

# Manual of PEARLNEQ v5

J.J.T.I. Boesten  
M.M.S. ter Horst

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Wettelijke Onderzoekstaken Natuur & Milieu



## Manual of PEARLNEQ v5

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WOT Working Document **304** presents the findings of a research project commissioned by the Netherlands Environmental Assessment Agency (PBL) and funded by the Dutch Ministry of Economic Affairs, Agriculture and Innovation (EL&I). This document contributes to the body of knowledge which will be incorporated in more policy-oriented publications such as the National Nature Outlook and Environmental Balance reports, and thematic assessments.

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**Working Document 304**

Wettelijke Onderzoekstaken Natuur & Milieu

Wageningen, Juni 2012

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The Working Documents series is published by the Statutory Research Tasks Unit for Nature & the Environment (WOT Natuur & Milieu), part of Wageningen UR. This document is available from the secretary's office, and can be downloaded from [www.wotnatuurenmilieu.wur.nl](http://www.wotnatuurenmilieu.wur.nl).

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## Summary

This manual describes the PEARLNEQ v5 software package . This package can estimate long-term sorption parameters using results of aged-sorption studies with soil, using a submodel for sorption and transformation that is identical to the submodel used for that purpose in the FOCUS\_PEARL v3.3.3.

The submodel assumes two types of sorption sites: equilibrium sites and non-equilibrium sites. The sorption isotherms for both sites are described with Freundlich equations. The content sorbed at the equilibrium site is assumed to be continuously at equilibrium and the content sorbed at the non-equilibrium site is described with a pseudo first-order sorption rate equation. The software package offers two options for describing the transformation rate in soil. The first option is that the transformation rate in soil is proportional to the amount in the liquid phase plus the amount sorbed at the equilibrium site. The second option is that the transformation rate in soil is proportional to the amount in the liquid phase. So for both options the content sorbed at the non-equilibrium site is not subject to transformation.

The mathematical equations describing the submodel are solved via a FORTRAN programme. An additional FORTRAN programme generates the necessary input files for the PEST optimisation package. Instructions are given how to obtain optimized parameters using an example dataset and how to obtain parameters using your own data.



# 1 Introduction

This document describes a PEARLNEQ-PEST combination, which can be used to estimate the parameters for long-term sorption kinetics in the PEARL model on the basis of an incubation experiment for a certain soil and a certain pesticide. The combination provides also the transformation half-life at reference temperature (when long-term sorption kinetics are included in PEARL, the definition of this half-life changes so it has to be recalculated; see Boesten and van der Linden, 2001). If the incubation experiment has been carried out at multiple temperatures, the Arrhenius activation energy for the transformation rate in soil can be optimised simultaneously.

The differences with the previous release (PEARLNEQ v4) are:

- An option is offered to define the transformation half-life on the basis of the concept that the transformation rate is proportional to the amount of substance in the liquid phase
- The equilibrium sorption coefficient has become a parameter that is optimised.



## 2 Precautionary remark

This PEARLNEQ-PEST software tool should be seen as an introduction to fitting results of experiments on long-term sorption kinetics to the sorption submodel used in the PEARL model. The tool shows you how PEST can be coupled to a fortran programme that contains this PEARL sorption submodel (i.e. PEARLNEQ.EXE) but it should not be seen as a ready-to-use tool. The tool provides you with example input files for the PEST optimisation package and shows you how to organise this optimisation. We had to make a number of assumptions for generating these PEST input files (e.g. upper and lower bounds of parameters, weighing factors for each measurement, etc.). We do not claim that these assumptions are defensible for your problem; they are our best guesses but they may not be appropriate for your problem. It is your responsibility to check the appropriateness of the result obtained. We do not accept any responsibility for use of PEARLNEQ.



### **3 Description of the incubation experiment**

The PEARLNEQ-PEST tool can be used to fit the results of the following experiment. A number of jars is filled with soil. Each jar contains the same mass of moist soil. At the start of the experiment the same initial mass of pesticide is added to the moist soil in all jars. The jars are incubated at a fixed temperature (or at a few temperatures). At certain time points the remaining total amount of pesticide is measured via an extraction with organic solvent. At the same time the concentration in the liquid phase of the moist soil is measured. The liquid phase can be collected by centrifuging the moist soil over a filter. As an alternative for centrifuging, a desorption experiment can be carried out by adding a certain volume of water and subsequent shaking for about 24 h.

It may also be useful to have additional results of measurements of an adsorption isotherm with an equilibration time of about 24 h using the same soil and pesticide.





## 4 Theoretical background

PEARLNEQ assumes a Freundlich two-site sorption submodel: one site for equilibrium sorption and the second site for long-term sorption kinetics. The operational definition for the equilibrium sorption sites is that they have reached equilibrium after about 24 h shaking of a well-stirred suspension of the soil in water. The long-term sorption sites do not reach equilibrium within 24 h. PEARLNEQ assumes first order degradation kinetics; it offers two options for describing the degradation kinetics. The first option is that the degradation rate is proportional to the number of molecules present in liquid phase and those sorbed to the equilibrium site. The second option is that the degradation rate is proportional to only the number of molecules present in liquid phase (see Beltman *et al.*, 2008). However, molecules sorbed on the kinetic site are assumed not to degrade in both options. This conceptual model is presented in Figure 1. The submodel for sorption and degradation kinetics used in PEARLNEQ can be described as follows (Leistra *et al.*, 2001):

$$M_p = V c_L + M_s (X_{EQ} + X_{NE}) \quad (1)$$

$$X_{EQ} = K_{F,EQ} c_{L,R} \frac{c_L}{c_{L,R}} \frac{\ddot{o}^N}{\emptyset} \quad (2)$$

$$\frac{dX_{NE}}{dt} = k_{des} (K_{F,NE} c_{L,R} \frac{c_L}{c_{L,R}} \frac{\ddot{o}^N}{\emptyset} - X_{NE}) \quad (3)$$

$$K_{F,NE} = f_{NE} K_{F,EQ} \quad (4)$$

$$\frac{dM_p}{dt} = -k_t (V c_L + M_s X_{EQ}) \quad (5A)$$

$$\frac{dM_p}{dt} = -k_t V c_L \quad (5B)$$

$$K_{F,EQ} = m_{OM} K_{OM,EQ} \quad (6)$$

Where:

- $M_p$  = total mass of pesticide in each jar (mg), acronym Mas
- $V$  = the volume of water in the soil incubated in each jar (mL), acronym VolLiq
- $M_s$  = the mass of dry soil incubated in each jar (g), acronym MasSol
- $c_L$  = concentration in the liquid phase (mg/L), acronym ConLiq
- $c_{L,R}$  = reference concentration in the liquid phase (mg/L), acronym ConLiqRef
- $X_{EQ}$  = content sorbed at equilibrium sites (mg/g)
- $X_{NE}$  = content sorbed at non-equilibrium sites (mg/g)
- $K_{F,EQ}$  = equilibrium Freundlich sorption coefficient (mL/g), acronym CoffFreEq
- $K_{F,NE}$  = non-equilibrium Freundlich sorption coefficient (mL/g), acronym CoffFreNeg

