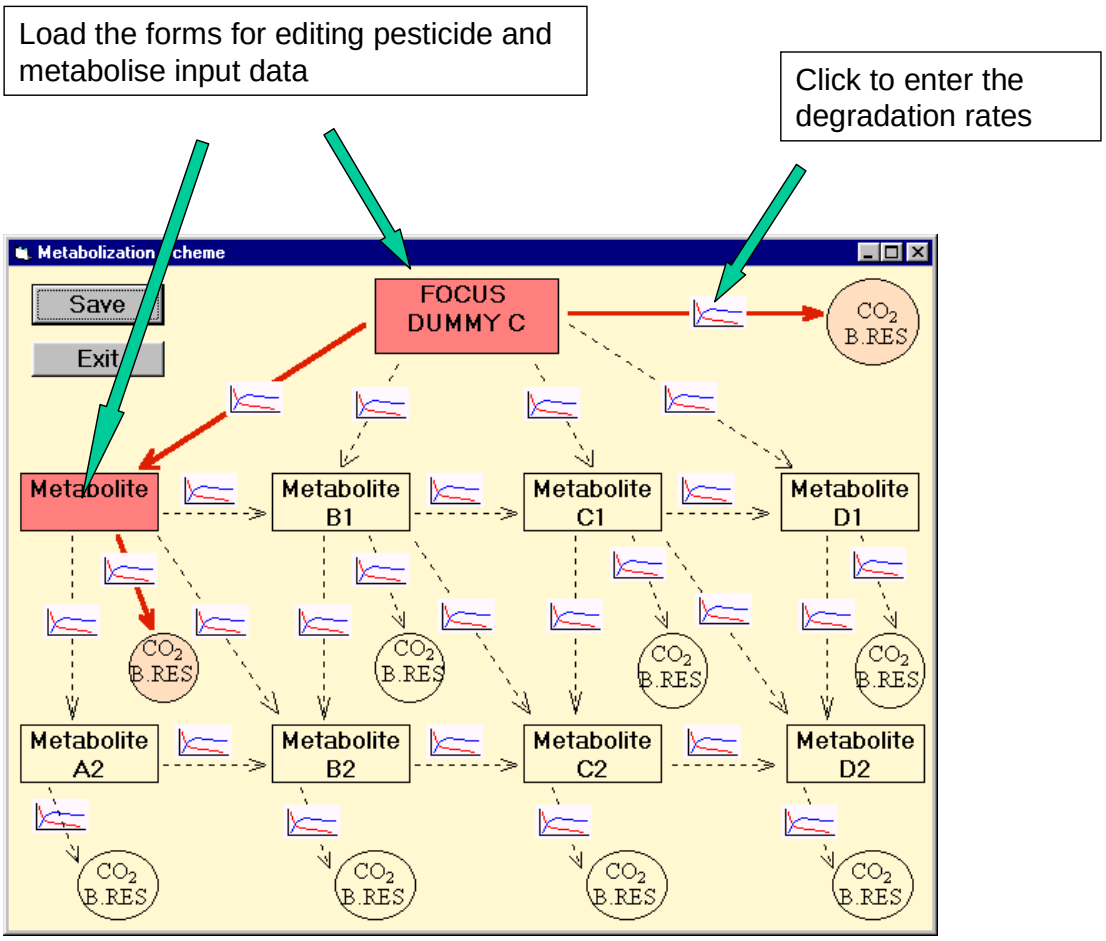


**Figure 3: PELMO 4: metabolism scheme**

The metabolism scheme shows 9 boxes which represent the parent compound together with 8 transformation products. The boxes can be activated after defining a transformation rate by clicking at the diagrams attached to the dotted arrows (see Figure 4).

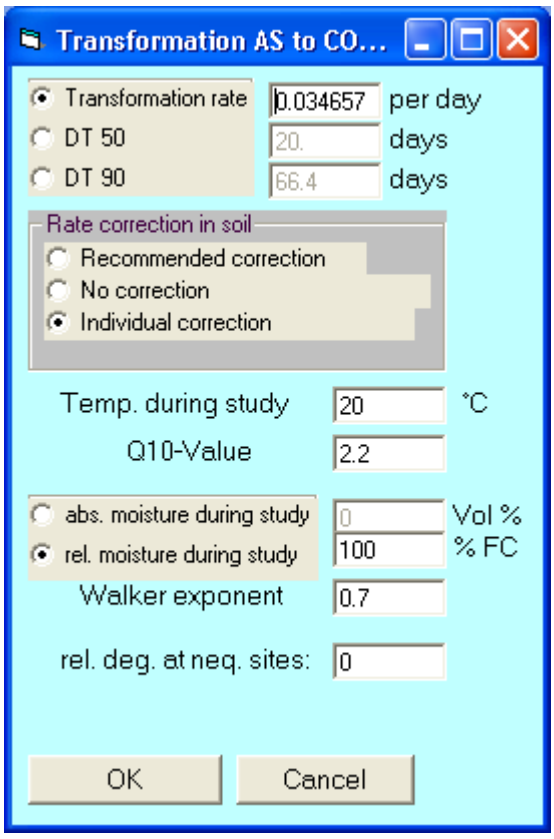


**Figure 4: PELMO 4: Editing transformation rates**

PELMO always considers SFO kinetics which means that the transformation rate can be expressed also by DT50 or DT90 values. If one of the first three fields is modified, the remaining two will be automatically updated. For the temperature and soil moisture correction PELMO offers a "recommended" parameter setting which is suggested by FOCUS (2000) and FOCUS(2009):

- moisture: transformation rate related to field capacity, Walker exponent: 0.7
- temperature: Q10 – factor: 2.58 related to 20 °C.
- relative degradation at non-equilibrium sites set to 0

If a transformation rate other than zero has been entered and the form closed, the black dotted arrow on the metabolism scheme turns into a bold red arrow and the respective red box turns into red.
If a certain transformation pathway should be switched off the respective transformation rate has to be set to "0".
In the second step substance specific input data should be entered for each activated box.

