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Title Utilities for Pesticide Fate Modelling

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Description Utilities for simple calculations of predicted environmental concentrations ('PEC' values) and for dealing with data from some FOCUS pesticide fate modelling software packages.

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Imports graphics, readr, methods

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License GPL

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Contents

`chent_focus_sw` *Create a chemical compound object for FOCUS Step 1 calculations*

Description

Create a chemical compound object for FOCUS Step 1 calculations

Usage

```
chent_focus_sw(
  name,
  Koc,
  DT50_ws = NA,
  DT50_soil = NA,
  DT50_water = NA,
  DT50_sediment = NA,
  cwsat = 1000,
  mw = NA,
  max_soil = 1,
  max_ws = 1
)
```

Arguments

name	Length one character vector containing the name
Koc	Partition coefficient between organic carbon and water in L/kg.
DT50_ws	Half-life in water/sediment systems in days
DT50_soil	Half-life in soil in days
DT50_water	Half-life in water in days (Step 2)
DT50_sediment	Half-life in sediment in days (Step 2)
cwsat	Water solubility in mg/L
mw	Molar weight in g/mol.
max_soil	Maximum observed fraction (dimensionless) in soil
max_ws	Maximum observed fraction (dimensionless) in water/sediment systems

Value

A list with the substance specific properties

---

drift_data_JKI *Deposition from spray drift expressed as percent of the applied dose as published by the JKI*

Description

Deposition from spray drift expressed as percent of the applied dose as published by the German Julius-Kühn Institute (JKI).

Usage

```
drift_data_JKI
```

Format

A list currently containing matrices with spray drift percentage data for field crops (Ackerbau), and Pome/stone fruit, early and late (Obstbau frueh, spaet).

Details

The data were extracted from the spreadsheet cited below using the R code given in the file `data_generation/drift_data_J` installed with this package. The file itself is not included in the package, as its licence is not clear.

Additional spray drift values were taken from the publication by Rautmann et al. (2001). Specifically, these are the values for early vines, and the values for a 3 m buffer which are incomplete in the spreadsheet.

Note that for vegetables, ornamentals and small fruit, the values for field crops are used for crops < 50 cm, and the vales for late vines are used for crops > 50 cm. In the JKI spreadsheet, it is indicated that these values are used for spray applications with handheld/knapsack equipment (tragbare Spritz- und Sprühgerate).

Values for non-professional use listed in the JKI spreadsheet were not included.

Source

JKI (2010) Spreadsheet 'Tabelle der Abdrifteckwerte.xls', retrieved from http://www.jki.bund.de/no_cache/de/startseite/instit eckwerte.html on 2015-06-11, not present any more 2024-01-31

Rautmann, D., Streloke, M and Winkler, R (2001) New basic drift values in the authorization procedure for plant protection products Mitt. Biol. Bundesanst. Land- Forstwirtsch. 383, 133-141

Examples

```
drift_data_JKI
```

---

drift_parameters_focus

Regression parameters for the Rautmann drift data

Description

The parameters were extracted from Appendix B to the FOCUS surface water guidance using the R code given in the file `data_generation/drift_parameters_focus.R` installed with this package. The appendix itself is not included in the package, as its licence is not clear.

Usage

```
drift_parameters_focus
```

Format

A tibble::tibble.

Details

For the hinge distance, `Inf` was substituted for the cases where no hinge distance is given in the data, in this way parameters C and D are never used for any distance if A and B are used for the case that the distance is smaller than the hinge distance.

References

FOCUS (2014) Generic guidance for Surface Water Scenarios (version 1.4). FOrum for the Co-ordination of pesticde fate models and their USe. http://esdac.jrc.ec.europa.eu/public_path/projects_data/focus/sw/docs/Generic%20FOCUS_SWS_vc1.4.pdf

FOCUS (2001) FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC. Report of the FOCUS Working Group on Surface Water Scenarios, EC Document Reference SANCO/4802/2001-rev.2. 245, Appendix B. https://esdac.jrc.ec.europa.eu/public_path/projects_data/focus/sw/docs/FOCUS_SWS_APPENDIX_B.doc

Rautmann, D., Streloke, M and Winkler, R (2001) New basic drift values in the authorization procedure for plant protection products Mitt. Biol. Bundesanst. Land- Forstwirtsch. 383, 133-141

See Also

drift_percentages_rautmann, PEC_sw_drift

Examples

```
drift_parameters_focus
unique(drift_parameters_focus$crop_group)
```

---

drift_percentages_rautmann

Calculate drift percentages based on Rautmann data

Description

Calculate drift percentages based on Rautmann data

Usage

```
drift_percentages_rautmann(
  distances,
  applications = 1,
 crop_group_focus = c("arable", "hops", "vines, late", "vines, early", "fruit, late",
    "fruit, early", "aerial"),
  formula = c("Rautmann", "FOCUS"),
  widths = 1
)
```

Arguments

distances	The distances in m for which to get PEC values
applications	Number of applications for selection of drift percentile
crop_group_focus	One of the crop groups as used in drift_parameters_focus
formula	By default, the original Rautmann formula is used. If you specify "FOCUS", mean drift input over the width of the water body is calculated as described in Chapter 5.4.5 of the FOCUS surface water guidance
widths	The widths of the water bodies (only used in the FOCUS formula)

References

FOCUS (2014) Generic guidance for Surface Water Scenarios (version 1.4). FOrum for the Co-ordination of pesticde fate models and their USe. http://esdac.jrc.ec.europa.eu/public_path/projects_data/focus/sw/docs/Generic%20FOCUS_SWS_vc1.4.pdf

See Also

drift_parameters_focus, PEC_sw_drift

Examples

```
# Compare JKI data with Rautmann formula
# One application on field crops, for 1 m, 3 m and 5 m distance
drift_data_JKI[[1]][as.character(c(1, 3, 5)), "Ackerbau"]
drift_percentages_rautmann(c(1, 3, 5))
drift_percentages_rautmann(c(1, 3, 5), formula = "FOCUS")

# One application to early or late fruit crops
drift_data_JKI[[1]][as.character(c(3, 5, 20, 50)), "Obstbau frueh"]
drift_percentages_rautmann(c(3, 5, 20, 50), crop_group = "fruit, early")
drift_percentages_rautmann(c(3, 5, 20, 50), crop_group = "fruit, early",
  formula = "FOCUS")
drift_data_JKI[[1]][as.character(c(3, 5, 20, 50)), "Obstbau spaet"]
drift_percentages_rautmann(c(3, 5, 20, 50), crop_group = "fruit, late")
drift_percentages_rautmann(c(3, 5, 20, 50), crop_group = "fruit, late",
  formula = "FOCUS")

# We get a continuum if the waterbody covers the hinge distance
# (11.4 m for 1 early app to fruit)
x <- seq(3, 30, by = 0.1)
d <- drift_percentages_rautmann(x, crop_group = "fruit, early", formula = "FOCUS")
plot(x, d, type = "l",
  xlab = "Distance of near edge [m]",
  ylab = "Mean drift percentage over waterbody width",
  main = "One application to fruit, early")
abline(v = 11.4, lty = 2)
```

EFSA_GW_interception_2014

Subset of EFSA crop interception default values for groundwater modelling

Description

Subset of EFSA crop interception default values for groundwater modelling

Usage

```
EFSA_GW_interception_2014
```

Format

A matrix containing interception values, currently only for some selected crops

Source

European Food Safety Authority (2014) EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. *EFSA Journal* **12**(5):3662, 37 pp., doi:10.2903/j.efsa.2014.3662

Examples

```
EFSA_GW_interception_2014
```

EFSA_washoff_2017 *Subset of EFSA crop washoff default values*

Description

Subset of EFSA crop washoff default values

Usage

```
EFSA_washoff_2017
```

Format

A matrix containing wash-off factors, currently only for some selected crops

Source

European Food Safety Authority (2017) EFSA guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. *EFSA Journal* **15**(10) 4982 doi:10.2903/j.efsa.2017.4982

Examples

```
EFSA_washoff_2017
```

`endpoint` *Retrieve endpoint information from the chyaml field of a chent object*

Description

R6 class objects of class chent represent chemical entities and can hold a list of information loaded from a chemical yaml file in their chyaml field. Such information is extracted and optionally aggregated by this function.