$N$  = Freundlich exponent (-), acronym ExpFre

$k_{des}$  = desorption rate coefficient ( $d^{-1}$ ), acronym CofRatDes

$f_{NE}$  = a factor for describing the ratio between the equilibrium and non-equilibrium Freundlich coefficients (-), acronym FacSorNeqEqI

$k_t$  = degradation rate coefficient ( $d^{-1}$ )

$m_{OM}$  = mass fraction of organic matter in the soil (kg/kg), acronym CntOm

$K_{OM,EQ}$  = coefficient of equilibrium sorption on organic matter (mL/g), acronym KomEqI

PEARLNEQ does not use the transformation rate coefficient ( $k_t$ ) as input parameter, but the half-life at reference temperature (acronym DT50Ref,  $dt50$ ). They are related as follows (assuming first order kinetics):

$$dt50 = \ln(2) / k_t \quad (7)$$

The effect of soil temperature on the transformation rate coefficient in soil is described by the Arrhenius equation:

$$f_T = \exp\left(\frac{-E}{R} \left(\frac{1}{T} - \frac{1}{T_{REF}}\right)\right) \quad (8)$$

Where

$f_T$  = the multiplication factor for the rate coefficient (-)

$E$  = Arrhenius activation energy (kJ/mol)

$T$  = temperature of the soil (K)

$T_{REF}$  = the reference temperature for the specified  $DT50$  (K)

$R$  = the gas constant ( $kJ\ mol^{-1}\ K^{-1}$ ).

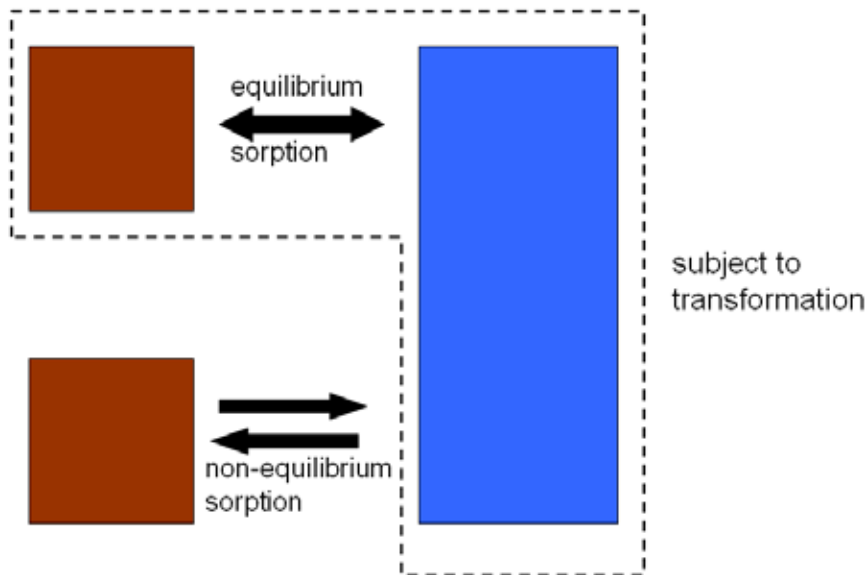


Figure 1. Conceptual representation of the PEARLNEQ model showing the soil solution on the right and the equilibrium and non-equilibrium sorption sides on the left. Note that there are two options for the transformation process as described by Eqns 5-A and 5-B. Only the option described by Eqn 5-A is shown here.

Often no concentration measurements in the soil pore water are available but instead at each sampling point in time a certain volume of water (usually a CaCl<sub>2</sub> solution) is added to soil and the suspension is shaken for about 24 h after which the concentration in the supernatant is measured. In such a case the fit has to be based on these concentration measurements in the supernatant of the soil-water suspension.

This is simulated in PEARLNEQ as follows:

- A. It is assumed that full equilibrium is reached for the equilibrium sorption site during the desorption experiment (i.e., shaking for 24 h)
- B. It is assumed that desorption from the non-equilibrium sorption site can be ignored during the desorption experiment.

Assumption A is justifiable because this is exactly the operational definition of the equilibrium sorption site. Assumption B is justifiable because desorption coefficients for long-term kinetics are usually in the order of 0.01 d<sup>-1</sup>, which implies that amounts desorbed within 1 day are negligibly small.

Using these assumptions, the concentration in the liquid phase of the supernatant after desorption can be estimated by stating that (i) the total content of substance in the moist soil and the soil-water suspension have to be equal, and (ii) the content sorbed at the non-equilibrium sites in the moist soil and in the soil-water suspension are equal. Using Equation 1 then results in the following equation

$$V c_{L,MS} + M_s (X_{EQ,MS} + X_{NE}) = (V + V_{ADD}) c_{L,SUS} + M_s (X_{EQ,SUS} + X_{NE}) \quad (9)$$

Where:

The subscript MS indicates the moist-soil system

The subscript SUS indicates the soil-water suspension system and

$V_{ADD}$  = volume of liquid (usually CaCl<sub>2</sub> solution) added to the soil at each sampling point just before starting the 24 h desorption experiment (mL), acronym VolLiqAdd.

At each sampling point in time, Equation 9 can be rewritten (using Eqn 2) into an equation that contains only one unknown variable, i.e. the concentration in the liquid phase of the soil suspension ( $c_{L,SUS}$ ). PEARLNEQ provides as output always the concentration in the soil-water suspension as a function of time. If  $V_{ADD} = 0$ , then this implies that the concentration in the moist soil is given.

PEARLNEQ provides as output also the so-called apparent sorption coefficient ( $K_{D,APP}$ ). This is used for studies in which a certain volume of water (usually a CaCl<sub>2</sub> solution) is added to soil and the suspension is shaken for about 24 h. It is then defined as the total content sorbed at the end of the shaking period divided by  $c_{L,SUS}$ . This is calculated by PEARLNEQ as:

$$K_{D,APP} = \frac{X_{EQ,SUS} + X_{NE}}{c_{L,SUS}} \quad (10)$$

PEARLNEQ solves the set of Eqn 1 to Eqn 9 numerically using Euler's method for integration of the state variables  $M_p$  and  $X_{NE}$ . The time step for integration,  $\Delta t$ , is calculated as:

$$Dt = \frac{A}{\max(k_i f_T, k_{des})} \quad (11)$$

Where  $A$  is an accuracy parameter (·) which was set to 0.003. Leistra *et al.* (2001, p. 84) have shown that such a value of  $A$  should give accurate results.

The concentration in the liquid phase is calculated via an iteration procedure as described in Appendix 4 of FOCUS (2006). Appendix 3 shows a test of the PEARLNEQ results against an analytical solution for the case of a linear isotherm ( $N=1$ ), indicating good correspondence between numerical and analytical results.

## 5 Fitting procedure for parameters with PEST

The provided package assumes that the following variables need to be optimized:

- The initial mass of the pesticide (MasIni)
- The ratio between the equilibrium and non-equilibrium Freundlich coefficients (FacSorNeqEq)
- The desorption rate coefficient (CofRatDes)
- The half-life at reference temperature (DT50Ref) for the selected transformation option (Eqn 5-A or Eqn 5-B)
- The coefficient of equilibrium sorption on organic matter (KomEq)
- The molar activation energy (MolEntTra); this can only be optimized if the experiment has been carried out at multiple temperatures.