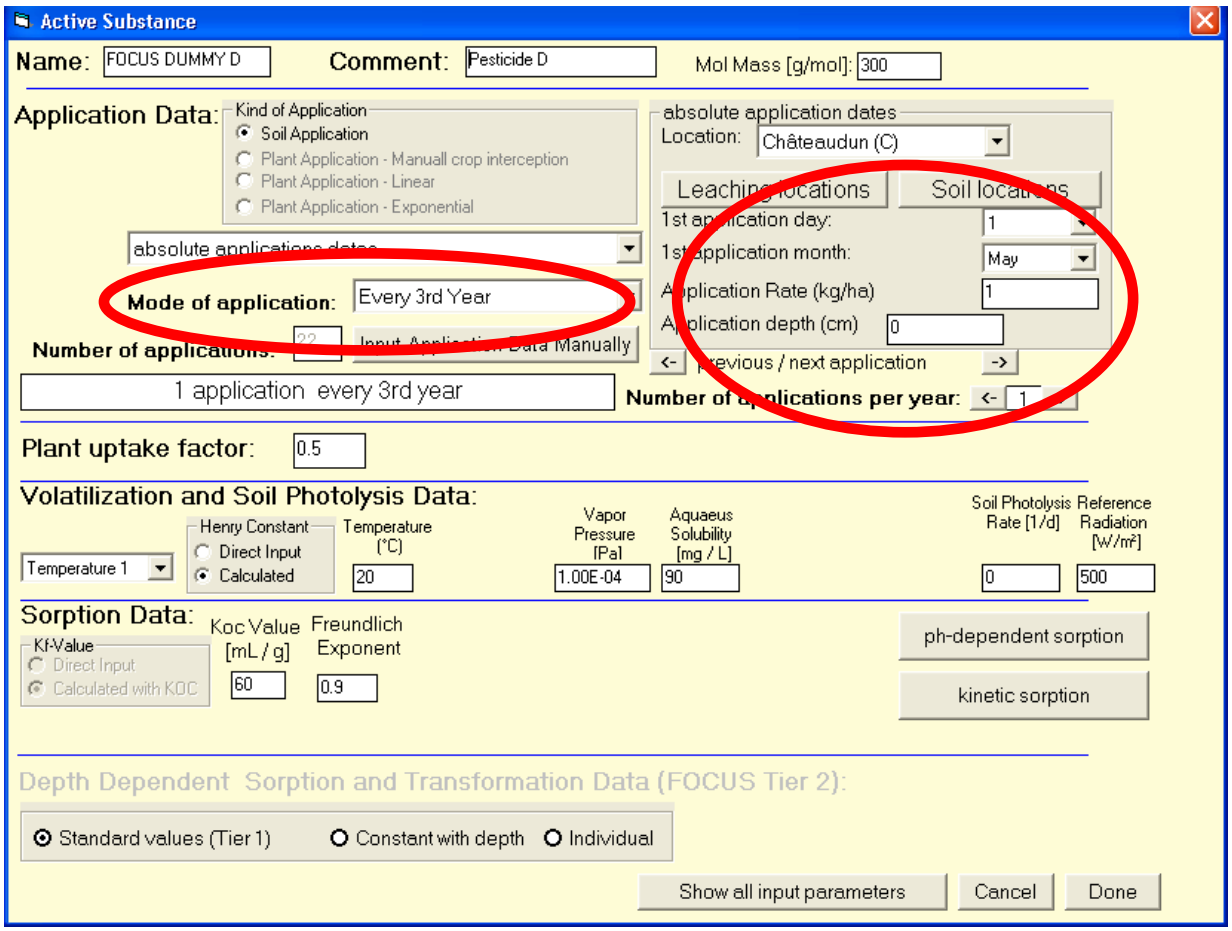


**Figure 5: PELMO 4: Editing pesticide input data (absolute application pattern)**

The form shown in Figure 5 is loaded when after a click at the box for the active compound. For the application mode the user can decide between absolute applications (application dates related to a certain location independent on the crop) or relative applications (application dates related to a certain crop independent on the location).
For absolute application patterns the location must be selected first followed by additional information on the application pattern (application date, rate and depth). For each location a different number of applications within a year can be defined. If more than one application per year is to be simulated the total number of application per year must be entered first. Afterwards a certain application within the sequence can be reached by clicking at the arrows “previous/next application”.

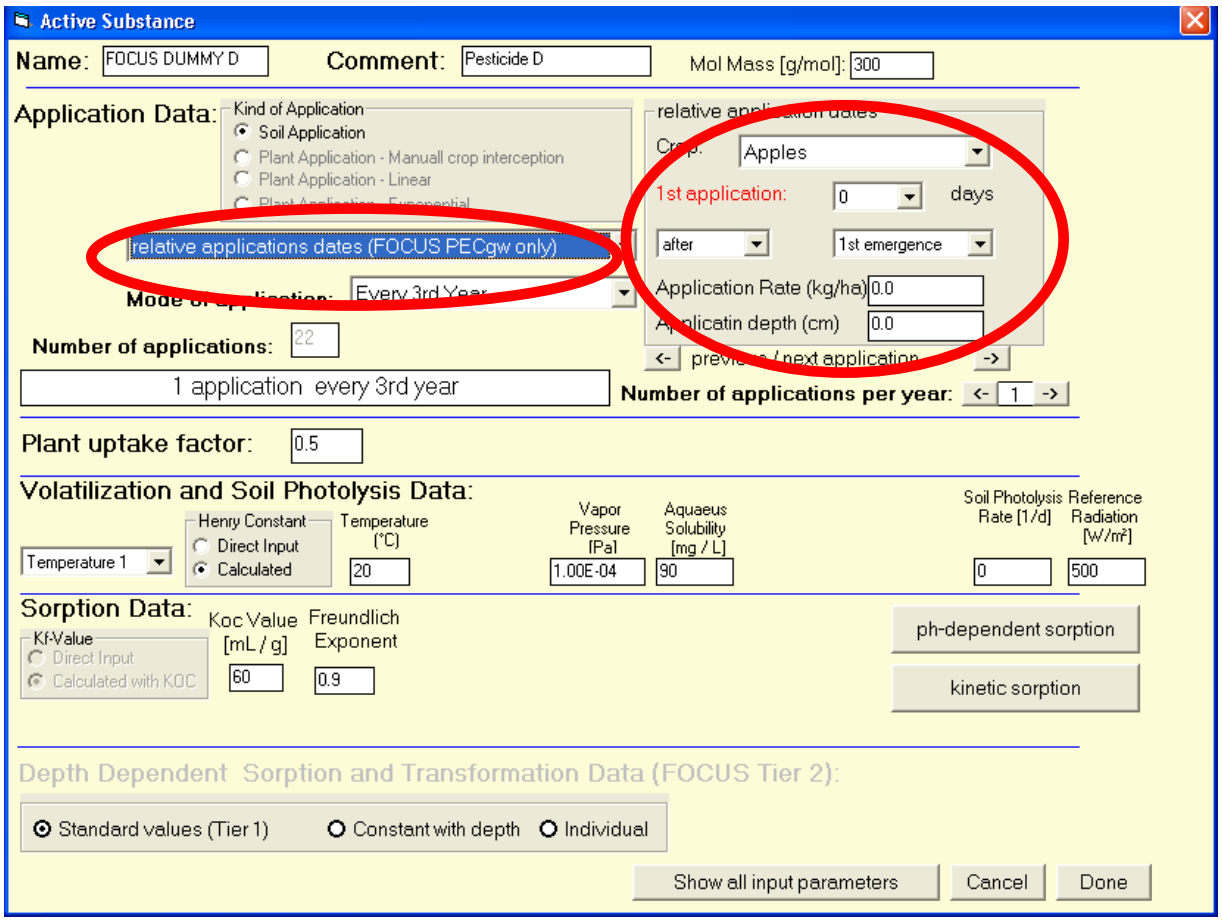


**Figure 6: PELMO 4: Editing pesticide input data (relative application pattern)**

For relative application patterns (Figure 6) the crop must be selected first followed by the information on the application pattern as described before. However, the application dates are entered relatively to crop development stages. The crop development stages in the database are based on the FOCUS scheme (FOCUS 2009). If a specific crop is planted more than one time per year (e.g. carrots) the application dates are always related to the first cropping period.

According to the FOCUS recommendations regular applications can be applied annually, biennially, or triennially.

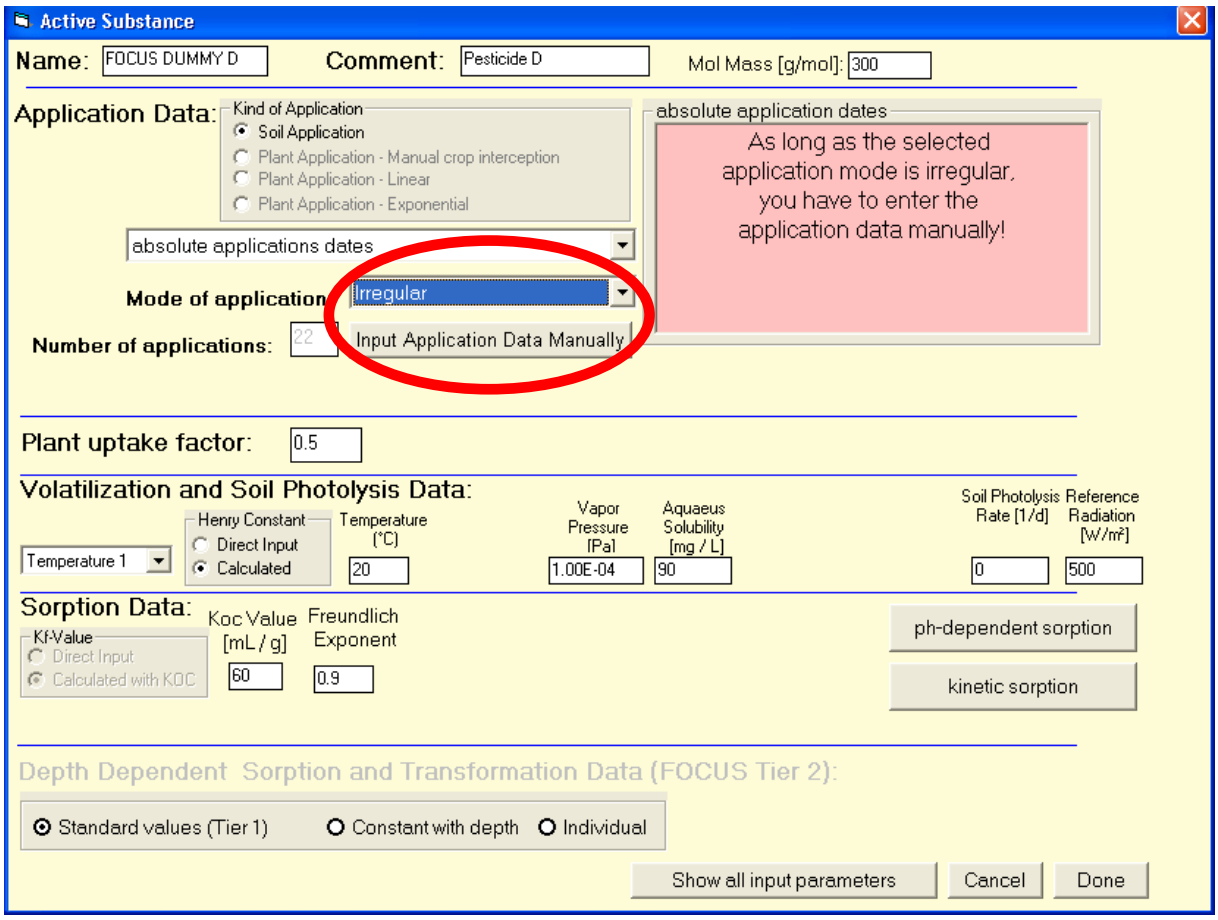


**Figure 7: PELMO 4: Editing pesticide input data (irregular application pattern)**

If pesticides are applied irregularly (what means that the pattern changes in a different way than described earlier) the application dates must be entered in a specific table which can be called when clicking at the button “Input Application Data Manually”.