Usage

```
endpoint(
  chent,
  medium = "soil",
  type = c("degradation", "sorption"),
  lab_field = c(NA, "laboratory", "field"),
  redox = c(NA, "aerobic", "anaerobic"),
  value = c("DT50ref", "Kfoc", "N"),
  aggregator = geomean,
  raw = FALSE,
  signif = 3
)

soil_DT50(
  chent,
  aggregator = geomean,
  signif = 3,
  lab_field = "laboratory",
  value = "DT50ref",
  redox = "aerobic",
  raw = FALSE
)

soil_Kfoc(chent, aggregator = geomean, signif = 3, value = "Kfoc", raw = FALSE)

soil_N(chent, aggregator = mean, signif = 3, raw = FALSE)

soil_sorption(
```

```
  chent,
  values = c("Kfoc", "N"),
  aggregators = c(Kfoc = geomean, Koc = geomean, N = mean),
  signif = c(Kfoc = 3, N = 3),
  raw = FALSE
)
```

Arguments

chent	The chent object to get the information from
medium	The medium for which information is sought
type	The information type
lab_field	If not NA, do we want laboratory or field endpoints
redox	If not NA, are we looking for aerobic or anaerobic data
value	The name of the value we want. The list given in the usage section is not exclusive
aggregator	The aggregator function. Can be mean, geomean, or identity, for example.
raw	Should the number(s) be returned as stored in the chent object (could be a character value) to retain original information about precision?
signif	How many significant digits do we want
values	The values to be returned
aggregators	A named vector of aggregator functions to be used

Details

The functions soil_* are functions to extract soil specific endpoints. For the Freundlich exponent, the capital letter N is used in order to facilitate dealing with such data in R. In pesticide fate modelling, this exponent is often called 1/n.

Value

The result from applying the aggregator function to the values converted to a numeric vector, rounded to the given number of significant digits, or, if raw = TRUE, the values as a character value, retaining any implicit information on precision that may be present.

FOCUS_GW_scenarios_2012

A very small subset of the FOCUS Groundwater scenario definitions

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Description

Currently, only scenario names with acronyms and a small subset of the soil definitions are provided. The soil definitions are from page 46ff. from FOCUS (2012).

Usage

```
FOCUS_GW_scenarios_2012
```

Format

An object of class `list` of length 2.

References

FOCUS (2012) Generic guidance for Tier 1 FOCUS ground water assessments. Version 2.1. FOrum for the Co-ordination of pesticde fate models and their USe. http://focus.jrc.ec.europa.eu/gw/docs/Generic_guidance_FOCV2

Examples

```
FOCUS_GW_scenarios_2012
```

FOCUS_Step_12_scenarios

Step 1/2 scenario data as distributed with the FOCUS Step 1/2 calculator

---

Description

The data were extracted from the scenario.txt file using the R code shown below. The text file is not included in the package as its licence is not clear.

Format

A list containing the scenario names in a character vector called 'names', the drift percentiles in a matrix called 'drift', interception percentages in a matrix called 'interception' and the runoff/drainage percentages for Step 2 calculations in a matrix called 'rd'.

Examples

```
## Not run:
  # This is the code that was used to extract the data
  scenario_path <- "inst/extdata/FOCUS_Step_12_scenarios.txt"
  scenarios <- readLines(scenario_path)[9:38]
  FOCUS_Step_12_scenarios <- list()
  sce <- read.table(text = scenarios, sep = "\t", header = TRUE, check.names = FALSE,
    stringsAsFactors = FALSE)
  FOCUS_Step_12_scenarios$names = sce$Crop
  rownames(sce) <- sce$Crop
  FOCUS_Step_12_scenarios$drift = sce[, 3:11]
  FOCUS_Step_12_scenarios$interception = sce[, 12:15]
  sce_2 <- readLines(scenario_path)[41:46]
  rd <- read.table(text = sce_2, sep = "\t")[1:2]
  rd_mat <- matrix(rd$V2, nrow = 3, byrow = FALSE)
  dimnames(rd_mat) = list(Time = c("Oct-Feb", "Mar-May", "Jun-Sep"),
```

```
                          Region = c("North", "South"))
  FOCUS_Step_12_scenarios$rd = rd_mat
  save(FOCUS_Step_12_scenarios, file = "data/FOCUS_Step_12_scenarios.RData")

## End(Not run)

# And this is the resulting data
FOCUS_Step_12_scenarios
```

`FOMC_actual_twa` *Actual and maximum moving window time average concentrations for FOMC kinetics*

Description

Actual and maximum moving window time average concentrations for FOMC kinetics

Usage

```
FOMC_actual_twa(
  alpha = 1.0001,
  beta = 10,
  times = c(0, 1, 2, 4, 7, 14, 21, 28, 42, 50, 100)
)
```

Arguments

`alpha`	Parameter of the FOMC model
`beta`	Parameter of the FOMC model
`times`	The output times, and window sizes for time weighted average concentrations

Author(s)

Johannes Ranke

Source

FOCUS (2014) Generic Guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration, Version 1.1, 18 December 2014, p. 251

Examples

```
FOMC_actual_twa(alpha = 1.0001, beta = 10)
```

geomean *Calculate the geometric mean*

Description

Based on some posts in a thread on Stackoverflow http://stackoverflow.com/questions/2602583/geometric-mean-is-there-a-built-in This function returns NA if NA values are present and na.rm = FALSE (default). If negative values are present, it gives an error message. If at least one element of the vector is 0, it returns 0.

Usage

```
geomean(x, na.rm = FALSE)
```

Arguments

x	Vector of numbers
na.rm	Should NA values be omitted?

Value

The geometric mean

Author(s)

Johannes Ranke

Examples

```
geomean(c(1, 3, 9))
geomean(c(1, 3, NA, 9))
## Not run: geomean(c(1, -3, 9)) # returns an error
```

get_vertex *Fit a parabola through three points*

Description

This was inspired by an answer on stackoverflow https://stackoverflow.com/a/717791

Usage

```
get_vertex(x, y)
```

Arguments

x	Three x coordinates
y	Three y coordinates

GUS *Groundwater ubiquity score based on Gustafson (1989)*

Description

The groundwater ubiquity score GUS is calculated according to the following equation

$$GUS = \log_{10} DT50_{soil}(4 - \log_{10} K_{oc})$$

Usage

```
GUS(...)

## S3 method for class 'numeric'
GUS(DT50, Koc, ...)

## S3 method for class 'chent'
GUS(
  chent,
  degradation_value = "DT50ref",
  lab_field = "laboratory",
  redox = "aerobic",
  sorption_value = "Kfoc",
  degradation_aggregator = geomean,
  sorption_aggregator = geomean,
  ...
)

## S3 method for class 'GUS_result'
print(x, ..., digits = 1)
```

Arguments

`...`	Included in the generic to allow for further arguments later. Therefore this also had to be added to the specific methods.
`DT50`	Half-life of the chemical in soil. Should be a field half-life according to Gustafson (1989). However, leaching to the sub-soil can not completely be excluded in field dissipation experiments and Gustafson did not refer to any normalisation procedure, but says the field study should be conducted under use conditions.
`Koc`	The sorption constant normalised to organic carbon. Gustafson does not mention the nonlinearity of the sorption constant commonly found and usually described by Freundlich sorption, therefore it is unclear at which reference concentration the Koc should be observed (and if the reference concentration would be in soil or in porewater).
`chent`	If a chent is given with appropriate information present in its chyaml field, this information is used, with defaults specified below.