It is assumed that all other variables are known.

The provided package assumes that the measurements that are fitted, consist for each point in time of

- A mass of pesticide in **mg**
- A concentration in liquid phase in **mg/mL**.

In case one of the two measurements is missing a value of -99.9999 can be specified. The PEARLMK program will give the missing measurement a weight of zero, meaning that this measurement takes no part in the optimisation procedure.

PEST needs a number of input parameters for the fitting procedure (e.g. upper and lower bounds of parameters, weighing factor for each measurement, etc.). Our experience is that the weighing factor for each measurement is the most important input parameter.

Therefore we offer two options for weighing:

'equal' which gives a weight of 1.0 to all observations (so equal weights)

'inverse' which gives a weight that is proportional to the inverse of the observed value.

If the observed value is zero, the weight is set equal to 1.0 in any case.

The option 'equal' implies that high observed values get more weight than low observed values. As described above, the fitting procedure considers two quantities: mass of pesticide and the concentration in the liquid phase. This may lead to completely different weights for these two types of quantities.

E.g. if the mass is initially 50 **mg** and the concentration in the liquid phase is in the order of 1 **mg/mL**, then the fitting procedure will be completely dominated by the decline of the mass of pesticide. So if the option 'equal' is used, the user should choose a mass of solid phase such that the values of the mass of pesticide in **mg** should be in the same order of magnitude as the concentration in liquid phase in **mg/mL**.

The option 'inverse' implies that each measurement gets more or less equal weight for the parameter estimation. This 'inverse' option gave the best results in a few tests. However, we do not claim that this is the best choice for your dataset nor do we claim that the other PEST input parameters are the best choice for your dataset.

The provided package can handle multiple observations for each point in time. The user can specify up to nine replicate sets. A replicate set can contain measurements at different time points and different temperatures. There is no restriction in the number of measurements in a replicate set. The different replicate sets do not necessarily need to contain the same number of measurements or the same time points of measuring. However there is a restriction with respect to the temperatures. The user needs to specify in a separate table at which temperature the measurements are performed and each replicate set should contain at least one measurement performed at each of the temperatures specified in the list.

## 6 Installation of PEARLNEQ

PEARLNEQ is distributed in a zip file. Unzip the file and specify a path (e.g. c:\pearlneq). Be sure there is no space within the specified path, because this will cause failure. The package contains four directories, i.e. Neq\_Bin, Neq\_fortran\_source\_files, Neq\_Example and Pest.

- The Neq\_Bin directory contains the PEARLNEQ executables, PEARLNEQ.EXE and PEARLMK.EXE.
- The PEST optimisation software is available in the Pest directory. As PEST is now available freeware (<http://www.pesthomepage.org/Downloads.php>), we included relevant executables of the latest version as of 13-09-2010 (version 12). Separate installation of PEST is not necessary.
- The Neq\_fortran\_source\_files directory contains the fortran source files used to generate the PEST input files and the programme that calculates the sorption kinetics
- The Neq\_Example directory contains results from an example study; bentazon in a Dutch sandy soil: the Vredepeel dataset (Boesten and Van der Pas, 2000).





## 7 Running the example

The following steps must be followed.

- 1 Run the example, to check if everything works and get experience with the system. Go to the Neq\_Example directory, and run the example by double-clicking on example.bat.
  - The batch file will first call PEARLMK. This pre-processing program generates the input files for PEST, i.e. example.pst, example.tpl and example.ins (see Figure 2, RunId = "example"). The 'pst'-file is the PEST control file. The 'tpl'-file provides the template for the input file for PEARLNEQ and the 'ins'-file describes the location of the simulated values in the 'out'-file.
  - Next Pest programs PESTCHECK, TEMPCHECK and INCHECK are executed to check respectively the 'pst'-file, the 'tpl'-file and the 'ins'-file(s). Press 'enter' after each check to proceed.
  - Then, the optimisation starts. PEST calls PEARLNEQ several times (see Figure 2).
  - If you get an error message after the first step (PEARLMK), type control-break to stop the process and check the error messages available in the example.err file.
- 2 After successful optimisation, read the results from the file example.rec. Choose "select the program from the list" and open with Notepad. The relevant results, including parameter values, 95% confidence intervals and correlation matrices can be found at the end of this file (Section OPTIMISATION RESULTS, see Appendix 2). The meaning of the short acronyms in this rec-file is as follows:
  - fsne = FacSorNeqEqI
  - crd = CofRatDes
  - dt50 = DT50Ref
  - masini = MasIni
  - komeqI = KomEqI
  - met = MolEntTra.
  - PEST also generates parameter sensitivity files etc. Details can be found in the PEST manual, which is available in the PEST subdirectory of the package.
- 3 If you encounter errors during the second step, you can try running PEARLNEQ directly. PEARLMK has created a file example.neq (in ...\\Neq\_Example) which is the input file for pearnEq. You can run PEARLNEQ by typing "...\\Neq\_Bin\\pearlneq example" in a DOS-box.
- 4 PEARLNEQ will create an output file (example.out) and a log file (example.log). The output files are self-explaining. The output file contains the result of the last run which is in PEST by definition the run with the optimised parameters.
- 5 The results from the output file (example.out) are the source for the best fit and you can use the data in this file to create graphs.

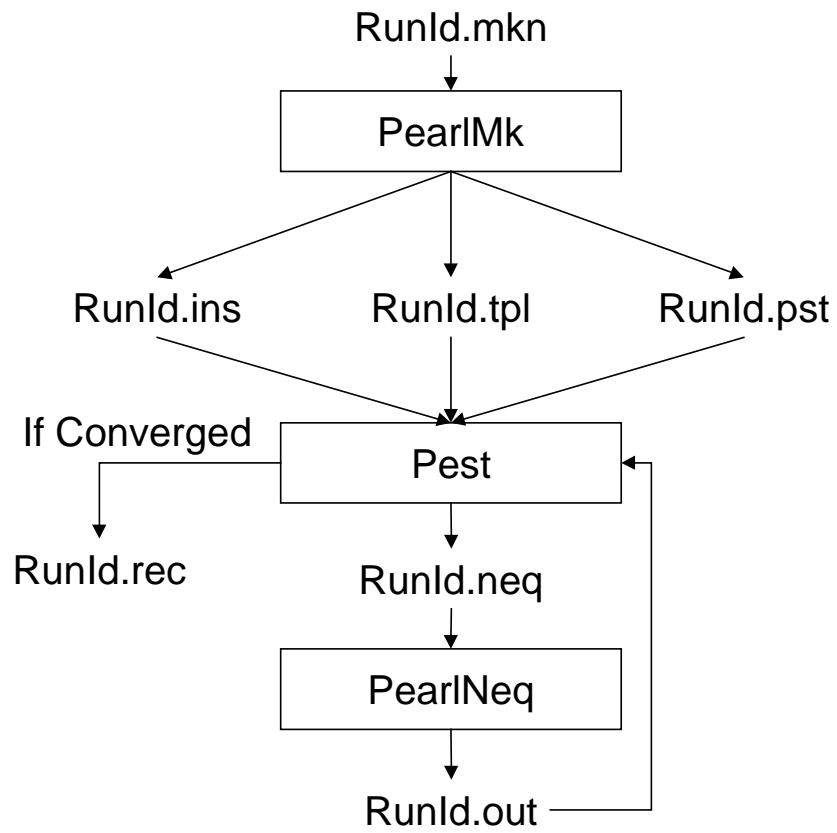


Figure 2. Dataflow diagram for the PEARLNEQ-PEST combination. The acronym RunId is "example" for the example provided.