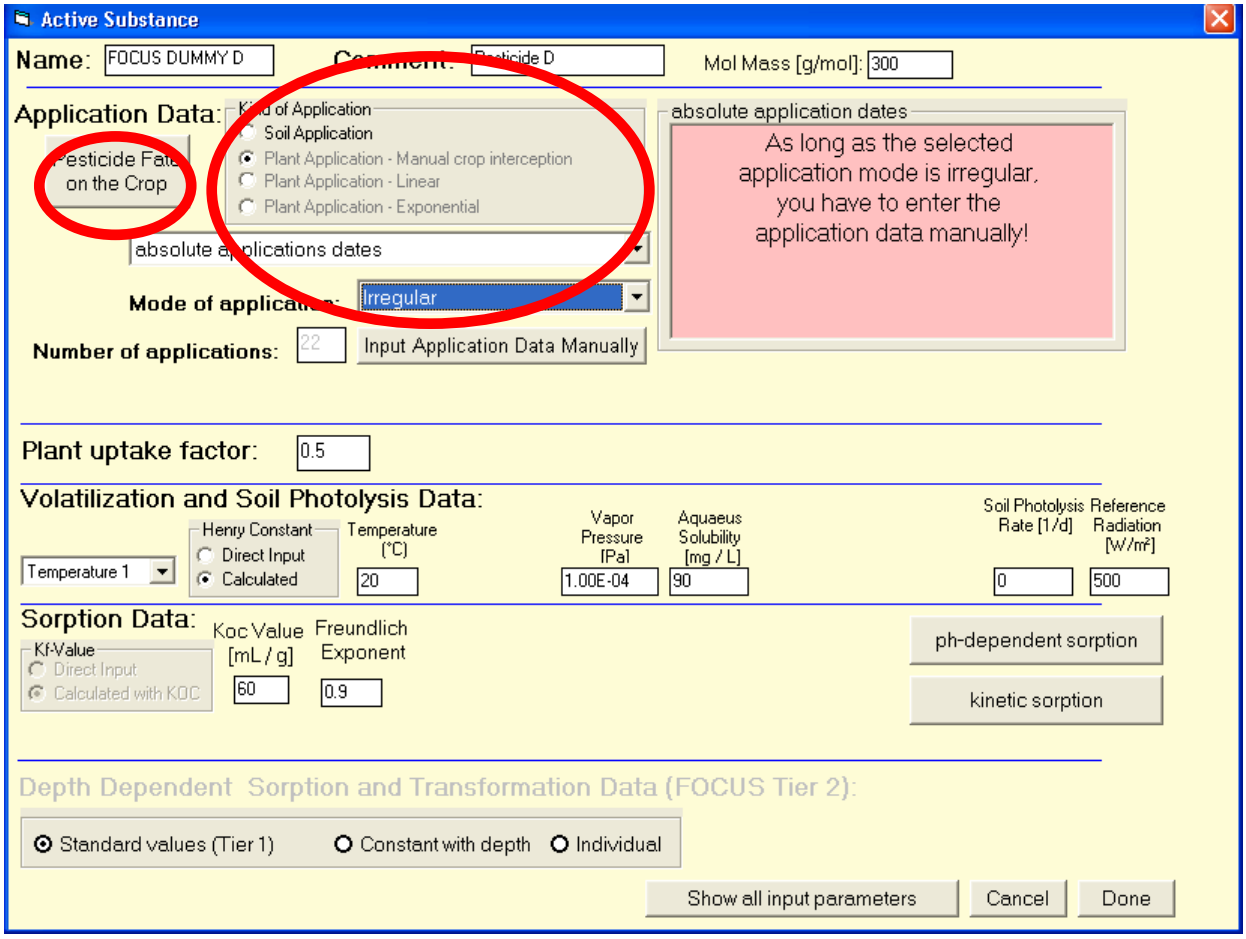

Figure 8: PELMO 4: Editing pesticide input data (Soil or plant application)

PELMO distinguishes between four different kinds of application

- soil application (which is the default for FOCUS groundwater simulations)
- plant application – manual crop interception
- plant application - linear model
- plant application - exponential model

“plant application – manual crop interception” is a new option which allows the definition of a percentile of the rate which remains on the crop but maybe reaches the soil later due to wash-off induced by rainfall and irrigation. The other two options define the crop interception automatically according to the actual development of the crop. The pesticide fate on plant surfaces can be described in a new form which is loaded after clicking at the button “pesticide fate on the crop” (see Figure 7).

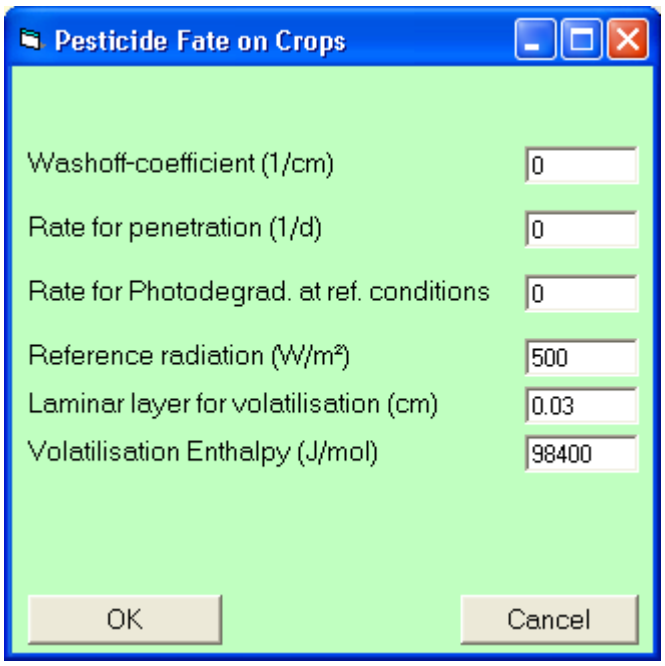

Figure 9: PELMO 4: Pesticide fate on the crop surface

Four different processes (wash-off from plants, penetration into plants, volatilisation from plants, photo-degradation on plants) can be simulated if the necessary input parameters are entered. If a certain process should be switched off, the respective rate constant has to be set to “0”.

PELMO considers the uptake of pesticides by plant roots (see Figure 10). The recommended value for systemic compounds is “0.5” which means that the pesticide concentration taken up by the plant root is 50 % of the soil water concentration in the respective soil layer.
If the parameter is set to “0” pesticide uptake by plant roots will be switched off.