`degradation_value`
: Which of the available degradation values should be used?

`lab_field`
: Should laboratory or field half-lives be used? This defaults to lab in this implementation, in order to avoid double-accounting for mobility. If comparability with the original GUS values given by Gustafson (1989) is desired, non-normalised first-order field half-lives obtained under actual use conditions should be used.

`redox`
: Aerobic or anaerobic degradation data

`sorption_value`
: Which of the available sorption values should be used? Defaults to Kfoc as this is what is generally available from the European pesticide peer review process. These values generally use a reference concentration of 1 mg/L in porewater, that means they would be expected to be Koc values at a concentration of 1 mg/L in the water phase.

`degradation_aggregator`
: Function for aggregating half-lives

`sorption_aggregator`
: Function for aggregation Koc values

`x`
: An object of class GUS_result to be printed

`digits`
: The number of digits used in the print method

Value

A list with the DT50 and Koc used as well as the resulting score of class GUS_result

Author(s)

Johannes Ranke

References

Gustafson, David I. (1989) Groundwater ubiquity score: a simple method for assessing pesticide leachability. *Environmental toxicology and chemistry* **8**(4) 339–57.

`max_twa` *The maximum time weighted average concentration for a moving window*

Description

If you generate your time series using `sawtooth`, you need to make sure that the length of the time series allows for finding the maximum. It is therefore recommended to check this using `plot.one_box` using the window size for the argument `max_twa`.

Usage

```
max_twa(x, window = 21)
```

Arguments

x	An object of type one_box
window	The size of the moving window

Details

The method working directly on fitted mkinfit objects uses the equations given in the PEC soil section of the FOCUS guidance and is restricted SFO, FOMC and DFOP models and to the parent compound

References

FOCUS (2006) "Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration" Report of the FOCUS Work Group on Degradation Kinetics, EC Document Reference Sanco/10058/2005 version 2.0, 434 pp, http://esdac.jrc.ec.europa.eu/projects/degradation-kinetics

See Also

twa

Examples

```
pred <- sawtooth(one_box(10),
  applications = data.frame(time = c(0, 7), amount = c(1, 1)))
max_twa(pred)
pred_FOMC <- mkinfit("FOMC", FOCUS_2006_C, quiet = TRUE)
max_twa(pred_FOMC)
```

---

one_box *Create a time series of decline data*

Description

Create a time series of decline data

Usage

```
one_box(x, ini, ..., t_end = 100, res = 0.01)

## S3 method for class 'numeric'
one_box(x, ini = 1, ..., t_end = 100, res = 0.01)

## S3 method for class 'character'
one_box(x, ini = 1, parms, ..., t_end = 100, res = 0.01)

## S3 method for class 'mkinfit'
one_box(x, ini = "model", ..., t_end = 100, res = 0.01)
```

Arguments

x	When numeric, this is the half-life to be used for an exponential decline. When a character string specifying a parent decline model is given e.g. FOMC, parms must contain the corresponding parameters. If x is an mkinfit object, the decline is calculated from this object.
ini	The initial amount. If x is an mkinfit object, and ini is 'model', the fitted initial concentrations are used. Otherwise, ini must be numeric. If it has length one, it is used for the parent and initial values of metabolites are zero, otherwise, it must give values for all observed variables.
...	Further arguments passed to methods
t_end	End of the time series
res	Resolution of the time series
parms	A named numeric vector containing the model parameters

Value

An object of class one_box, inheriting from ts.

Examples

```
# Only use a half-life
pred_0 <- one_box(10)
plot(pred_0)

# Use a fitted mkinfit model
require(mkin)
fit <- mkinfit("FOMC", FOCUS_2006_C, quiet = TRUE)
pred_1 <- one_box(fit)
plot(pred_1)

# Use a model with more than one observed variable
m_2 <- mkinmod(parent = mkinsub("SFO", "m1"), m1 = mkinsub("SFO"))
fit_2 <- mkinfit(m_2, FOCUS_2006_D, quiet = TRUE)
pred_2 <- one_box(fit_2, ini = "model")
plot(pred_2)
```

PEC_FOMC_accu_rel — *Get the relative accumulation of an FOMC model over multiples of an interval*

Description

Get the relative accumulation of an FOMC model over multiples of an interval

Usage

```
PEC_FOMC_accu_rel(n, interval, FOMC)
```

Arguments

n	number of applications
interval	Time between applications
FOMC	Named numeric vector containing the FOMC parameters alpha and beta

Value

A numeric vector containing all n accumulation factors for the n applications

---

PEC_soil *Calculate predicted environmental concentrations in soil*

Description

This is a basic calculation of a contaminant concentration in bulk soil based on complete, instantaneous mixing. If an interval is given, an attempt is made at calculating a long term maximum concentration using the concepts layed out in the PPR panel opinion (EFSA PPR panel 2012 and in the EFSA guidance on PEC soil calculations (EFSA, 2015, 2017).

Usage

```
PEC_soil(
  rate,
  rate_units = "g/ha",
  interception = 0,
  mixing_depth = 5,
  PEC_units = "mg/kg",
  PEC_pw_units = "mg/L",
  interval = NA,
  n_periods = Inf,
  tillage_depth = 20,
  leaching_depth = tillage_depth,
  crop = "annual",
  cultivation = FALSE,
  chent = NA,
  DT50 = NA,
  FOMC = NA,
  Koc = NA,
  Kom = Koc/1.724,
  t_avg = 0,
  t_act = NULL,
  scenarios = c("default", "EFSA_2017", "EFSA_2015"),
  leaching = scenarios == "EFSA_2017",
  porewater = FALSE
)
```

Arguments

rate	Application rate in units specified below
rate_units	Defaults to g/ha
interception	The fraction of the application rate that does not reach the soil
mixing_depth	Mixing depth in cm
PEC_units	Requested units for the calculated PEC. Only mg/kg currently supported
PEC_pw_units	Only mg/L currently supported
interval	Period of the deeper mixing. The default is NA, i.e. no deeper mixing. For annual deeper mixing, set this to 365 when degradation units are in days
n_periods	Number of periods to be considered for long term PEC calculations
tillage_depth	Periodic (see interval) deeper mixing in cm
leaching_depth	EFSA (2017) uses the mixing depth (ecotoxicological evaluation depth) to calculate leaching for annual crops where tillage takes place. By default, losses from the layer down to the tillage depth are taken into account in this implementation.
crop	Ignored for scenarios other than EFSA_2017. Only annual crops are supported when these scenarios are used. Only crops with a single cropping cycle per year are currently supported.
cultivation	Does mechanical cultivation in the sense of EFSA (2017) take place, i.e. twice a year to a depth of 5 cm? Ignored for scenarios other than EFSA_2017
chent	An optional chent object holding substance specific information. Can also be a name for the substance as a character string
DT50	If specified, overrides soil DT50 endpoints from a chent object If DT50 is not specified here and not available from the chent object, zero degradation is assumed
FOMC	If specified, it should be a named numeric vector containing the FOMC parameters alpha and beta. This overrides any other degradation endpoints, and the degradation during the interval and after the maximum PEC is calculated using these parameters without temperature correction
Koc	If specified, overrides Koc endpoints from a chent object
Kom	Calculated from Koc by default, but can explicitly be specified as Kom here
t_avg	Averaging times for time weighted average concentrations
t_act	Time series for actual concentrations
scenarios	If this is 'default', the DT50 will be used without correction and soil properties as specified in the REACH guidance (R.16, Table R.16-9) are used for porewater PEC calculations. If this is "EFSA_2015", the DT50 is taken to be a modelling half-life at 20°C and pF2 (for when 'chent' is specified, the DegT50 with destination 'PECgw' will be used), and corrected using an Arrhenius activation energy of 65.4 kJ/mol. Also model and scenario adjustment factors from the EFSA guidance are used.
leaching	Should leaching be taken into account? The default is FALSE, except when the EFSA_2017 scenarios are used.