## 8 Run PEARL\_Neq with your own data

- 1 We assume that you have carried out an appropriate incubation experiment as described before. The first step of optimising your own data consists of **editing the file `example.mkn`**, which can be found in the example subdirectory of the **PEARLNEQ directory**. Open the file with a text editor. *Please make a copy of this file before editing.* Make sure there is no space in the new name. This will give an error. An example of this input file is listed in Appendix 1. The following parameters must be provided:
  - **TimEnd** (d): The duration of the incubation experiment.
  - **MasSol** (g): The mass of dry soil incubated in each jar.
  - **VolLiqSol** (mL): Volume of liquid in the moist soil *during* incubation.
  - **VolLiqAdd** (mL): Volume of liquid added to the soil *after* incubation (i.e. the amount of liquid added to perform a conventional desorption equilibrium experiment).
  - **CntOm** (kg.kg<sup>-1</sup>): Mass fraction of organic matter in the soil.
  - **ConLiqRef** (mg L<sup>-1</sup>): Reference concentration in the liquid phase.
  - **ExpFre** (-): Freundlich exponent; use value taken from adsorption isotherm measured for this pesticide-soil combination
  - **KomEq** (L kg<sup>-1</sup>): coefficient of equilibrium sorption on organic matter. *This parameter will be optimised.* We suggest to use as initial guess a value taken from adsorption isotherm measured for this pesticide-soil combination; in case you have no organic matter content of the soil, set the organic matter to 1.0 and specify the measured Freundlich equilibrium coefficient (see Eqn 6)
  - **MasIni** (µg): The initial total mass of pesticide in each jar. *This parameter will be optimised.* There is no default value for this parameter because it depends on the setup of the experiment.
  - **FacSorNeqEq** (-): factor describing the ratio  $f_{NE} = K_{F,NE}/K_{F,EO}$  as defined by Eqn 4. *This parameter will be optimised*, but you have to specify an initial guess here. We suggest a value of 0.5.
  - **CofRatDes** (d<sup>-1</sup>): the desorption rate coefficient. *This parameter will be optimised*, but you have to specify an initial guess here. We suggest a value of 0.01 d<sup>-1</sup>.
  - Option **OptSor** ('Neq' or 'Eq'):\_option for the type of sorption process (i.e. Non-equilibrium or equilibrium) to be simulated. In case of 'Eq' FacSorNeqEq and CofRatDes are automatically set to zero in the optimisation procedure.
  - **DT50Ref** (d): the transformation half-life under reference conditions, applying to the equilibrium domain for the option of Eqn 5-A and to the liquid phase for the option of Eqn 5-B. *This parameter will be optimised*, but you have to specify an initial guess here. This initial guess could be the 'classical' half-life, which applies to the total soil system (i.e. the equilibrium domain + the non-equilibrium domain).
  - **TemRefTra** (C): The reference temperature, for which the half-life will be provided (set to incubation temperature if data for only one temperature are available and set to 20° C if you have data for multiple temperatures).
  - **MolEntTra** (kJ mol<sup>-1</sup>): the molar enthalpy of transformation. *This parameter will be optimised if you have carried out the experiment at multiple temperatures; otherwise it is a model-input.* In any case you have to specify a value (e.g. 60 kJ mol<sup>-1</sup>) which will be used as an initial guess in case of data for more than one temperature.
  - table **Tem** (C): List of temperatures at which the incubation experiment has been carried out. One temperature is OK if only data for one temperature are available.
  - table **Observations**: List of observations. The first column contains the time (d), the second column the temperature, column 3 contains the total mass of pesticide in the system (µg),

column 4 contains the concentration of pesticide ( $\mu\text{g mL}^{-1}$ ) measured in the pore water of moist soil (then VolLiqAdd = 0) or in the water phase after a desorption experiment (in which case VolLiqAdd is not zero). Column 5 contains the name (integer) of the replicate set and column 6 contains the characters 'OBS'. You can specify up to nine replicate sets. A replicate set can contain measurements at different time points and different temperatures. There is no restriction in the number of measurements in a replicate set. The different replicate sets do not necessarily need to contain the same number of measurements or the same time points of measuring. However each replicate set should contain at least one measurement performed at each of the temperatures specified in table Tem. Measurements in table Observations should be sorted: firstly sort by column 5 (name replicate set; integer), secondly sort by column 2 (temperature) and thirdly sort by column 1 (time).

- option Opt\_weights: options for weights. Two options for weighing are offered: 'equal' which gives a weight of 1.0 to all observations (so equal weights) and 'inverse' which gives a weight that is proportional to the inverse of the observed value; if the observed value is zero, the weight is set equal to 1.0 in any case; you can inspect the weights in the 'pst' file.
  - option Opt\_transformation: option for the concept of the degradation rate. The two options are 'EqIDom' (transformation in the equilibrium domain as described by Eqn 5-A) and 'LiqPhs' (transformation in the liquid phase only as described by Eqn 5-B).
2. Modify the contents of the example.bat file (right click with the mouse and then edit): **replace "example" everywhere it occurs by the name of the copied input file and delete last line of the file (which would generate the graph)**. Repeat step 1-5 of chapter 7.
  3. If the optimization is not successful, you can try re-running PEARLNEQ with different initial guesses of MasIni, DT50Ref, FacSorNeqEqI, KomEqI and CofRatDes.

## 9 Concluding remark

While using PEARLNEQ, we noticed that very regularly the results depend on the initial guesses of the parameters. Therefore we advise you to perform always a number of runs with different initial guesses. We advise you also to analyse the results very carefully, especially the 95% confidence intervals of your parameters. If the interval is wide for a certain parameter, this indicates that the estimated variable is very uncertain. As a consequence it is usually not meaningful to use it any further in the risk assessment.