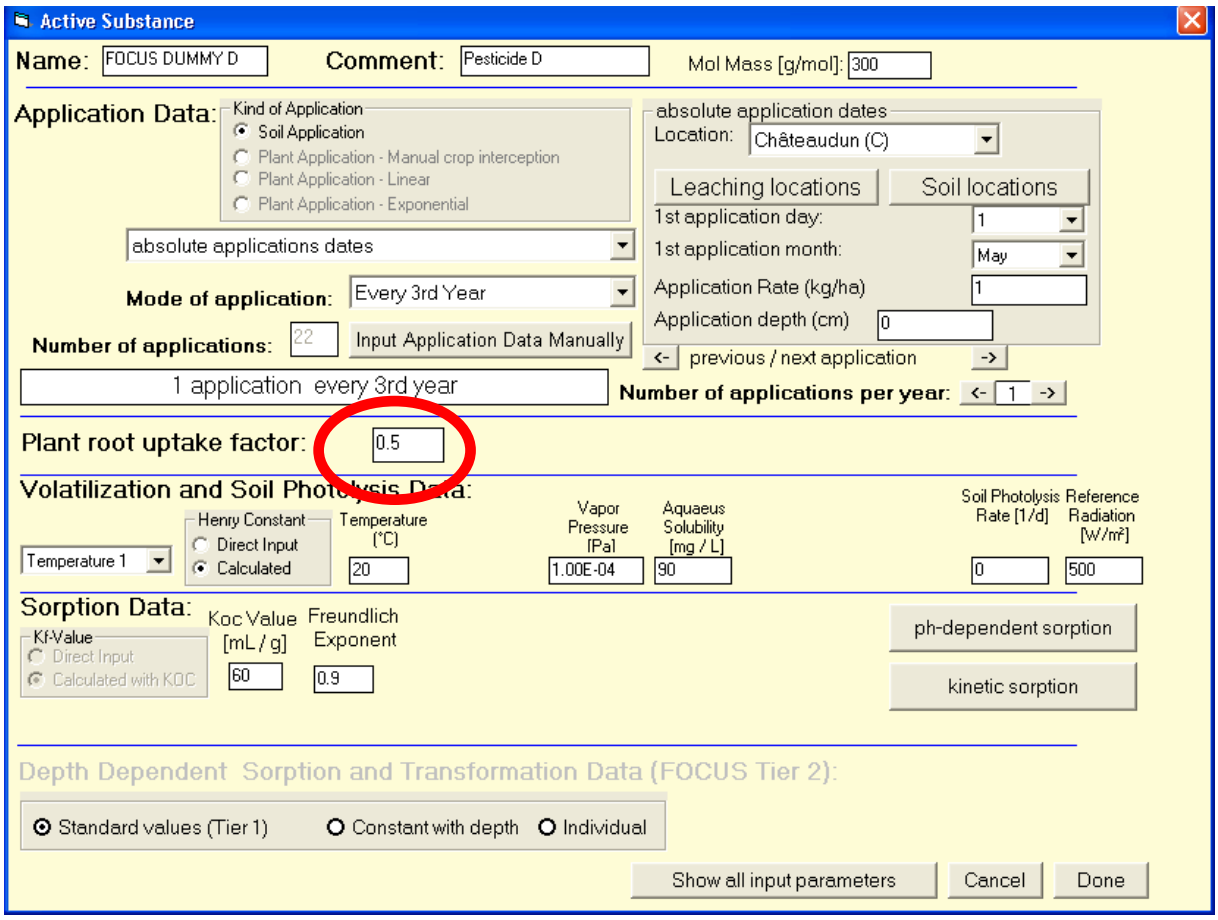

Figure 10: PELMO 4: Modifying the plant root uptake factor

For the estimation of temperature dependent volatilisation from soil surfaces and the transport in the soil air Henry's law constant (or alternatively: water solubility and vapour pressure) must be given for 2 different temperatures (see the rectangle in Figure 11). Photolysis on the soil surface can be considered when entering a soil photolysis rate together with the references radiation.

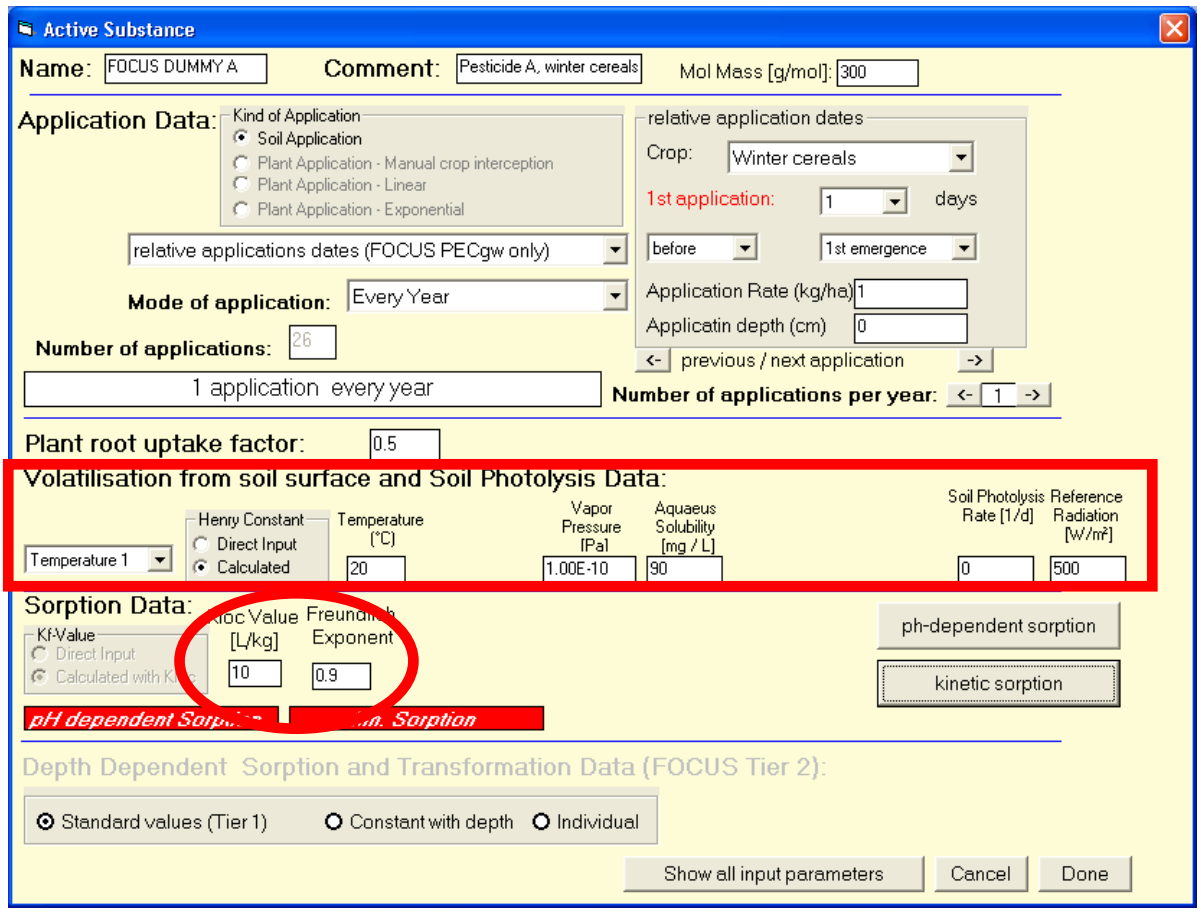

Figure 11: PELMO 4: Considering volatilisation and soil photolysis

The simplest way to consider sorption is to enter kfoc-value and the respective Freundlich exponent. If necessary, depth dependent Kf-values, kinetic sorption parameters or pH-dependent sorption in soil can be considered on additional forms which can be called by clicking at the respective buttons (see the arrows in Figure 12).