`porewater` Should equilibrium porewater concentrations be estimated based on Kom and the organic carbon fraction of the soil instead of total soil concentrations? Based on equation (7) given in the PPR panel opinion (EFSA 2012, p. 24) and the scenarios specified in the EFSA guidance (2015, p. 13).

Details

This assumes that the complete load to soil during the time specified by 'interval' (typically 365 days) is dosed at once. As in the PPR panel opinion cited below (EFSA PPR panel 2012), only temperature correction using the Arrhenius equation is performed.

Total soil and porewater PEC values for the scenarios as defined in the EFSA guidance (2017, p. 14/15) can easily be calculated.

Value

The predicted concentration in soil

Note

While time weighted average (TWA) concentrations given in the examples from the EFSA guidance from 2015 (p. 80) are be reproduced, this is not true for the TWA concentrations given for the same example in the EFSA guidance from 2017 (p. 92).

According to the EFSA guidance (EFSA, 2017, p. 43), leaching should be taken into account for the EFSA 2017 scenarios, using the evaluation depth (here mixing depth) as the depth of the layer from which leaching takes place. However, as the amount leaching below the evaluation depth (often 5 cm) will partly be mixed back during tillage, the default in this function is to use the tillage depth for the calculation of the leaching rate.

If temperature information is available in the selected scenarios, as e.g. in the EFSA scenarios, the DT50 for groundwater modelling (destination 'PECgw') is taken from the chent object, otherwise the DT50 with destination 'PECsoil'.

Author(s)

Johannes Ranke

References

EFSA Panel on Plant Protection Products and their Residues (2012) Scientific Opinion on the science behind the guidance for scenario selection and scenario parameterisation for predicting environmental concentrations of plant protection products in soil. *EFSA Journal* **10**(2) 2562, doi:10.2903/j.efsa.2012.2562

EFSA (European Food Safety Authority) 2017) EFSA guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. *EFSA Journal* **15**(10) 4982 doi:10.2903/j.efsa.2017.4982

EFSA (European Food Safety Authority) (2015) EFSA guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. *EFSA Journal* **13**(4) 4093 doi:10.2903/j.efsa.2015.4093

Examples

```
PEC_soil(100, interception = 0.25)

# This is example 1 starting at p. 92 of the EFSA guidance (2017)
# Note that TWA concentrations differ from the ones given in the guidance
# for an unknown reason (the values from EFSA (2015) can be reproduced).
PEC_soil(1000, interval = 365, DT50 = 250, t_avg = c(0, 21),
               Kom = 1000, scenarios = "EFSA_2017")
PEC_soil(1000, interval = 365, DT50 = 250, t_av = c(0, 21),
               Kom = 1000, scenarios = "EFSA_2017", porewater = TRUE)

# This is example 1 starting at p. 79 of the EFSA guidance (2015)
PEC_soil(1000, interval = 365, DT50 = 250, t_avg = c(0, 21),
               scenarios = "EFSA_2015")
PEC_soil(1000, interval = 365, DT50 = 250, t_av = c(0, 21),
               Kom = 1000, scenarios = "EFSA_2015", porewater = TRUE)

# The following is from example 4 starting at p. 85 of the EFSA guidance (2015)
# Metabolite M2
# Calculate total and porewater soil concentrations for tier 1 scenarios
# Relative molar mass is 100/300, formation fraction is 0.7 * 1
results_pfm <- PEC_soil(100/300 * 0.7 * 1 * 1000, interval = 365, DT50 = 250, t_avg = c(0, 21),
                        scenarios = "EFSA_2015")
results_pfm_pw <- PEC_soil(100/300 * 0.7 * 1000, interval = 365, DT50 = 250, t_av = c(0, 21),
                           Kom = 100, scenarios = "EFSA_2015", porewater = TRUE)
```

PEC_soil_mets *Calculate initial and accumulation PEC soil for a set of metabolites*

Description

Calculate initial and accumulation PEC soil for a set of metabolites

Usage

```
PEC_soil_mets(rate, mw_parent, mets, interval = 365, ...)
```

Arguments

rate	Application rate in units specified below
mw_parent	The molecular weight of the parent compound
mets	A dataframe with metabolite identifiers as rownames and columns "mw", "occ" and "DT50" holding their molecular weight, maximum occurrence in soil and their soil DT50
interval	The interval for accumulation calculations
...	Further arguments are passed to PEC_soil

PEC_sw_drainage_UK *Calculate initial predicted environmental concentrations in surface water due to drainage using the UK method*

Description

This implements the method specified in the UK data requirements handbook and was checked against the spreadsheet published on the CRC website

Usage

```
PEC_sw_drainage_UK(
  rate,
  interception = 0,
  Koc,
  latest_application = NULL,
  soil_DT50 = NULL,
  model = NULL,
  model_parms = NULL
)
```

Arguments

rate	Application rate in g/ha
interception	The fraction of the application rate that does not reach the soil
Koc	The sorption coefficient normalised to organic carbon in L/kg
latest_application	Latest application date, formatted as e.g. "01 July"
soil_DT50	Soil degradation half-life, if SFO kinetics are to be used
model	The soil degradation model to be used. Either one of "FOMC", "DFOP", "HS", or "IORE", or an mkinmod object
model_parms	A named numeric vector containing the model parameters

Value

The predicted concentration in surface water in µg/L

Author(s)

Johannes Ranke

References

HSE's Chemicals Regulation Division (CRD) Active substance PECsw calculations (for UK specific authorisation requests) https://www.hse.gov.uk/pesticides/topics/pesticide-approvals/pesticides-registration/data-requirements-handbook/fate/active-substance-uk.htm accessed 2019-09-27

Drainage PECs Version 1.0 (2015) Spreadsheet published at https://www.hse.gov.uk/pesticides/topics/pesticide-approvals/pesticides-registration/data-requirements-handbook/fate/pec-tools-2015/PEC%20sw-sed%20(drainage).xlsx accessed 2019-09-27

Examples

```
PEC_sw_drainage_UK(150, Koc = 100)
```

PEC_sw_drift *Calculate predicted environmental concentrations in surface water due to drift*

Description

This is a basic, vectorised form of a simple calculation of a contaminant concentration in surface water based on complete, instantaneous mixing with input via spray drift.