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## Appendix 1 Example input file

```

*-----
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* STANDARD FILE for pearlmk version 5
* Program to fit the half-life, activation energy and parameters for long-term sorption
* kinetics of pesticides in soil
*
* This file is intended for use with the PEST program (Doherty et al., 1991).
* Please refer to the manual of PEARLNEQ
*
* (c) /Alterra/PBL/RIVM 2011
*-----
--

* Model control
Yes          ScreenOutput
0.0          TimStart          (d)          Start time of experiment
500.0        TimEnd           (d)          End time of experiment
0.01         DelTim           (d)          Time step of Euler's integration
procedure

* System characterization
54.64        MasIni           (ug)         Initial guess of initial mass
45.36        MasSol           (g)          Mass of soil in incubation jar
6.64         VolLiqSol        (mL)         Volume of liquid in the moist soil
0.0          VolLiqAdd        (mL)         Volume of liquid ADDED
0.047        CntOm            (kg.kg-1)    Organic matter content

* Sorption parameter
1.0          ConLiqRef        (mg.L-1)     Reference liquid concentration
0.87         ExpFre           (-)          Freundlich exponent
2.1          KomEq1           (L.kg-1)     Initial guess of Coefficient for
equilibrium sorption
0.5          FacSorNeqEq1     (-)          Initial guess of ratio KfNeq/KfEq1
0.01         CofRatDes        (d-1)        Initial guess of desorption rate
constant
Neq1         OptSor           (-)          Option for type of sorption process
to be simulated

* Transformation parameters
14.00        DT50Ref          (d)          Initial guess of half-life at ref.
temperature
20.0         TemRefTra        (C)          Reference temperature

```

110.0                    MolEntTra                    (kJ.mol-1)                    Initial guess of molar activation energy

\* Temperature at which the incubation experiments have been carried out

table Tem (C)

1 5.0

2 15.0

end\_table

\* Number of replicate sets (range 1 - 9)

\* A set of replicates can contain observation at different time points and temperatures

\* Each replicate set should contain at least one measurement performed at each of the temperatures specified in table Tem

\* 1st sort by Rep. (column 5), 2nd sort by Tem (column 2), 3rd sort by Tim (column 1)

\* specify missing values or values you do not want to include in the optimisation procedure (e.g. outliers) as -99.999

\* PEARLMK will give these observations a weight of zero, meaning that the observation takes no part in the optimisation

2                    NumRepSet                    (-)

\* Provide the results of the measurements

\* Tim Tem Mas                    ConLiq                    Rep.                    observation ID

\* (d) (C) (ug)                    (ug/mL)

table Observations

2	5	52.2400	5.9340	1	OBS
10	5	50.7800	4.4670	1	OBS
42	5	46.0200	3.9340	1	OBS
87	5	37.8200	2.8560	1	OBS
157	5	33.1800	1.9390	1	OBS
244	5	25.5300	1.4640	1	OBS
358	5	18.1900	0.8660	1	OBS
451	5	10.4300	0.6360	1	OBS
2	15	51.5600	5.8530	1	OBS
6	15	48.3100	4.3540	1	OBS
10	15	44.6900	3.5730	1	OBS
42	15	23.9400	1.5650	1	OBS
87	15	10.9600	0.6560	1	OBS
157	15	3.2800	0.1500	1	OBS
244	15	1.4600	0.0310	1	OBS
2	5	51.0200	5.5230	2	OBS
10	5	50.4000	5.6450	2	OBS
42	5	-99.9999	3.3930	2	OBS
87	5	39.4000	3.0080	2	OBS
157	5	32.4500	1.9170	2	OBS

244	5	26.2100	1.4660	2	OBS
358	5	22.4400	0.8980	2	OBS
451	5	8.4200	0.5670	2	OBS
2	15	51.1000	5.9380	2	OBS
6	15	46.4800	4.5310	2	OBS
10	15	54.4400	4.3290	2	OBS
42	15	22.3400	1.7290	2	OBS
87	15	10.8300	0.6860	2	OBS
157	15	2.9900	0.1550	2	OBS
244	15	1.4200	0.0300	2	OBS

end\_table

\* Option for weights of Observations:

\*'equal' gives equal weights to all measurements

\*'inverse' gives weight equal to inverse value of each measurement (if measurement is zero then weight is 1.0)

inverse    Opt\_weights

\* Option for description of transformation rate

\* 'Eqldom' uses rate based on amount of substance in equilibrium domain

\* 'LiqPhs' uses rate based on amount of substance in liquid phase

Eqldom    Opt\_transformation



## Appendix 2 Results of the default example

### Results (taken from last section of REC-file)

These are the results of the default example, provided with the package.

#### OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits	
		lower limit	upper limit
fsne	0.397874	0.261110	0.534637
crd	5.645117E-03	2.658158E-03	8.632077E-03
dt50	15.2567	14.1241	16.3893
masini	56.5621	53.4596	59.6645
komeql	2.78833	2.34018	3.23648
met	105.667	101.813	109.522

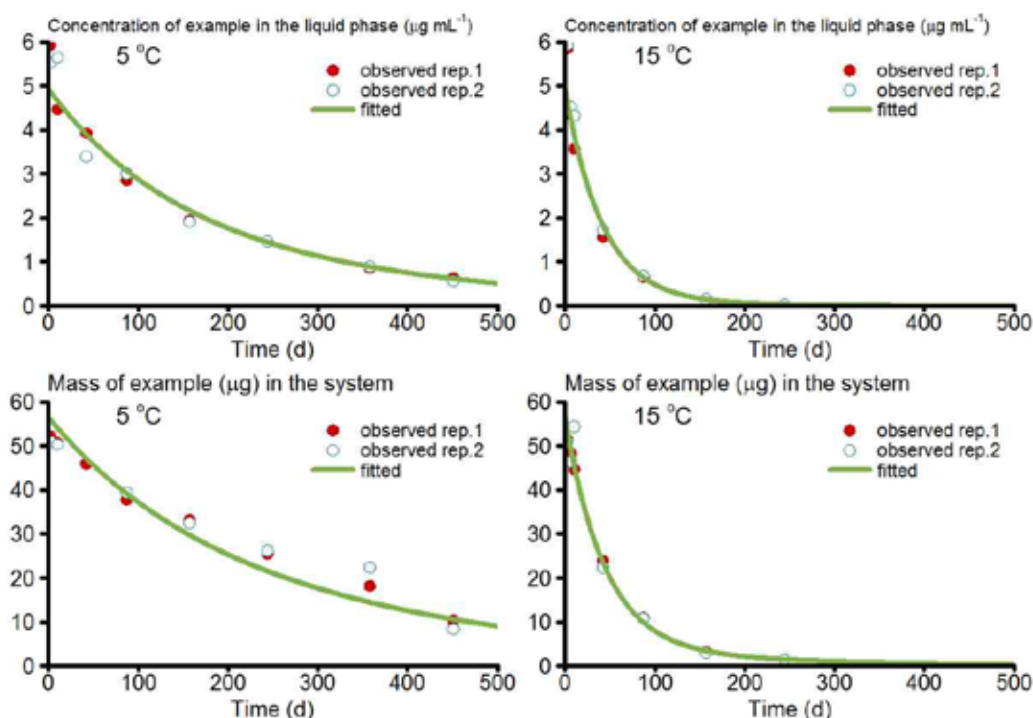
Note: confidence limits provide only an indication of parameter uncertainty. They rely on a linearity assumption which may not extend as far in parameter space as the confidence limits themselves - see PEST manual.