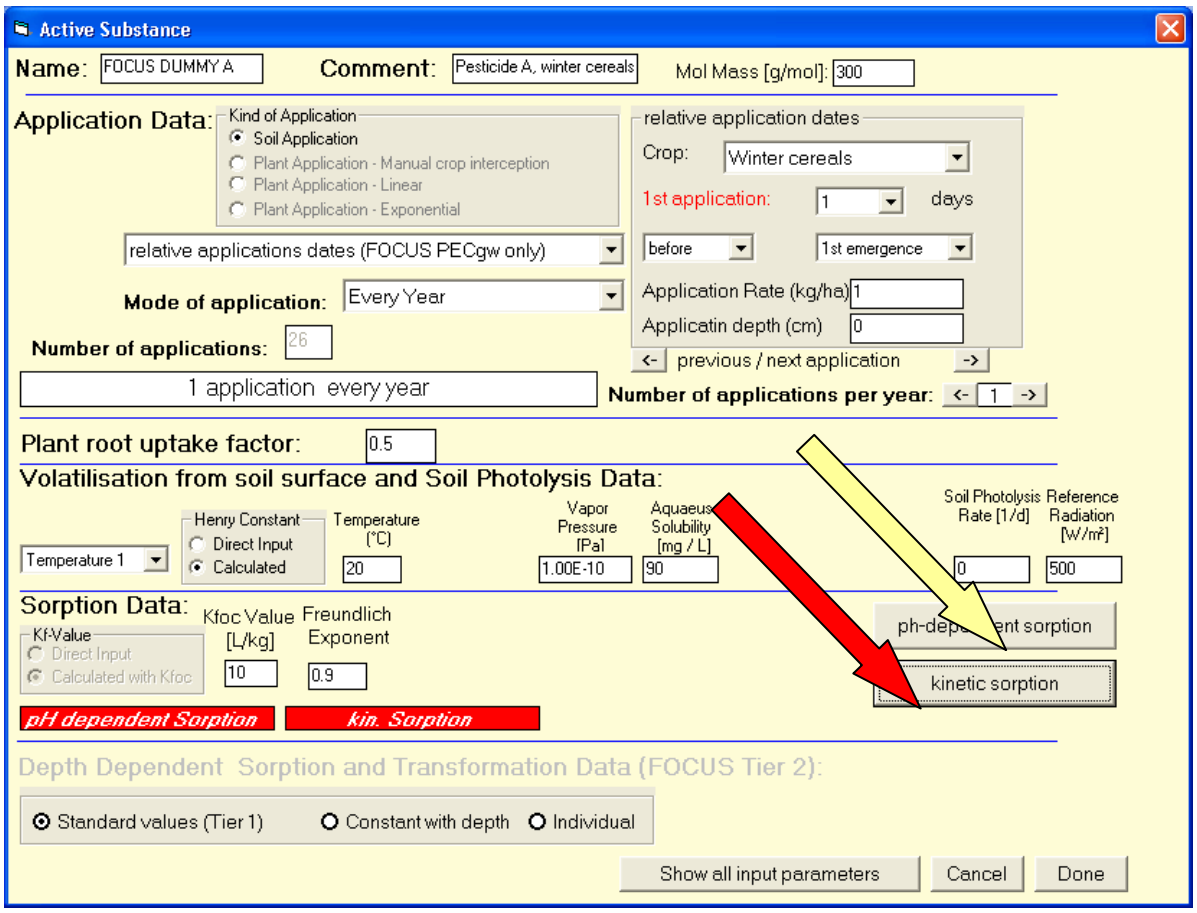


**Figure 12: PELMO 4: Extended Input sheet to consider kinetic sorption in PELMO**

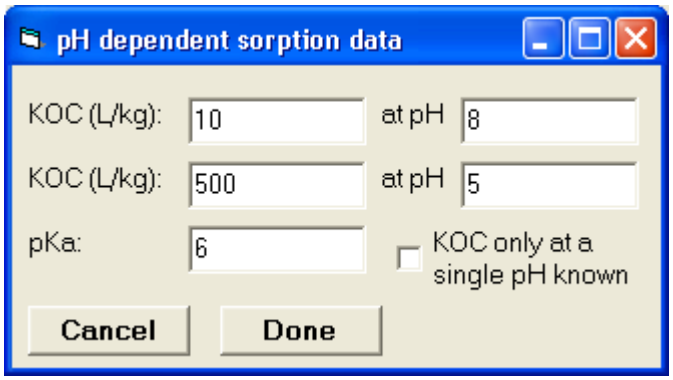


Figure 13: PELMO 4: Editing pH-dependent sorption parameters

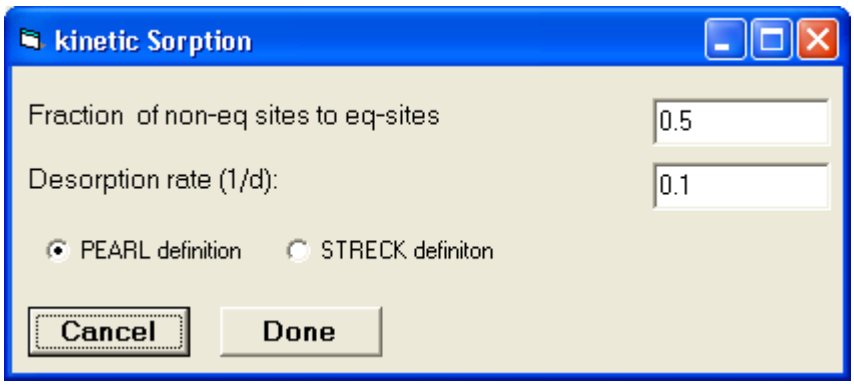

Figure 14: PELMO 4: Editing kinetic sorption parameters

The forms for pH-dependent sorption and kinetic sorption parameterisation are presented in Figure 13 and Figure 14, respectively. If pesticide input files include parameters for the estimation of these processes flags appear on the main pesticide input form (see Figure 11). It is possible to select PEARL or Streck parameter definitions by using the radio buttons on the form. Figure 14 shows the PEARL input parameters, Figure 15 the respective Streck variables. When switching between the two modes the parameters are automatically transferred according to the equations in the previous chapter.
When using the non-equilibrium sorption module in PELMO it has to be considered that - compared to the traditional definition of the sorption constant in PELMO - the Streck definition is different because it is related to the equilibrium domain in soil only and not (as in previous PELMO versions) to the total soil (equilibrium and non-equilibrium domain). That may lead to confusion when kinetic sorption is switched off (desorption rate set to "0"). Still overall sorption constants will depend on $f_{eq}$ (Streck). Therefore, in the field "KOC Value" (see the yellow arrow in Figure 12) always the (normal) equilibrium sorption constant related to the whole soil has to be entered (consistent with previous versions of PELMO).

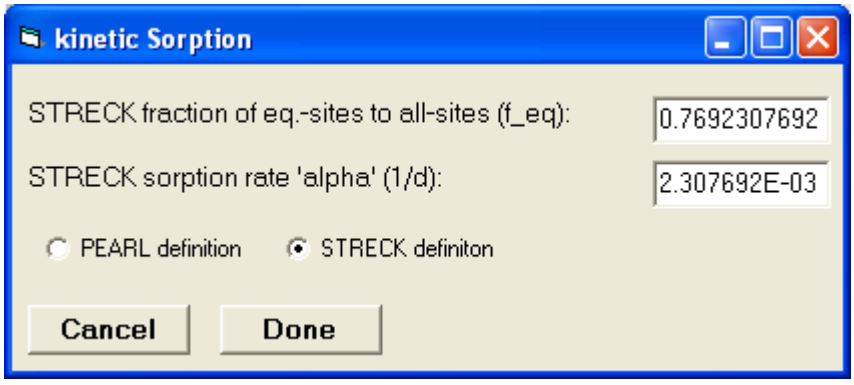

**Figure 15: Parameter setting using the Streck-model**

# 3. Parameterisation descriptions

The implemented scenario and parameter definitions are based on:

- **FOCUS DEFINITION** = Definitions made by the FOCUS working group
- **FOCUS SCENARIO SPECIFIC** = Definitions made by the FOCUS working group for a specific scenario
- **DEVELOPMENT DEFINITION** = Definitions made during the PELMO file development
- **USER INPUT** = Input to be specified by the user in the PELMO shell

## 3.1. Meteorological files (*.CLI)

| Parameter and description | | Value, source & comments |
|---|---|---|
| **RECORD 1** | | |
| TITLE: | label for meteorological file | **FOCUS SCENARIO SPECIFIC** |
| **RECORD 2 – REPEAT FOR EACH DAY OF A YEAR** | | |
| MMDDYY: | meteorological month/day/year | **FOCUS SCENARIO SPECIFIC**<br><br>Used are 9 location specific weather scenarios and 24 crop and location specific irrigated weather scenarios.<br><br>hourly data are not considered for FOCUS scenarios |
| PRECIP: | precipitation (cm $day^{-1}$) | |
| PEVP: | pan evaporation data (cm $day^{-1}$) | |
| TEMP: | 14h temperature per day (°C) | |
| AVTEMP: | mean temperature per day (°C) | |
| VATEMP: | difference between min. and max. temperature per day (°C) | |
| RELMOI: | rel. humidity (%) – not used | |
| RAD: | Radiation (kJ/m²) | |
| HOUR: | hour (only if hourly weather data available | |