Usage

```
PEC_sw_drift(
  rate,
  applications = 1,
  water_depth = 30,
  drift_percentages = NULL,
  drift_data = c("JKI", "RF"),
 crop_group_JKI = c("Ackerbau", "Obstbau frueh", "Obstbau spaet", "Weinbau frueh",
   "Weinbau spaet", "Hopfenbau", "Flaechenkulturen > 900 l/ha", "Gleisanlagen"),
 crop_group_focus = c("arable", "hops", "vines, late", "vines, early", "fruit, late",
    "fruit, early", "aerial"),
  distances = c(1, 5, 10, 20),
  formula = c("Rautmann", "FOCUS"),
  water_width = 100,
  side_angle = 90,
  rate_units = "g/ha",
  PEC_units = "µg/L"
)
```

Arguments

rate	Application rate in units specified below
applications	Number of applications for selection of drift percentile

water_depth	Depth of the water body in cm
drift_percentages	Percentage drift values for which to calculate PECsw. Overrides 'drift_data' and 'distances' if not NULL.
drift_data	Source of drift percentage data. If 'JKI', the drift_data_JKI included in the package is used. If 'RF', the Rautmann drift data are calculated either in the original form or integrated over the width of the water body, depending on the 'formula' argument.
crop_group_JKI	When using the 'JKI' drift data, one of the German names as used in drift_parameters_focus.
crop_group_focus	One of the crop groups as used in drift_parameters_focus
distances	The distances in m for which to get PEC values
formula	By default, the original Rautmann formula is used. If you specify "FOCUS", mean drift input over the width of the water body is calculated as described in Chapter 5.4.5 of the FOCUS surface water guidance
water_width	Width of the water body in cm
side_angle	The angle of the side of the water relative to the bottom which is assumed to be horizontal, in degrees. The SYNOPS model assumes 45 degrees here.
rate_units	Defaults to g/ha
PEC_units	Requested units for the calculated PEC. Only µg/L currently supported

Value

The predicted concentration in surface water

Author(s)

Johannes Ranke

See Also

drift_parameters_focus, drift_percentages_rautmann

Examples

```
PEC_sw_drift(100)
# Alternatively, we can use the formula for a single application to
# "Ackerbau" from the paper
PEC_sw_drift(100, drift_data = "RF")

# This makes it possible to also use different distances
PEC_sw_drift(100, distances = c(1, 3, 5, 6, 10, 20, 50, 100), drift_data = "RF")

# or consider aerial application
PEC_sw_drift(100, distances = c(1, 3, 5, 6, 10, 20, 50, 100), drift_data = "RF",
  crop_group_focus = "aerial")
```

```
# Using custom drift percentages is also supported
PEC_sw_drift(100, drift_percentages = c(2.77, 0.95, 0.57, 0.48, 0.29, 0.15, 0.06, 0.03))

# The influence of assuming a 45° angle of the sides of the waterbody and the width of the
# waterbody can be illustrated
PEC_sw_drift(100)
PEC_sw_drift(100, drift_data = "RF")
PEC_sw_drift(100, drift_data = "RF", formula = "FOCUS")
PEC_sw_drift(100, drift_data = "RF", formula = "FOCUS", side_angle = 45)
PEC_sw_drift(100, drift_data = "RF", formula = "FOCUS", side_angle = 45, water_width = 200)
```

`PEC_sw_exposit_drainage` *Calculate PEC surface water due to drainage as in Exposit 3*

Description

This is a reimplementation of the calculation described in the Exposit 3.02 spreadsheet file, in the worksheet "Konzept Drainage". Although there are four groups of compounds ("Gefährdungsgruppen"), only one distinction is made in the calculations, between compounds with low mobility (group 1) and compounds with modest to high mobility (groups 2, 3 and 4). In this implementation, the group is derived only from the Koc, if not given explicitly. For details, see the discussion of the function arguments below.

Usage

```
PEC_sw_exposit_drainage(
  rate,
  interception = 0,
  Koc = NA,
  mobility = c(NA, "low", "high"),
  DT50 = Inf,
  t_drainage = 3,
  V_ditch = 30,
  V_drainage = c(spring = 10, autumn = 100),
  dilution = 2
)
```

Arguments

`rate`	The application rate in g/ha
`interception`	The fraction intercepted by the crop
`Koc`	The sorption coefficient to soil organic carbon used to determine the mobility. A trigger value of 550 L/kg is used in order to decide if Koc » 500.
`mobility`	Overrides what is determined from the Koc.
`DT50`	The soil half-life in days

t_drainage	The time between application and the drainage event, where degradation occurs, in days
V_ditch	The volume of the ditch is assumed to be 1 m * 100 m * 30 cm = 30 m3
V_drainage	The drainage volume, equivalent to 1 mm precipitation on 1 ha for spring/summer or 10 mm for autumn/winter/early spring.
dilution	The dilution factor

Value

A list containing the following components

perc_runoff The runoff percentages for dissolved and bound substance

runoff A matrix containing dissolved and bound input for the different distances

PEC_sw_runoff A matrix containing PEC values for dissolved and bound substance for the different distances. If the rate was given in g/ha, the PECsw are in microg/L.

Source

Excel 3.02 spreadsheet available from https://www.bvl.bund.de/SharedDocs/Downloads/04_Pflanzenschutzmittel/zul_umwelt_exposit.html

See Also

perc_runoff_exposit for runoff loss percentages and perc_runoff_reduction_exposit for runoff reduction percentages used

Examples

```
PEC_sw_exposit_drainage(500, Koc = 150)
```

PEC_sw_exposit_runoff *Calculate PEC surface water due to runoff and erosion as in Exposit 3*

Description

This is a reimplementation of the calculation described in the Exposit 3.02 spreadsheet file, in the worksheet "Konzept Runoff".

Usage

```
PEC_sw_exposit_runoff(
  rate,
  interception = 0,
  Koc,
  DT50 = Inf,
  t_runoff = 3,
```

```
  exposit_reduction_version = c("3.02", "3.01a", "3.01a2", "2.0"),
  V_ditch = 30,
  V_event = 100,
  dilution = 2
)
```

Arguments

rate	The application rate in g/ha
interception	The fraction intercepted by the crop
Koc	The sorption coefficient to soil organic carbon
DT50	The soil half-life in days
t_runoff	The time between application and the runoff event, where degradation occurs, in days
exposit_reduction_version	The version of the reduction factors to be used. "3.02" is the current version used in Germany, "3.01a" is the version with additional percentages for 3 m and 6 m buffer zones used in Switzerland. "3.01a2" is a version introduced for consistency with previous calculations performed for a 3 m buffer zone in Switzerland, with the same reduction being applied to the dissolved and the bound fraction.
V_ditch	The volume of the ditch is assumed to be 1 m * 100 m * 30 cm = 30 m3
V_event	The unreduced runoff volume, equivalent to 10 mm precipitation on 1 ha
dilution	The dilution factor

Value

A list containing the following components

perc_runoff The runoff percentages for dissolved and bound substance

runoff A matrix containing dissolved and bound input for the different distances

PEC_sw_runoff A matrix containing PEC values for dissolved and bound substance for the different distances. If the rate was given in g/ha, the PECsw are in microg/L.

Source

Excel 3.02 spreadsheet available from https://www.bvl.bund.de/SharedDocs/Downloads/04_Pflanzenschutzmittel/zul_umwelt_exposit.html

See Also

perc_runoff_exposit for runoff loss percentages and perc_runoff_reduction_exposit for runoff reduction percentages used

Examples

```
PEC_sw_exposit_runoff(500, Koc = 150)
PEC_sw_exposit_runoff(600, Koc = 10000, DT50 = 195, exposit = "3.01a")
```

PEC_sw_focus *Calculate PEC surface water at FOCUS Step 1*

Description

This is a reimplementation of the FOCUS Step 1 and 2 calculator version 3.2, authored by Michael Klein, in R. Note that results for multiple applications should be compared to the corresponding results for a single application. At current, this is not done automatically in this implementation. Only Step 1 PECs are calculated. However, input files can be generated that are suitable as input for the FOCUS calculator.