See file example.sen for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	52.2400	56.0685	-3.82855	1.9000E-02	group_1
o2	5.93400	4.87561	1.05839	0.1690	group_1
o3	50.7800	54.1461	-3.36612	2.0000E-02	group_1
o4	4.46700	4.66163	-0.194625	0.2240	group_1
o5	46.0200	47.2145	-1.19446	2.2000E-02	group_1
o6	3.93400	3.90830	2.570465E-02	0.2540	group_1
o7	37.8200	39.1978	-1.37783	2.6000E-02	group_1
o8	2.85600	3.07724	-0.221241	0.3500	group_1
o9	33.1800	29.7477	3.43230	3.0000E-02	group_1
o10	1.93900	2.16419	-0.225189	0.5160	group_1
o11	25.5300	21.5225	4.00753	3.9000E-02	group_1
o12	1.46400	1.44167	2.232551E-02	0.6830	group_1
o13	18.1900	14.4310	3.75896	5.5000E-02	group_1
o14	0.866000	0.884960	-1.896006E-02	1.155	group_1
o15	10.4300	10.5691	-0.139077	9.6000E-02	group_1
o16	0.636000	0.611774	2.422601E-02	1.572	group_1
o17	51.5600	54.1928	-2.63284	1.9000E-02	group_2
o18	5.85300	4.70303	1.14997	0.1710	group_2
o19	48.3100	49.7606	-1.45061	2.1000E-02	group_2
o20	4.35400	4.27852	7.547846E-02	0.2300	group_2
o21	44.6900	45.7072	-1.01722	2.2000E-02	group_2
o22	3.57300	3.89246	-0.319459	0.2800	group_2
o23	23.9400	23.5344	0.405612	4.2000E-02	group_2
o24	1.56500	1.83077	-0.265773	0.6390	group_2
o25	10.9600	9.92738	1.03262	9.1000E-02	group_2
o26	0.656000	0.643818	1.218180E-02	1.524	group_2
o27	3.28000	3.36159	-8.159186E-02	0.3050	group_2
o28	0.150000	0.140302	9.697650E-03	6.667	group_2
o29	1.46000	1.41916	4.084043E-02	0.6850	group_2
o30	3.100000E-02	3.173072E-02	-7.307200E-04	32.26	group_2

o31	51.0200	56.0685	-5.04855	2.0000E-02	group_3
o32	5.52300	4.87561	0.647387	0.1810	group_3
o33	50.4000	54.1461	-3.74612	2.0000E-02	group_3
o34	5.64500	4.66163	0.983375	0.1770	group_3
o35	-99.9999	47.2145	-147.214	0.000	group_3
o36	3.39300	3.90830	-0.515295	0.2950	group_3
o37	39.4000	39.1978	0.202166	2.5000E-02	group_3
o38	3.00800	3.07724	-6.924076E-02	0.3320	group_3
o39	32.4500	29.7477	2.70230	3.1000E-02	group_3
o40	1.91700	2.16419	-0.247189	0.5220	group_3
o41	26.2100	21.5225	4.68753	3.8000E-02	group_3
o42	1.46600	1.44167	2.432551E-02	0.6820	group_3
o43	22.4400	14.4310	8.00896	4.5000E-02	group_3
o44	0.898000	0.884960	1.303994E-02	1.114	group_3
o45	8.42000	10.5691	-2.14908	0.1190	group_3
o46	0.567000	0.611774	-4.477399E-02	1.764	group_3
o47	51.1000	54.1928	-3.09284	2.0000E-02	group_4
o48	5.93800	4.70303	1.23497	0.1680	group_4
o49	46.4800	49.7606	-3.28061	2.2000E-02	group_4
o50	4.53100	4.27852	0.252478	0.2210	group_4
o51	54.4400	45.7072	8.73278	1.8000E-02	group_4
o52	4.32900	3.89246	0.436541	0.2310	group_4
o53	22.3400	23.5344	-1.19439	4.5000E-02	group_4
o54	1.72900	1.83077	-0.101773	0.5780	group_4
o55	10.8300	9.92738	0.902617	9.2000E-02	group_4
o56	0.686000	0.643818	4.218180E-02	1.458	group_4
o57	2.99000	3.36159	-0.371592	0.3340	group_4
o58	0.155000	0.140302	1.469765E-02	6.452	group_4
o59	1.42000	1.41916	8.404300E-04	0.7040	group_4
o60	3.000000E-02	3.173072E-02	-1.730720E-03	33.33	group_4



*Observed values of mass and concentration of the default example for the two replicate sets and two different temperatures and fitted values of mass and concentration of the default example for two different temperatures.*

## Appendix 3 Comparison between an analytical solution and PearlNeq

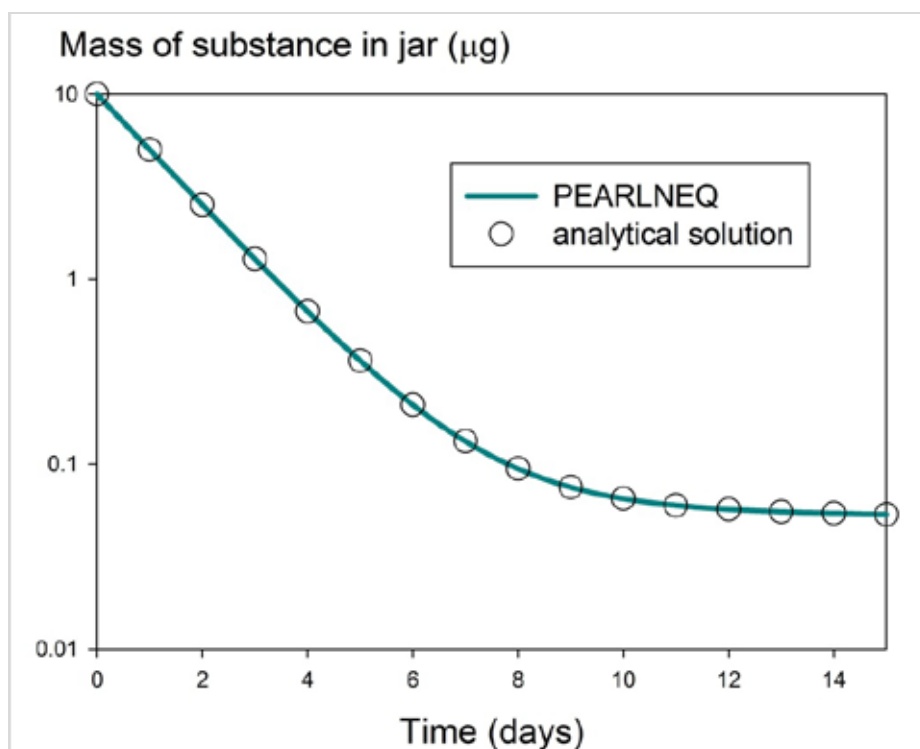
In this appendix an analytical solution for the remaining mass of pesticide is compared with the PearlNeq solution (Appendix 4). The system properties were:

* Mass of dry soil (MasSol) (g)	1.0000
* Volume of water in moist soil (VolLiqsol) (mL)	0.2000
* Volume of water added (VolLiqAdd) (mL)	0.0000
* Initial mass of pesticide (MasIni) (ug)	10.0000
* Reference concentration (ConLiqRef) (ug.mL-1)	1.0000
* Equilibrium sorption coefficient (CofFreEq) (mL.g-1)	1.0000
* Non-equili. sorption coefficient (CofFreNeq) (mL.g-1)	0.5000
* Freundlich exponent (ExFre) (-)	1.0000
* Desorption rate coefficient (CofRatDes) (d-1)	0.0100
* Half-life transformation (DT50Ref) (d)	1.0000
* Reference temperature (TemRefTra) (K)	293.1500

The transformation rate concept of Eqn 5-A was used.