## 3.2.

## Soil scenario files (*.SZE)

| Parameter and description | Value, source & comments |
|---|---|
| **RECORD 1**<br>TITLE: label for scenario title | **FOCUS SCENARIO SPECIFIC** |
| **RECORD 2**<br>PFAC(0): pan factor when no crop is present used to estimate the daily potential evapotranspiration (ET) from the daily pan evaporation. | **FOCUS DEFINITION** - crop specific values are defined by the kc_year factors (see table with CN in record 9). These calibration factors reflect the soil surface and aerodynamic resistance as effective annual averages. |
| SFAC: snowmelt factor in cm/degrees Celsius above freezing.<br>IPEIND: Pan evaporation flag. | set to **0.46** - **DEVELOPMENT DEFINITION** - SFAC is an empirical factor with wide variation. The value 0.46 represents an appropriate average based on data in the PRZM 3.12 manual and on Anderson, E.A.; 0.46 is also default value in PELMO 3.0 |
| IPEIND: | set to 0 = daily pan evaporation is read from the meteorological file - **FOCUS DEFINITION** |
| ANETD: minimum depth for soil evaporation (cm) | **DEVELOPMENT DEFINITION** - This location specific factor is highly correlated to the climatic conditions; based on the US distribution map and the relevant 20 year average annual air temperature following values are suggested for the specific FOCUS scenarios: |
| INICROP: initial crop number | set to 1 = simulate initial crop<br>- **DEVELOPMENT DEFINITION** |
| ISCOND: surface condition of initial crop | set to 1 = fallow **DEVELOPMENT DEFINITION** |
| PFAC(1): pan factor at maturation used to estimate the daily potential evapotranspiration (ET) from the daily pan evaporation. | **FOCUS DEFINITION** - crop specific values are defined by the kc_year factors (see table with CN in record 9). These calibration factors reflect the soil surface and aerodynamic resistance as effective annual averages. |
| PFAC(2): pan factor at senescence used to estimate the daily potential evapotranspiration (ET) from the daily pan evaporation. | **FOCUS DEFINITION** - crop specific values are defined by the kc_year factors (see table with CN in record 9). These calibration factors reflect the soil surface and aerodynamic resistance as effective annual averages. |

| | | |
|---|---|---|
| **RECORD 3** | | |
| ERFLAG: | flag to select simulation of erosion. | set to 0 = **no** erosion - **FOCUS DEFINITION** |
| **RECORD 4** | | |
| NDC: | number of different crops in the simulation. | set to 1 = only **one** crop - **FOCUS DEFINITION** |
| **RECORD 5 – REPEAT UP TO NDC** | | |
| ICNCN: | crop number of the different crop. | set to 1 = the crop used - **FOCUS DEFINITION** |
| CINTCP: | maximum interception storage of the crop (cm). | set to zero = no rainfall interception - **FOCUS DEFINITION**<br><br>**FOCUS SCENARIO SPECIFIC** |
| AMXDR: | maximum rooting depth of the crop (cm). | **FOCUS SCENARIO SPECIFIC** - is set to the maximum interception percentages (crop and location specific values vary from 45% to 90%) |
| COVMAX: | maximum areal coverage of the canopy (percent). | |
| ICNAH: | surface condition of the crop after harvest date (fallow, cropping, residue). | set to 3 = residue **DEVELOPMENT DEFINITION** |
| CN: | runoff curve numbers of antecedent moisture condition II for fallow, cropping, residue (3 values). | Runoff is calculated by a modification of the USDA Soil Conservation Service curve number approach (Haith *et al.*, 1979). The curve numbers were selected based on two definitions:<br><br>1) **SCS hydraulic Soil Group:** The SCS group was chosen for Piacenza to be **A**, Hamburg to be **B** and for all the rest locations to be **C** - **FOCUS DEFINITION**<br><br>2) **Curve Numbers:** Crop and soil specific CN are defined corresponding to values of PELMO 4.0, the original USDA definition and the PRZM 4 manual. – **DEVELOPMENT DEFINITION**<br><br>**THOUGH THE NECESSARY INPUT DATA IS PROVIDED RUNOFF IS NORMALLY NOT CONSIDERED FOR TIER 1 SIMULATIONS (SEE RECORD 13)** |

| | SCS soil group: | A | B | C | D | HTMAX | PFAC |
|---|---|---|---|---|---|---|---|
| | - fallow + residue | 77 | 86 | 91 | 94 | - | 1.00 |
| | – apples (orchards) | 36 | 60 | 73 | 79 | 250 | 0.99 |
| | – grass (+alfalfa) | 30 | 58 | 71 | 78 | 40 | 1.00 |
| | – potatoes | 62 | 83 | 89 | 93 | 100 | 0.94 |
| | – sugar beet | 58 | 72 | 81 | 85 | 40 | 0.93 |
| | – winter cereals | 54 | 70 | 80 | 85 | 100 | 0.84 |
| | - beans (field+vegetable) | 67 | 78 | 85 | 89 | 150 | 0.89 |
| | – bush berries | 36 | 60 | 73 | 79 | 130 | 1.00 |
| | – cabbage | 58 | 72 | 81 | 85 | 30 | 0.97 |
| | – carrots | 58 | 72 | 81 | 85 | 40 | 0.96 |
| | – citrus | 36 | 60 | 73 | 79 | 250 | 0.73 |
| | – cotton | 67 | 78 | 85 | 89 | 120 | 0.95 |
| | – linseed | 54 | 70 | 80 | 85 | 150 | 0.84 |
| | – maize | 62 | 83 | 89 | 93 | 250 | 0.94 |
| | – oil seed rape (sum) | 54 | 70 | 80 | 85 | 140 | 0.93 |
| | – oil seed rape (win) | 54 | 70 | 80 | 85 | 140 | 0.78 |
| | – onions | 58 | 72 | 81 | 85 | 60 | 0.91 |
| | – peas (animals) | 67 | 78 | 85 | 89 | 100 | 0.96 |
| | – soybean | 67 | 78 | 85 | 89 | 170 | 0.92 |
| | – spring cereals | 54 | 70 | 80 | 85 | 110 | 0.92 |
| | – strawberries | 58 | 72 | 81 | 85 | 40 | 1.00 |
| | – sunflower | 62 | 83 | 89 | 93 | 150 | 0.86 |
| | – tobacco | 67 | 78 | 85 | 89 | 250 | 0.98 |
| | – tomatoes | 62 | 74 | 81 | 86 | 110 | 0.97 |
| | – vines | 45 | 62 | 73 | 79 | 170 | 0.89 |

| | | |
|---|---|---|
| | | For all perennial crops (alfalfa, apples, bushberries citrus, grass, strawberries, vines) the same CN are used for fallow and residue! |
| USLEC: | Universal soil loss equation cover management factor for fallow, crop and residue. | Only required if ERFLAG = 1<br>set to 1 – **DEVELOPMENT DEFINITION** |
| WFMAX: | maximum dry weight of the crop at full canopy (kg $m^{-2}$). | set to 0.0 = not used - **FOCUS DEFINITION**<br>(only required if non-linear foliar application). |
| RRPPEX: | poorly exposed transformation fraction | set to 0.0 = not used - **FOCUS DEFINITION**<br>(only required if non-linear foliar application). |
| RRRPEX: | poorly exposed penetration fraction | set to 0.0 = not used - **FOCUS DEFINITION**<br>(only required if non-linear foliar application). |
| RRVPEX: | poorly exposed volatilisation fraction | set to 0.0 = not used - **FOCUS DEFINITION**<br>(only required if non-linear foliar application). |
| RRWPEX: | poorly exposed wash-off fraction | set to 0.0 = not used - **FOCUS DEFINITION**<br>(only required if non-linear foliar application). |
| IRRFLG: | | set to 0.0 for non-irrigated crops<br>set to 1.0 for irrigated crops- **FOCUS DEFINITION** |
| PEREN: | | set to 0.0 for non-irrigated crops<br>set to 1.0 for irrigated crops- **FOCUS DEFINITION** |

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|---|---|
| **RECORD 6** | |
| | set to 66 (= longest possible simulation period) - |

| | |
|---|---|
| NCPDS: number of cropping periods. | **FOCUS DEFINITION** |
| **RECORD 7 - REPEAT UP TO NCPDS** | |
| E_MMDDYY: crop emergence date (month/day/year). | **FOCUS SCENARIO SPECIFIC** |
| M_MMDDYY: crop maturation date. | **FOCUS SCENARIO SPECIFIC** |
| H_MMDDYY: crop harvest date. | **FOCUS SCENARIO SPECIFIC** |
| INCROP: crop number associated with NDC | set to 1 (only one crop) - **FOCUS DEFINITION** |
| H_MMDDYY: crop senescence date. | **FOCUS SCENARIO SPECIFIC** |
| T_MMDDYY: crop tillage date. | **not used in FOCUS** |