Usage

```
PEC_sw_focus(
  parent,
  rate,
  n = 1,
  i = NA,
  comment = "",
  met = NULL,
  f_drift = NA,
  f_rd = 0.1,
  scenario = FOCUS_Step_12_scenarios$names,
  region = c("n", "s"),
  season = c(NA, "of", "mm", "js"),
  interception = c("no interception", "minimal crop cover", "average crop cover",
    "full canopy"),
  met_form_water = TRUE,
  txt_file = "pesticide.txt",
  overwrite = FALSE,
  append = FALSE
)
```

Arguments

parent	A list containing substance specific parameters, e.g. conveniently generated by chent_focus_sw.
rate	The application rate in g/ha. Overriden when applications are given explicitly
n	The number of applications
i	The application interval
comment	A comment for the input file
met	A list containing metabolite specific parameters. e.g. conveniently generated by chent_focus_sw. If not NULL, the PEC is calculated for this compound, not the parent.

f_drift	The fraction of the application rate reaching the waterbody via drift. If NA, this is derived from the scenario name and the number of applications via the drift data defined by the FOCUS_Step_12_scenarios
f_rd	The fraction of the amount applied reaching the waterbody via runoff/drainage. At Step 1, it is assumed to be 10%, be it the parent or a metabolite
scenario	The name of the scenario. Must be one of the scenario names given in FOCUS_Step_12_scenarios
region	'n' for Northern Europe or 's' for Southern Europe. If NA, only Step 1 PECsw are calculated
season	'of' for October to February, 'mm' for March to May, and 'js' for June to September. If NA, only step 1 PECsw are calculated
interception	One of 'no interception' (default), 'minimal crop cover', 'average crop cover' or 'full canopy'
met_form_water	Should the metabolite formation in water be taken into account? This can be switched off to check the influence and to compare with previous versions of the Steps 12 calculator
txt_file	the name, and potentially the full path to the Steps.12 input text file to which the specification of the run(s) should be written
overwrite	Should an existing file a the location specified in txt_file be overwritten? Only takes effect if append is FALSE.
append	Should the input text file be appended, if it exists?

Note

The formulas for input to the waterbody via runoff/drainage of the parent and subsequent formation of the metabolite in water is not documented in the model description coming with the calculator. As one would expect, this appears to be (as we get the same results) calculated by multiplying the application rate with the molar weight correction and the formation fraction in water/sediment systems.

Step 2 is not implemented.

References

FOCUS (2014) Generic guidance for Surface Water Scenarios (version 1.4). FOrum for the Co-ordination of pesticde fate models and their USe. http://esdac.jrc.ec.europa.eu/public_path/projects_data/focus/sw/docs/Gene

Website of the Steps 1 and 2 calculator at the Joint Research Center of the European Union: http://esdac.jrc.ec.europa.eu/projects/stepsonetwo

Examples

```
# Parent only
dummy_1 <- chent_focus_sw("Dummy 1", cwsat = 6000, DT50_ws = 6, Koc = 344.8)
PEC_sw_focus(dummy_1, 3000, f_drift = 0)

# Metabolite
new_dummy <- chent_focus_sw("New Dummy", mw = 250, Koc = 100)
```

```
M1 <- chent_focus_sw("M1", mw = 100, cwsat = 100, DT50_ws = 100, Koc = 50,
  max_ws = 0, max_soil = 0.5)
PEC_sw_focus(new_dummy, 1000, scenario = "cereals, winter", met = M1)
```

`PEC_sw_sed` *Calculate predicted environmental concentrations in sediment from surface water concentrations*

Description

The method 'percentage' is equivalent to what is used in the CRD spreadsheet PEC calculator

Usage

```
PEC_sw_sed(
  PEC_sw,
  percentage = 100,
  method = "percentage",
  sediment_depth = 5,
  water_depth = 30,
  sediment_density = 1.3,
  PEC_sed_units = c("µg/kg", "mg/kg")
)
```

Arguments

`PEC_sw`	Numeric vector or matrix of surface water concentrations in µg/L for which the corresponding sediment concentration is to be estimated
`percentage`	The percentage in sediment, used for the percentage method
`method`	The method used for the calculation
`sediment_depth`	Depth of the sediment layer
`water_depth`	Depth of the water body in cm
`sediment_density`	The density of the sediment in L/kg (equivalent to g/cm3)
`PEC_sed_units`	The units of the estimated sediment PEC value

Value

The predicted concentration in sediment

Author(s)

Johannes Ranke

Examples

```
PEC_sw_sed(PEC_sw_drift(100, distances = 1), percentage = 50)
```

perc_runoff_exposit *Runoff loss percentages as used in Exposit 3*

Description

A table of the loss percentages used in Exposit 3 for the twelve different Koc classes

Usage

```
perc_runoff_exposit
```

Format

A data frame with percentage values for the dissolved fraction and the fraction bound to eroding particles, with Koc classes used as row names

Koc_lower_bound The lower bound of the Koc class

dissolved The percentage of the applied substance transferred to an adjacent water body in the dissolved phase

bound The percentage of the applied substance transferred to an adjacent water body bound to eroding particles

Source

Excel 3.02 spreadsheet available from https://www.bvl.bund.de/SharedDocs/Downloads/04_Pflanzenschutzmittel/zul_umwelt_exposit.html

Examples

```
print(perc_runoff_exposit)
```

perc_runoff_reduction_exposit *Runoff reduction percentages as used in Exposit*

Description

A table of the runoff reduction percentages used in Exposit 3 for different vegetated buffer widths

Usage

```
perc_runoff_reduction_exposit
```

Format

A named list of data frames with reduction percentage values for the dissolved fraction and the fraction bound to eroding particles, with vegetated buffer widths as row names. The names of the list items are the Exposit versions from which the values were taken.

dissolved The reduction percentage for the dissolved phase

bound The reduction percentage for the particulate phase

Source

Excel 3.02 spreadsheet available from https://www.bvl.bund.de/SharedDocs/Downloads/04_Pflanzenschutzmittel/zul_umwelt_exposit.html

Agroscope version 3.01a with additional runoff factors for 3 m and 6 m buffer zones received from Muris Korkaric (not published). The variant 3.01a2 was introduced for consistency with previous calculations performed by Agroscope for a 3 m buffer zone.

Examples

```
print(perc_runoff_reduction_exposit)
```

`pfm_degradation` *Calculate a time course of relative concentrations based on an mkinmod model*

Description

Calculate a time course of relative concentrations based on an mkinmod model

Usage

```
pfm_degradation(
  model = "SFO",
  DT50 = 1000,
  parms = c(k_parent = log(2)/DT50),
  years = 1,
  step_days = 1,
  times = seq(0, years * 365, by = step_days)
)
```

Arguments

`model`	The degradation model to be used. Either a parent only model like 'SFO' or 'FOMC', or an mkinmod object
`DT50`	The half-life. This is only used when simple exponential decline is calculated (SFO model).
`parms`	The parameters used for the degradation model

years	For how many years should the degradation be predicted?
step_days	What step size in days should the output have?
times	The output times

Author(s)

Johannes Ranke

Examples

```
head(pfm_degradation("SFO", DT50 = 10))
```

---

plot.one_box *Plot time series of decline data*

Description

Plot time series of decline data

Usage

```
## S3 method for class 'one_box'
plot(
  x,
  xlim = range(time(x)),
  ylim = c(0, max(x)),
  xlab = "Time",
  ylab = "Residue",
  max_twa = NULL,
  max_twa_var = dimnames(x)[[2]][1],
  ...
)
```