The analytical solution was taken from Appendix 4 of FOCUS (2006).

The figure shows that the PearlNeq solution coincides very well with the analytical solution.



*Comparison between the analytical solution and the PearlNeq solution*





## Appendix 4 Listing of Fortran program PearlNeq

```
program PearlNeq
!=====
==
!
! PEARLNEQ program - simulates pesticide behaviour in a closed incubation system
! assuming
! a two-site Freundlich sorption submodel and first-order
! transformation
! kinetics
!
! version 5.0 of 9 February 2012
!=====
==

use Sishell          ! General routines
use CompilerSpecific ! Compiler specific statements

implicit none

character (len=LineLength) :: Path

integer :: T,Steps,StepsToPrint,NumStep

double precision, parameter :: RGas=8.31432d0 ! Molar gas constant
double precision, parameter :: TimeStart=0.d0 ! Start time
double precision, parameter :: DelTimPrint=1.d0/24.d0 ! Print time step

double precision :: CntOm,CofFreEql,CofFreNeq,CofRatDes,CofRatTra,DelTim, &
DT50Ref,ExpFre,Mas,MasEql,MasIni,MasSol,VolLiqAdd,MolEntTra,TimeEnd,&
VolLiqSol,VolLiqSus,XNeq,ConLiqRef,Tim,Tem,FacTem,TemRefTra,KomEql, FacSorNeqEql,ConPor,C
onSus, &
DeltimNum, XEq,XeqSus,KdApp

type (TableType) :: TemTab

save

IOMode = IOMode_Full
ShowScreen = .false.

! Initial part of program
!-----

! Set the model stamp (version numbers etc)
Call SetModelStamp ()

! Open the input file
call InitCh (Path)
Call OpenPearlNeqFiles(Path)

! System properties
!-----

! Initial mass of pesticide
call GetInput (MasIni,'MasIni','(ug)',Valmin=0.d0)

! Mass of dry soil
call GetInput (MasSol,'MasSol','(g)',Valmin=0.d0)

! Volume of liquid in moist soil and volume of liquid added
call GetInput (VolLiqSol,'VolLiqSol','(mL)',Valmin=0.d0)
call GetInput (VolLiqAdd,'VolLiqAdd','(mL)',Valmin=0.d0)
```

```

! Calculate the volume of the suspension
VolLiqSus = VolLiqSol + VolLiqAdd

! Organic matter content
call GetInput (CntOm,'CntOm','(kg.kg-1)',ValMin=0.d0)

! Sorption parameters
!-----

! Reference concentration
call GetInput (ConLiqRef,'ConLiqRef','(mg.L-1)',ValMin=0.1d0)

! Freundlich N
call GetInput (ExpFre,'ExpFre','(-)',ValMin=0.01d0,ValMax=1.3d0)

! Equilibrium Kom
call GetInput (KomEq1,'KomEq1','(L.kg-1)',ValMin=0.d0)
CofFreEq1 = KomEq1 * CntOm

!
! Ratio Kf,neq/Kf,eq
call GetInput (FacSorNeqEq1,'FacSorNeqEq1','(-)',Valmin=0.d0)

CofFreNeq = FacSorNeqEq1 * CofFreEq1

! Desorption rate coefficient
call GetInput (CofRatDes,'CofRatDes','(d-1)',ValMin=0.d0,ValMax=0.5d0)

! Transformation parameters
!-----

! Molar activation energy
call GetInput &
(MolEntTra,'MolEntTra','(kJ.mol-1)',ValMin=0.d0,ValMax=200.d0)
MolEntTra = 1.d3*MolEntTra

! Pesticide half-life
call GetInput (DT50Ref,'DT50Ref','(d)',ValMin=1.d-1,ValMax=1.d6)

! Reference temperature
call GetInput (TemRefTra,'TemRefTra','(C)')
TemRefTra = TemRefTra + 273.15d0

! Experimental temperatures
!-----
call GetInput (TemTab,'Tem','(C)',Col=1)

! Time parameters
!-----
! End time
call GetInput (TimeEnd,'TimEnd','(d)',ValMin=0.d0)

! Main part of programme
!-----

write (FilOut,'(a)') ' '
write (FilOut,'(a)') '-----'
write (FilOut,'(a)') '* System properties'
write (FilOut,'(a,f10.4)') '* Mass of dry soil (g) :',MasSol
write (FilOut,'(a,f10.4)') '* Volume of water in moist soil (mL) :',VolLiqSol
write (FilOut,'(a,f10.4)') '* Volume of water added (mL) :',VolLiqAdd
write (FilOut,'(a,f10.4)') '* Initial mass of pesticide (ug) :',MasIni
write (FilOut,'(a,f10.4)') '* Reference concentration (ug.mL-1) :',ConLiqRef
write (FilOut,'(a,f10.4)') '* Equilibrium sorption coeff (mL.g-1) :',CofFreEq1
write (FilOut,'(a,f10.4)') '* Non-equili. sorption coeff (mL.g-1) :',CofFreNeq
write (FilOut,'(a,f10.4)') '* Freundlich exponent (-) :',ExpFre
write (FilOut,'(a,f10.4)') '* Desorption rate coefficient (d-1) :',CofRatDes
write (FilOut,'(a,f10.4)') '* Half-life transformation (d) :',DT50Ref

```

```

    if (OptTra() == 1) write (FilOut,'(a)') '* Half-life based on substance in
equilibrium domain'
    if (OptTra() == 2) write (FilOut,'(a)') '* Half-life based on substance in liquid
phase'
write (FilOut,'(a,f10.4)') '* Arrhenius activation energy (kJ mol-1):',MolEntTra/1.d3
write (FilOut,'(a,f10.4)') '* Reference temperature (K)           :',TemRefTra
write (FilOut,'(a)') '-----'
write (FilOut,'(a)') ' '

write (FilOut,'(" ",a6,1x,a8,5(1x,a20))')
'Temp','Time','Mas','ConLiq','XNeq','XEq','Kd_app'
write (FilOut,'(" ",a6,1x,a8,5(1x,a20))') '(C)','(d)','(ug)','(ug.mL-1)','(ug.g-
1)','(ug.g-1)','(mL.g-1)'

Temperatures: do T = 1,TemTab%NumRow

! Calculate the coefficient at ambient temperature
Tem = TemTab%Y(1,T) + 273.15d0
FacTem = exp((-MolEntTra/RGas)*((1.d0/Tem)-(1.d0/TemRefTra)))

CofRatTra = FacTem*log(2.d0)/DT50Ref

! DelTimNum = timestep prescribed by numerical accuracy criterion (d)
DelTimNum = (0.0003d0)/max(CofRatTra, CofRatDes)

! NumStep = number of timesteps within 1 h
NumStep = int((1.0d0/24.d0)/DelTimNum) + 1

! DelTim = timestep (d)
DelTim = (1.0d0/24.d0)/NumStep
StepsToPrint = max(1,int((DelTimPrint+1.d-10)/DelTim))

! Initialize the time loop
Mas = MasIni
XNeq = 0.d0

Tim = TimeStart
Steps = 0
TimeLoop: do

    MasEqL = Mas - MasSol*XNeq
    XEq = MasEqL/MasSol
    ConPor = Freundlich (MasEqL,MasSol,VolLiqSol,CofFreEqL,ConLiqRef,ExpFre)
    ConSus = Freundlich (MasEqL,MasSol,VolLiqSus,CofFreEqL,ConLiqRef,ExpFre)
! calculation of apparent Kd: ratio adsorbed amount:dissolved concentration in
the suspension
    XEqSus=CofFreEqL*ConLiqRef*(ConSus/ConLiqRef)**ExpFre
    KdApp = (XEqSus + XNeq)/ConSus

    if ((mod(Steps,StepsToPrint)) == 0) then
! ConSus is always the only output concentration allowing direct fits of
desorption
! measurements
        write (FilOut,'(f6.1,f10.3,5(1x,f20.8))') Tem-
273.15d0,Tim,Mas,ConSus,XNeq,XEqSus,KdApp
    end if

! Integration of total mass
    if (OptTra() == 1) Mas = Mas + DelTim * (-1.d0*CofRatTra*(Mas-MasSol*XNeq ))
    if (OptTra() == 2) Mas = Mas + DelTim * (-1.d0*CofRatTra*(ConPor*VolLiqSol))

! Integration of non-equilibrium domain
    XNeq = XNeq + DelTim *
(CofRatDes*(CofFreNeq*ConLiqRef*(ConPor/ConLiqRef)**ExpFre-XNeq))

! Increase time
    Tim = Tim + DelTim
    Steps = Steps + 1