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| **RECORD 8** | |
| CORED: total depth of soil core (cm) | **FOCUS SCENARIO SPECIFIC** |
| DUMMY: dummy number | former plant uptake factor, not considered here any more, this parameter is now read in from the pesticide data file. |
| NCOM2 total number of simulation compartments in the soil core | **FOCUS SCENARIO SPECIFIC** |
| BDFLAG | set to 0 = not used |
| THFLAG: field capacity and wilting point flag. | set to 0 = **the FOCUS SCENARIO SPECIFIC soil water contents are used** -<br><u>Comment:</u> another PELMO option would be to calculate field capacity and wilting point by internal pedotransfer rules using scenario specific clay and sand contents. |
| HSWZT: drainage flag. | set to 0 = free draining - **FOCUS DEFINITION** |
| **RECORD 9** | |
| NHORIZ: total number of horizons | **FOCUS SCENARIO SPECIFIC** |
| DELXFLG: layer thickness flag | SET TO 0 = NOT USED |

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|---|---|---|
| **RECORD 10A –REPEAT 10A-10B UP TO NHORIZ** | | |
| HORIZN: | horizon number in relation to NRHORIZ. | **FOCUS SCENARIO SPECIFIC** |
| THKNS: | soil horizon thickness (cm). | **FOCUS SCENARIO SPECIFIC** |
| BD: | soil bulk density [g $cm^{-3}$] | **FOCUS SCENARIO SPECIFIC** |
| DISP: | Dispersion length ($cm^2$ $day^{-1}$) | set to 5 cm– **FOCUS DEFINITION** |
| THETO: | initial soil water content in the soil horizon ($cm^3$ $cm^{-3}$) | set to THEFC – **DEVELOPMENT DEFINITION** |
| AD: : | drainage parameter ($1/d^3$) | **NOT USED FOCUS DEFINITION** |
| **RECORD 10B –REPEAT 10A-10B UP TO NHORIZ** | | |
| THEFC: | field capacity ($cm^3$ $cm^{-3}$). | **FOCUS SCENARIO SPECIFIC** |
| THEWP: | wilting point ($cm^3$ $cm^{-3}$). | **FOCUS SCENARIO SPECIFIC** |
| OC: | organic carbon content (%) | **FOCUS SCENARIO SPECIFIC** |
| PH: | pH value | **FOCUS SCENARIO SPECIFIC** |
| Biodeg: | relative biodegradation factor | depth dependent correction factor applied to the substance(s) degradation rates **FOCUS DEFINITION**<br>0 – 30 cm depth 1<br>30 – 60 cm depth 0.5<br>60 – 100 cm depth 0.3<br>> 100 cm depth 0 |
| **RECORD 11** | | |
| ILP: | Initial level of substance indicator | set to 0 = no initial substance levels input – **DEVELOPMENT DEFINITION** |
| **RECORD 12** | | |
| ITEM1: | Hydrology output summary indicator | **DEVELOPMENT DEFINITION** |
| STEP1: | Time step of hydrology output | set to YEARLY **– DEVELOPMENT DEFINITION** |
| LFREQ1: | Frequency of soil compartment reporting | set to 1 = every compartment is output – **DEVELOPMENT DEFINITION** |
| ITEM2: | Substance output summary indicator | **DEVELOPMENT DEFINITION** |
| STEP2: | Time step of substance output | set to YEARLY **– DEVELOPMENT DEFINITION** |
| LFREQ2: | Frequency of soil compartment reporting | set to 1 = every compartment is output – **DEVELOPMENT DEFINITION** |
| ITEM3: | Substance concentration profile indicator | **DEVELOPMENT DEFINITION** |
| STEP3: | Time step of substance concentration profile output | set to YEARLY **– DEVELOPMENT DEFINITION** |
| LFREQ3: | Frequency of soil compartment reporting | set to 1 = every compartment is output – |

| | | DEVELOPMENT DEFINITION |
|---|---|---|
| **RECORD 13** | | |
| ROFLAG: | runoff flag | set to 0 = no runoff **–FOCUS DEFINITION** |
| DEPRO: | runoff depth (cm) | NOT USED (IF RUN-OFF FLAG = 0) |
| DOC: | dissolved organic carbon (mg/L) | **NOT USED FOCUS DEFINITION** D |
| DOCFLG: | doc flag | **NOT USED FOCUS DEFINITION** |
| DEPMA: | depth of macro pores (cm) | **NOT USED FOCUS DEFINITION** |
| IC: | threshould rainfall that produces macro pore flow (cm) | **NOT USED FOCUS DEFINITION** |
| FMAC: | fraction routed into macro pores (cm) | **NOT USED FOCUS DEFINITION** |
| **RECORD 14** | | |
| GEOBREI: | Latitude | **FOCUS SCENARIO SPECIFIC**<br><br>Comment: The geographical latitude is usually required only for calculation of the evapotranspiration by the methods of Hamon or Haude, whereas the **FOCUS DEFINITION** is to use daily pan evaporation data. |

## 3.3. Substance file (*.PSM)

| Parameter and description | Value, source & comments |
|---|---|
| Comment: Text and / or lines in the substance file that are given in brackets (< >) are comments for easier understanding of the file structure and mark the beginning or end of a parameter section. These lines should not be changed.<br><br>The compound parameters are described here only for the parent compound. In principle, all processes except from volatilisation are taken into account also for each metabolite. Therefore, for each metabolite to be simulated, a similar set of parameters needs to be included, leaving out only the volatilisation data. | |
| **COMMENT**<br>CTITLE: label for substance | **USER INPUT** |
| **SOIL HORIZONS**<br>NHORIZ: total number of soil horizons | set to 0 = not used - **DEVELOPMENT DEFINITION**<br><br>Comment: This parameter is required if depth dependent biodegradation factors are specified in the substance file instead of the scenario file. The parameter has then to be set to the scenario specific number of horizons. |
| **NUMBER OF LOCATIONS**<br>N_LOC: number of locations for which applications will be defined (1-10)<br><br>DUMMY:<br><br>REL_ABS_APP: | **FOCUS SCENARIO SPECIFIC / USER INPUT**<br><br>not used<br><br>0: absolute application dates<br>9: relative application dates |
| **APPLICATIONS - REPEAT UP TO N_LOC**<br>NAPS: total number of substance applications occurring at different dates (1 – 200). | **FOCUS SCENARIO SPECIFIC / USER INPUT** |

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| **APPLICATIONS – REPEAT UP TO NAPS (IF ABSOLUTE APPLICATIONS ARE SELECTED)** | |
| APD: Day of the month of application | **USER INPUT** |
| APM: Month of application | **USER INPUT** |
| IAPYR: Year of application | **USER INPUT** |
| TAPP: Total application rate (kg $ha^{-1}$) | **USER INPUT** |
| DEPI: Depth of incorporation (cm) | **USER INPUT** |
| COVAPP: crop interception during application (%) | **NOT USED FOR FOCUS SIMULATIONS** |
| FRPEC: fraction of poorly exposed pesticide | **NOT USED FOR FOCUS SIMULATIONS** |
| APT: application hour | **NOT USED FOR FOCUS SIMULATIONS** |
| **APPLICATIONS – REPEAT UP TO NAPS (IF RELATIVE APPLICATIONS ARE SELECTED)** | |
| APD: Day relative to crop status | **USER INPUT** |
| APM: crop development type (emergence, harvest) | **USER INPUT** |
| IAPYR: Year of application | **USER INPUT** |
| TAPP: Total application rate (kg $ha^{-1}$) | **USER INPUT** |
| DEPI: Depth of incorporation (cm) | **USER INPUT** |
| COVAPP: crop interception during application (%) | **NOT USED FOR FOCUS SIMULATIONS** |
| FRPEC: fraction of poorly exposed pesticide | **NOT USED FOR FOCUS SIMULATIONS** |
| APT: application hour | **NOT USED FOR FOCUS SIMULATIONS** |
| **APPLICATION MODE** | |
| FAM: Substance application model | **USER INPUT**<br><br>Selectable chemical application methods are:<br>**1** = application to soil only<br>**2** = foliar application using the linear model<br>**3** = non-linear foliar application using exponential filtration model<br>**4** = application to the foliar, manual crop interception<br><br>**Note:** Foliar application needs to be activated to simulate washoff from plant foliage and degradation of foliage substance. |

| | | |
|---|---|---|
| **FOLIAR APPLICATION PARAMETERS (ONLY IF FAM = 2 OR 3)** | | |
| PLDKRT: | Decay rate on the plant foliate ($days^{-1}$) | Not used for FOCUS scenarios |
| FEXTRC: | Foliar extraction coefficient for substance washoff per cm of precipitation | Not used for FOCUS scenarios |
| FILTRA: | Filtration parameter. Only required for exponential model (FAM = 3). | Not used for FOCUS scenarios |
| FILTRA: | Filtration parameter. Only required for exponential model (FAM = 3). | Not used for FOCUS scenarios |
| FPENET: | Penetration rate into the plant foliate ($day^{-1}$) FPENET | Not used for FOCUS scenarios |
| PHRATE: | Photodegardation rate (1/d) | Not used for FOCUS scenarios |
| RADREF: | Reference radiation ($W/m^2$) | Not used for FOCUS scenarios |
| DLAM: | Laminar layer for volatilisation from foliate ($W/m^2$) | Not used for FOCUS scenarios |
| **FLAGS** | | |
| VAPFLG: | Henry's constant flag | **USER INPUT**<br>**0** = Henry's constant input by user<br>**1** = Henry's constant calculated |
| KDFLAG: | $K_D$ flag | **USER INPUT**<br>**0** = $K_D$ input by user<br>**1** = $K_D$ calculated from $K_{OC}$ |