Arguments

x	The object of type one_box to be plotted
xlim	Limits for the x axis
ylim	Limits for the y axis
xlab	Label for the x axis
ylab	Label for the y axis
max_twa	If a numeric value is given, the maximum time weighted average concentration(s) is/are shown in the graph.
max_twa_var	Variable for which the maximum time weighted average should be shown if max_twa is not NULL.
...	Further arguments passed to methods

See Also

sawtooth

Examples

```
dfop_pred <- one_box("DFOP", parms = c(k1 = 0.2, k2 = 0.02, g = 0.7))
plot(dfop_pred)
plot(sawtooth(dfop_pred, 3, 7), max_twa = 21)

# Use a fitted mkinfit model
m_2 <- mkinmod(parent = mkinsub("SFO", "m1"), m1 = mkinsub("SFO"))
fit_2 <- mkinfit(m_2, FOCUS_2006_D, quiet = TRUE)
pred_2 <- one_box(fit_2, ini = 1)
pred_2_saw <- sawtooth(pred_2, 2, 7)
plot(pred_2_saw, max_twa = 21, max_twa_var = "m1")
```

---

plot.TOXSWA_cwa *Plot TOXSWA surface water concentrations*

Description

Plot TOXSWA hourly concentrations of a chemical substance in a specific segment of a TOXSWA surface water body.

Usage

```
## S3 method for class 'TOXSWA_cwa'
plot(
  x,
  time_column = c("datetime", "t", "t_firstjan", "t_rel_to_max"),
  xlab = "default",
  ylab = "default",
  add = FALSE,
  threshold_factor = 1000,
  thin_low = 1,
  total = FALSE,
  LC_TIME = "C",
  ...
)
```

Arguments

x	The TOXSWA_cwa object to be plotted.
time_column	What should be used for the time axis. If "t_firstjan" is chosen, the time is given in days relative to the first of January in the first year.
xlab, ylab	Labels for x and y axis.
add	Should we add to an existing plot?

threshold_factor
: The factor by which the data have to be lower than the maximum in order to get thinned for plotting (see next argument).

thin_low
: If an integer greater than 1, the data close to zero (smaller than 1/threshold_factor of the maximum) in the series will be thinned by this factor in order to decrease the amount of data that is included in the plots

total
: Should the total concentration in water be plotted, including substance sorbed to suspended matter?

LC_TIME
: Specification of the locale used to format dates

...
: Further arguments passed to `plot` if we are not adding to an existing plot

Author(s)

Johannes Ranke

Examples

```
H_sw_D4_pond  <- read.TOXSWA_cwa("00001p_pa.cwa",
  basedir = "SwashProjects/project_H_sw/TOXSWA",
  zipfile = system.file("testdata/SwashProjects.zip", package = "pfm"))
plot(H_sw_D4_pond)
plot(H_sw_D4_pond, time_column = "t")
plot(H_sw_D4_pond, time_column = "t_firstjan")
plot(H_sw_D4_pond, time_column = "t_rel_to_max")

H_sw_R1_stream  <- read.TOXSWA_cwa("00003s_pa.cwa",
  basedir = "SwashProjects/project_H_sw/TOXSWA",
  zipfile = system.file("testdata/SwashProjects.zip", package = "pfm"))
plot(H_sw_R1_stream, time_column = "t_rel_to_max")
```

---

read.TOXSWA_cwa *Read TOXSWA surface water concentrations*

Description

Read TOXSWA hourly concentrations of a chemical substance in a specific segment of a TOXSWA surface water body. Per default, the data for the last segment are imported. As TOXSWA 4 reports the values at the end of the hour (ConLiqWatLayCur) in its summary file, we use this value as well instead of the hourly averages (ConLiqWatLay). In TOXSWA 5.5.3 this variable was renamed to ConLiqWatLay in the out file.

Usage

```
read.TOXSWA_cwa(
  filename,
  basedir = ".",
  zipfile = NULL,
```

```
  segment = "last",
  substance = "parent",
  total = FALSE,
  windows = NULL,
  thresholds = NULL
)
```

Arguments

filename	The filename of the cwa file (TOXSWA 2.x.y or similar) or the out file when using FOCUS TOXSWA 4 (i.e. TOXSWA 4.4.2) or higher.
basedir	The path to the directory where the cwa file resides.
zipfile	Optional path to a zip file containing the cwa file.
segment	The segment for which the data should be read. Either "last", or the segment number.
substance	For .out files, the default value "parent" leads to reading concentrations of the parent compound. Alternatively, the substance of interested can be selected by its code name.
total	Set this to TRUE in order to read total concentrations as well. This is only necessary for .out files as generated by TOXSWA 4.4.2 or similar, not for .cwa files. For .cwa files, the total concentration is always read as well.
windows	Numeric vector of width of moving windows in days, for calculating maximum time weighted average concentrations and areas under the curve.
thresholds	Numeric vector of threshold concentrations in µg/L for generating event statistics.

Value

An instance of an R6 object of class TOXSWA_cwa.

Author(s)

Johannes Ranke

Examples

```
H_sw_D4_pond  <- read.TOXSWA_cwa("00001p_pa.cwa",
                                 basedir = "SwashProjects/project_H_sw/TOXSWA",
                                 zipfile = system.file("testdata/SwashProjects.zip",
                                                       package = "pfm"))
```

sawtooth *Create decline time series for multiple applications*

Description

If the application pattern is specified in `applications`, `n` and `i` are disregarded.

Usage

```
sawtooth(
  x,
  n = 1,
  i = 365,
  applications = data.frame(time = seq(0, (n - 1) * i, length.out = n), amount = 1)
)
```

Arguments

`x`	A one_box object
`n`	The number of applications. If `applications` is specified, `n` is ignored
`i`	The interval between applications. If `applications` is specified, `i` is ignored
`applications`	A data frame holding the application times in the first column and the corresponding amounts applied in the second column.

Examples

```
applications = data.frame(time = seq(0, 14, by = 7), amount = c(1, 2, 3))
pred <- one_box(10)
plot(sawtooth(pred, applications = applications))

m_2 <- mkinmod(parent = mkinsub("SFO", "m1"), m1 = mkinsub("SFO"))
fit_2 <- mkinfit(m_2, FOCUS_2006_D, quiet = TRUE)
pred_2 <- one_box(fit_2, ini = 1)
pred_2_saw <- sawtooth(pred_2, 2, 7)
plot(pred_2_saw, max_twa = 21, max_twa_var = "m1")

max_twa(pred_2_saw)
```

SFO_actual_twa *Actual and maximum moving window time average concentrations for SFO kinetics*

Description

Actual and maximum moving window time average concentrations for SFO kinetics

Usage

```
SFO_actual_twa(DT50 = 1000, times = c(0, 1, 2, 4, 7, 14, 21, 28, 42, 50, 100))
```

Arguments

DT50	The half-life.
times	The output times, and window sizes for time weighted average concentrations

Author(s)

Johannes Ranke

Source

FOCUS (2014) Generic Guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration, Version 1.1, 18 December 2014, p. 251

Examples

```
SFO_actual_twa(10)
```

---

soil_scenario_data_EFSA_2015

Properties of the predefined scenarios from the EFSA guidance from 2015

Description

Properties of the predefined scenarios used at Tier 1, Tier 2A and Tier 3A for the concentration in soil as given in the EFSA guidance (2015, p. 13/14). Also, the scenario and model adjustment factors from p. 15 and p. 17 are included.

Usage

```
soil_scenario_data_EFSA_2015
```

Format

A data frame with one row for each scenario. Row names are the scenario codes, e.g. CTN for the Northern scenario for the total concentration in soil. Columns are mostly self-explanatory. rho is the dry bulk density of the top soil.