```

```

        if (Tim .dge. TimeEnd) exit
    end do TimeLoop

    write (FilOut, '(f6.1,f10.3,5(1x,f20.8))') Tem-
273.15d0, Tim, Mas, ConSus, XNeq, XEqSus, KdApp

    end do Temperatures

!=====
==
!=====
==

contains

    double precision function Freundlich (Mas, MasSol, VolLiq, CofFreEql, ConLiqRef, ExpFre)
    ! This function calculates the Freundlich equilibrium concentration in the liquid
    phase of a system
    !-----
    --

    implicit none

    double precision, parameter :: Err=1.d-4

    double precision :: ConLiqOld, ConLiq, CofFre
    double precision, intent(in) :: Mas, MasSol, VolLiq, CofFreEql, ConLiqRef, ExpFre

    ConLiq=ConLiqRef
    do
        ConLiqOld = ConLiq
        CofFre = &
        CofFreEql * ConLiqRef**(1.d0-ExpFre) * (max(ConLiq,1.d-30) )**(ExpFre-1.d0)
        ConLiq=Mas/(VolLiq+MasSol*CofFre)
        if (abs(ConLiq-ConLiqOld) < Err*abs(ConLiq)) exit
    end do

    Freundlich = ConLiq

end function Freundlich

!=====
==
!=====
==

    subroutine SetModelStamp ()
    ! Set the model stamp

!=====

    implicit none

    Model%ExtInp = '.neq'
    Model%ExtOut = '.out'
    Model%ExtLog = '.log'
    Model%ExtErr = '.err'
    Call InitCh (Model%Date)
    Model%Date = '9-Feb-2012'

end subroutine SetModelStamp

!=====
==
!=====
==

    subroutine OpenPearlNeqFiles (ProgramPath)
    ! Performs the following tasks:

```

```

! (1) Opens the input and output files
! (2) Prints the date-and-time and the Run Id to all opened output files.
! (3) Reads the start-time and end-time, gets the print interval
! (5) Sets the begin CPU time in seconds
!
! The following input and output files are used by the model:
! Unit FilInp:   The input file (extension prl)
! Unit FilOut:   The output file (extension out)
! Unit FilLog:   The log file (extension log)

```

```
!-----
```

```

implicit none

! Declaration of local variables
!-----
character (len=LineLength) :: InFile,OutFile,LogFile,SumFile,ErrFile,RunName
integer :: IOS
character (len=WordLength) :: DateVal,TimeVal,ZoneVal
character (len=LineLength) :: ProgramName,ProgramPath
integer :: F
integer, dimension(8) :: TimArray

! Main part of procedure
!-----

! Create Memory Space for the Words variable
Words%Allocated = .false.
Call Create (Words,NumWords)

! Date and time
Call Date_And_Time (Date=DateVal,Time=TimeVal,Zone=ZoneVal,Values=TimArray)

! Get the run ID
Call InitCh (RunName)
RunName = GetRun()

! Get the path for the program
Call GetProgramName (ProgramName)
Call GetPath (ProgramName,ProgramPath)

! Construct the file names (add the extensions)
call InitCh (InFile)
call InitCh (OutFile)
call InitCh (LogFile)
call InitCh (SumFile)
call InitCh (ErrFile)
InFile = trim(RunName)//Model%ExtInp
OutFile = trim(RunName)//Model%ExtOut
LogFile = trim(RunName)//Model%ExtLog
ErrFile = trim(RunName)//Model%ExtErr

! Open the input file
Open (FilInp,file=trim(InFile),status='old',IOStat=IOS)
if (IOS /= 0) then
  ! Error condition - abort program execution
  Error%Code = -1
  write ( Error%ml,('Cannot find file ",a," with status old')) trim(InFile)
  stop 'Illegal run id - no error file generated'
end if
rewind (FilInp)

! Open the error file
Call OpenAfterDelete (FilErr,trim(ErrFile))

! Open the output file
Call OpenAfterDelete (FilOut,trim(OutFile))

! Open the log file
Call OpenAfterDelete (FilLog,trim(LogFile))

```

```

write (*, ' ("* ")')
write (*, ' ("* -----")')
write (*, ' ("* PEARLNEQ (c) Alterra")')
write (*, ' ("* -----")')
write (*, ' ("*")')
write (*, ' ("* PEARLNEQ version 5.0")')
write (*, ' ("* PEARLNEQ created on ",a)') trim (Model%Date)
write (*, ' ("* ")')
write (*, ' ("* -----")')
write (*, ' ("* ")')

! Write the Run ID, file-names and date-and-time to the output file
do F = 21,22
  write (F, ' ("* -----&
&-----")')
  write (F, ' ("* Results from PEARLNEQ (c) Alterra")')
  write (F, ' ("* PEARLNEQ version 5.0")')
  write (F, ' ("* PEARLNEQ created on ",a)') trim (Model%Date)
  write (F, ' ("* ")')
  write (F, ' ("* Run ID           : ",a)') trim
(GetRun())
  write (F, ' ("* Input file generated on           : ",a2,"-",a2,"-
",a4)') &
  DateVal(7:8),DateVal(5:6),DateVal(1:4)
  write (F, ' ("* -----&
&-----")')
  write (F, ' ("* ")')

end do

end subroutine OpenPearlNEQFiles

!=====
==
!=====
==

integer function OptTra()

! Gets the option for the transformation rate

!=====

implicit none

! Declaration of local variables
!-----
integer :: OptTraLoc
logical :: First=.true.

save

! Initial part of procedure
!-----

if (First) then
  Call GetInput('Opt_transformation','Eqldom LiqPhs',OptTraLoc)
  first=.false.
end if

! Return part of procedure
!-----

OptTra=OptTraLoc

end function OptTra

end program PearlNeq

```

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