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|---|---|---|
| **VOLATILISATION 2 RECORDS, ONE FOR EACH TEMPERATURE** | | |
| HENRYK: | normalised Henry's law constant of the active substance (dimensionless). | Comment: Henry's constant **H** is a ratio of a chemical's vapour pressure to its solubility. It represents the equilibrium between the vapour and solution phases.<br><br>):<br><br>HENRYK = H / (R*T) = P*M / (C*R*T)<br><br>P = vapour pressure (Pa) - **USER INPUT**<br>M = mol weight (g $mole^{-1}$) - **USER INPUT**<br>C = water solubility (mg $L^{-1}$) - **USER INPUT**<br>R = gas constant = 8.3144 J $K^{-1}$ $mole^{-1}$<br>T = absolute temperature (K) |
| SOLUB: | Solubility in water (mg $L^{-1}$) | **USER INPUT** |
| MOLMAS: | Molar mass (g $mol^{-1}$) | **USER INPUT** |
| VAPPRE: | Vapour pressure (Pa) | required for calculation of Henry's constant - **USER INPUT** |
| DAIR: | molecular diffusion coefficient for the substance(s) in the air ($cm^2$ $sec^{-1}$) | required for calculation of Henry's constant - **USER INPUT** |
| VOLGRE: | depth for volatilisation (cm) | set to 0.1 cm – **FOCUS DEFINITION** |
| T_VOL: | Related Temperature (°C) | **USER INPUT** |
| **PLANT UPTAKE** | | |
| UPTKF: | plant uptake factor<br>(between 0.000 and 1.0; describes uptake as a fraction of transpiration* dissolved phase concentration) | **USER INPUT**<br>set to 0.5 for systemic compounds (default)<br>set to 0 = **no** plant uptake for other compounds<br>Other values not to be used for TIER 1 modelling! |
| **DEGRADATION - REPEAT FOR METABOLISATION PATHS A1 – D1 AND BOUND RESIDUES / $CO_2$** | | |
| DKRATE: | degradation rate constant ($day^{-1}$) | **USER INPUT -** Can also be entered as a DT50 value |
| TEMP0: | reference temperature for the degradation rate constant (°C) | **USER INPUT** |
| Q10: | Q10-factor for degradation rate increase when temperature increases by 10°C | **USER INPUT**<br>default = 2.2 - **FOCUS DEFINITION** |
| ABSFEU: | absolute reference moisture content during the degradation studies (%Vol) | **USER INPUT** |
| FELFEU: | relative reference moisture content during the degradation studies (% of FC (field capacity)) | **USER INPUT**<br>Comment: either absolute or relative soil moisture has to be specified, the other parameter should be set to 0 |
| FEUEXP: | Exponent for the moisture dependent correction of the degradation rate constant | **USER INPUT**<br>default = 0.7 – **FOCUS DEFINITION** |

| | | |
|---|---|---|
| | (moisture relationship according to WALKER) | |
| **FLAG** | | |
| DEGFLAG: | flag controlling depth dependent degradation | **USER INPUT**<br>0: degradation according to degradation factors in the scenario file<br>1: degradation constant with depth<br>2: degradation according to individual factors in the pesticide data file<br>For TIER 1 modelling the flag should be set to 0. |
| **ADSORPTION (IF KDFLAG = 1)** | | |
| KOC: | $K_{OC}$ value (ml $g^{-1}$) | **USER INPUT** |
| FRNEXKOC: | Freundlich exponent 1/n (dimensionless) | **USER INPUT** |
| PH_KOC: | pH value | **USER INPUT**<br>default = 7 |
| PKA: | pKA value | **USER INPUT**<br>default = 20, ie in practice not used |
| FRNMIN: | lower limit concentration for the non-linear sorption according to Freundlich (µg $L^{-1}$) | **USER INPUT**<br>default = $10^{-20}$ µg $L^{-1}$ |
| ALTERN: | annual increase of adsorption (%) | **USER INPUT**<br>default = 0 (no increase of sorption with time) |
| K_DOC: | Equilibrium constant for DOC (L/kg) | **not used for FOCUS simulations** |
| KOC_MOI: | Increase when soil is air dried (-) | **USER INPUT**<br>default = 0 (no increase of sorption with mositure) |
| KOC2: | second $K_{OC}$ value at a different pH (ml $g^{-1}$) | **USER INPUT** |
| PHKOC2: | pH value related to the second KOC | **USER INPUT** |
| FNEQ: | fraction of non-equilibrium sites | **USER INPUT** |
| KDES | desorption rate (1/d) | **USER INPUT** |

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| **DEPTH DEPENDENT SORPTION AND DEGRADATION (ONLY IF DEGFLAG=2) – REPEAT FOR EACH SOIL HORIZON** | | |
| KD : | $K_D$ value (ml $g^{-1}$) | **USER INPUT**<br>(only considered by PELMO if kdflag = 0) |
| FRNEXP: | Freundlich exponent 1/n (dimensionless) | **USER INPUT**<br>(only considered by PELMO if kdflag = 0) |
| DEG(1): | depth dependent correction of degradation rate for metabolism path A1 | **USER INPUT** |
| DEG(2): | depth dependent correction of degradation rate for metabolism path B1 | **USER INPUT** |
| DEG(3): | depth dependent correction of degradation rate for metabolism path C1 | **USER INPUT** |
| DEG(4): | depth dependent correction of degradation rate for metabolism path D1 | **USER INPUT** |
| DEG(5): | depth dependent correction of degradation rate for metabolism path BR/CO2 | **USER INPUT**<br><br>Comment: the depth dependent correction of degradation can also be specified in the scenario file. According to **FOCUS DEFINITION** the depth dependent correction factors are<br>0 – 30 cm depth 1<br>30 – 60 cm depth 0.5<br>60 – 100 cm depth 0.3<br>> 100 cm depth 0 |

## 3.4. Control file PELMO.INP

| Parameter and description | | Value, source & comments |
|---|---|---|
| **RECORD 1** | | |
| IYEAR: | number of years of simulation period | 26, 46, or 66 years - **FOCUS DEFINITION** |
| ISDAY: | start day of simulation | 1 – **DEVELOPMENT DEFINITION** |
| ISMON: | start month of simulation | 1 - **DEVELOPMENT DEFINITION** |
| IEDAY: | end day of simulation | 31 - **DEVELOPMENT DEFINITION** |
| IEMON: | end month of simulation | 12 - **DEVELOPMENT DEFINITION** |
| **RECORD 2** | | |
| APPLIK: | scenario parameter file name | **USER INPUT, FOCUS DEFINITION** |
| **RECORD 3** | | |
| CHEM: | substance parameter file name | **USER INPUT** |
| **RECORD 4 - REPEAT UP TO (NUMBER OF SIMULATION YEARS)** | | |
| KLIMA: | climate file name | **USER INPUT, FOCUS DEFINITION** |
| **RECORD 13** | | |
| NPLOTS: | Number of time series to be written to plotting file | 22 - **DEVELOPMENT DEFINITION** |
| **RECORD 14 – REPEAT UP TO NPLTOTS** | | |
| PLNAME: | Identifier of time series | **DEVELOPMENT DEFINITION** |
| MODE: | Plotting mode | Comment: The time series identified here are requirements for the graphical output and analysis within the Graphical User Interface. They cannot be changed. |
| IARG: | Argument of variable identified in PLNAME | |
| CONST: | Constant used for unit conversion | |

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