Source

EFSA (European Food Safety Authority) (2015) EFSA guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. *EFSA Journal* **13**(4) 4093 doi:10.2903/j.efsa.2015.4093

Examples

```
soil_scenario_data_EFSA_2015
```

`soil_scenario_data_EFSA_2017`
Properties of the predefined scenarios from the EFSA guidance from 2017

Description

Properties of the predefined scenarios used at Tier 1, Tier 2A and Tier 3A for the concentration in soil as given in the EFSA guidance (2017, p. 14/15). Also, the scenario and model adjustment factors from p. 16 and p. 18 are included.

Usage

```
soil_scenario_data_EFSA_2017
```

Format

A data frame with one row for each scenario. Row names are the scenario codes, e.g. CTN for the Northern scenario for the total concentration in soil. Columns are mostly self-explanatory. `rho` is the dry bulk density of the top soil.

Source

EFSA (European Food Safety Authority) (2017) EFSA guidance document for predicting environmental concentrations of active substances of plant protection products and transformation products of these active substances in soil. *EFSA Journal* **15**(10) 4982 doi:10.2903/j.efsa.2017.4982

Examples

```
soil_scenario_data_EFSA_2017

waldo::compare(soil_scenario_data_EFSA_2017, soil_scenario_data_EFSA_2015)
```

`SSLRC_mobility_classification` *Determine the SSLRC mobility classification for a chemical substance from its Koc*

Description

This implements the method specified in the UK data requirements handbook and was checked against the spreadsheet published on the CRD website

Usage

```
SSLRC_mobility_classification(Koc)
```

Arguments

`Koc`	The sorption coefficient normalised to organic carbon in L/kg

Value

A list containing the classification and the percentage of the compound transported per 10 mm drain water

Author(s)

Johannes Ranke

References

HSE's Chemicals Regulation Division (CRD) Active substance PECsw calculations (for UK specific authorisation requests) https://www.hse.gov.uk/pesticides/topics/pesticide-approvals/pesticides-registration/data-requirements-handbook/fate/active-substance-uk.htm accessed 2019-09-27

Drainage PECs Version 1.0 (2015) Spreadsheet published at https://www.hse.gov.uk/pesticides/topics/pesticide-approvals/pesticides-registration/data-requirements-handbook/fate/pec-tools-2015/PEC%20sw-sed%20(drainage).xlsx accessed 2019-09-27

Examples

```
SSLRC_mobility_classification(100)
SSLRC_mobility_classification(10000)
```

TOXSWA_cwa *R6 class for holding TOXSWA water concentration data and associated statistics*

Description

An R6 class for holding TOXSWA water concentration (cwa) data and some associated statistics. like maximum moving window average concentrations, and dataframes holding the events exceeding specified thresholds. Usually, an instance of this class will be generated by `read.TOXSWA_cwa`.

Format

An `R6Class` generator object.

Public fields

`filename` Length one character vector holding the filename.

`basedir` Length one character vector holding the directory where the file came from.

`zipfile` If not null, giving the path to the zip file from which the file was read.

`segment` Length one integer, specifying for which segment the cwa data were read.

`substance` The TOXSWA name of the substance.

`cwas` Dataframe holding the concentrations.

`events` List of dataframes holding the event statistics for each threshold.

`windows` Matrix of maximum time weighted average concentrations (TWAC_max) and areas under the curve in µg/day * h (AUC_max_h) or µg/day * d (AUC_max_d) for the requested moving window sizes in days.

Methods

Public methods:

- `TOXSWA_cwa$new()`
- `TOXSWA_cwa$moving_windows()`
- `TOXSWA_cwa$get_events()`
- `TOXSWA_cwa$print()`
- `TOXSWA_cwa$clone()`

Method `new()`**:** Create a TOXSWA_cwa object from a file

Usage:

```
TOXSWA_cwa$new(
  filename,
  basedir,
  zipfile = NULL,
  segment = "last",
  substance = "parent",
  total = FALSE
)
```

Arguments:

`filename` The filename

`basedir` The directory to look in

`zipfile` Optional path to a zipfile holding the file

`segment` Either "last" or the number of the segment for which to read the data

`substance` The TOXSWA substance name (for TOXSWA 4 or higher)

`total` Should total concentrations be read in? If FALSE, free concentrations are read

Method `moving_windows()`**:** Add to the `windows` field described above.

Usage:

```
TOXSWA_cwa$moving_windows(windows, total = FALSE)
```

Arguments:

`windows` Window sizes in days

`total` If TRUE, the total concentration including the amount adsorbed to suspended matter will be used.

Method `get_events()`**:** Populate a datataframe with event information for the specified threshold value. The resulting dataframe is stored in the `events` field of the object.

Usage:

```
TOXSWA_cwa$get_events(thresholds, total = FALSE)
```

Arguments:

`thresholds` Threshold values in µg/L.

`total` If TRUE, the total concentration including the amount adsorbed to suspended matter will be used.

Method `print()`**:** Print a `TOXSWA_cwa` object

Usage:

```
TOXSWA_cwa$print()
```

Method `clone()`**:** The objects of this class are cloneable with this method.

Usage:

```
TOXSWA_cwa$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
H_sw_R1_stream  <- read.TOXSWA_cwa("00003s_pa.cwa",
                                   basedir = "SwashProjects/project_H_sw/TOXSWA",
                                   zipfile = system.file("testdata/SwashProjects.zip",
                                             package = "pfm"))
H_sw_R1_stream$get_events(c(2, 10))
H_sw_R1_stream$moving_windows(c(7, 21))
print(H_sw_R1_stream)
```

TSCF *Estimation of the transpiration stream concentration factor*

Description

The FOCUS groundwater guidance (FOCUS 2014, p. 41) states that a reliable measured log Kow for neutral pH must be available in order to apply the Briggs equation. It is not clarified when it can be regarded reliable, but the equation is stated to be produced for non-ionic compounds, suggesting that the compound should not be ionogenic (weak acid/base) or ionic.

Usage

```
TSCF(log_Kow, method = c("briggs82", "dettenmaier09"))
```

Arguments

log_Kow	The decadic logarithm of the octanol-water partition constant
method	Short name of the estimation method.

Details

The Dettenmaier equation is given to show that other views on the subject exist.

References

FOCUS (2014) Generic Guidance for Tier 1 FOCUS Ground Water Assessments. Version 2.2, May 2014 Dettenmaier EM, Doucette WJ and Bugbee B (2009) Chemical hydrophobicity and uptake by plant roots. Environ. Sci. Technol 43, 324 - 329

Examples

```
plot(TSCF, -1, 5, xlab = "log Kow", ylab = "TSCF", ylim = c(0, 1.1))
TSCF_2 <- function(x) TSCF(x, method = "dettenmaier09")
curve(TSCF_2, -1, 5, add = TRUE, lty = 2)
legend("topright", lty = 1:2, bty = "n",
  legend = c("Briggs et al. (1982)", "Dettenmaier et al. (2009)"))
```

twa *Calculate a time weighted average concentration*

Description

The moving average is built only using the values in the past, so the earliest possible time for the maximum in the time series returned is after one window has passed.

Usage

```
twa(x, window = 21)

## S3 method for class 'one_box'
twa(x, window = 21)
```

Arguments

x	An object of type one_box
window	The size of the moving window

See Also

max_twa

Examples

```
pred <- sawtooth(one_box(10),
  applications = data.frame(time = c(0, 7), amount = c(1, 1)))
max_twa(pred)
```

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