Package 'lemna'

October 13, 2022

Title Lemna Ecotox Effect Model

Version 1.0.0

Description The reference implementation of model equations and default
parameters for the toxicokinetic-toxicodynamic (TKTD) model of the Lemna
(duckweed) aquatic plant. Lemna is a standard test macrophyte used in ecotox
effect studies. The model was described and published by the SETAC Europe
Interest Group Effect Modeling. It is a refined description of the Lemna
TKTD model published by Schmitt et al. (2013)
<doi:10.1016/j.ecolmodel.2013.01.017>.

URL https://github.com/nkehrein/lemna

BugReports https://github.com/nkehrein/lemna/issues

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R topics documented:

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effect   *Effects on biomass*

Description

Two endpoints are calculated which describe the effects on biomass:

- BM, percent effect on biomass at the last time step of the simulation
- r, percent effect on the average growth rate of biomass

Usage

```
effect(...)

## Default S3 method:
effect(init, times, param, envir, duration, ...)

## S3 method for class 'lemna_scenario'
effect(x, init, times, param, envir, duration, ...)
```

Arguments

...	additional parameters passed on to lemna() and deSolve::ode()
init	initial state of the model variables
times	numeric vector, output times for which model results are returned
param	named list, Lemna model parameters
envir	named list, contains time series data for each of the five environmental variables
duration	optional numeric, length of the simulated period to consider for effect calculation, period starts at the beginning of the simulation
x	a lemna_scenario object

Value

numeric, effect on biomass in percent (%) [0,100]

Methods (by class)

- `default`: All scenario parameters supplied as arguments

- `lemna_scenario`: Scenario parameters supplied as a `lemna_scenario` object

Examples

```
# effects in sample scenario
effect(metsulfuron)

# effects with modified environmental data
myenvir <- metsulfuron$envir
myenvir$tmp <- 20   # increase to 20°C
myenvir$conc <- 0.3  # constant exposure of 0.3 ug/L
effect(metsulfuron, envir=myenvir)

# calculate effects for the first seven days
effect(metsulfuron, duration=7)
```

---

focusd1 *A Lemna scenario using FOCUS D1 Ditch environmental conditions*

Description

The dataset consists of a named `list` which contains vectors describing initial state, parameters, output times, and environmental variables of the Lemna model. The scenario represents conditions of the FOCUS D1 Ditch exposure scenario.

Usage

```
focusd1
```

Format

An object of class `lemna_scenario` of length 4.

Details

The scenario will simulate a period of 365 days with hourly outputs, a start population of 80 g/m² dry weight, variable environmental conditions, and a complex, time-varying exposure pattern.

The scenario setup was published by Hommen *et al.* (2015). Exposure pattern and substance specific parameters are of exemplary character and represent the herbicide *metsulfuron-methyl*.

References

Hommen U., Schmitt W., Heine S., Brock Theo C.M., Duquesne S., Manson P., Meregalli G., Ochoa-Acuña H., van Vliet P., Arts G., 2015: How TK-TD and Population Models for Aquatic Macrophytes Could Support the Risk Assessment for Plant Protection Products. Integr Environ Assess Manag 12(1), pp. 82-95. doi: 10.1002/ieam.1715

Examples

```
# Simulate the example scenario
lemna(focusd1)
```

---

focusd2   *A Lemna scenario using FOCUS D2 Ditch environmental conditions*

Description

The dataset consists of a named `list` which contains vectors describing initial state, parameters, output times, and environmental variables of the Lemna model. The scenario represents conditions of the FOCUS D2 Ditch exposure scenario.

Usage

```
focusd2
```

Format

An object of class `lemna_scenario` of length 4.

Details

The scenario will simulate a period of 365 days with hourly outputs, a start population of 100 g/m² dry weight, variable environmental conditions, and a complex, time-varying exposure pattern.

The scenario setup was published by Hommen *et al.* (2015). Exposure pattern and substance specific parameters are of exemplary character and represent the herbicide *metsulfuron-methyl*.

References

Hommen U., Schmitt W., Heine S., Brock Theo C.M., Duquesne S., Manson P., Meregalli G., Ochoa-Acuña H., van Vliet P., Arts G., 2015: How TK-TD and Population Models for Aquatic Macrophytes Could Support the Risk Assessment for Plant Protection Products. Integr Environ Assess Manag 12(1), pp. 82-95. doi: 10.1002/ieam.1715

Examples

```
# Simulate the example scenario
lemna(focusd2)
```

---

focusr3	*A Lemna scenario using FOCUS R3 Stream environmental conditions*

Description

The dataset consists of a named `list` which contains vectors describing initial state, parameters, output times, and environmental variables of the Lemna model. The scenario represents conditions of the FOCUS R3 Stream exposure scenario.

Usage

```
focusr3
```

Format

An object of class `lemna_scenario` of length 4.

Details

The scenario will simulate a period of 365 days with hourly outputs, a start population of 100 g/m² dry weight, variable environmental conditions, and a complex, time-varying exposure pattern.

The scenario setup was published by Hommen *et al*. (2015). Exposure pattern and substance specific parameters are of exemplary character and represent the herbicide *metsulfuron-methyl*.

References

Hommen U., Schmitt W., Heine S., Brock Theo C.M., Duquesne S., Manson P., Meregalli G., Ochoa-Acuña H., van Vliet P., Arts G., 2015: How TK-TD and Population Models for Aquatic Macrophytes Could Support the Risk Assessment for Plant Protection Products. Integr Environ Assess Manag 12(1), pp. 82-95. doi: 10.1002/ieam.1715

Examples

```
# Simulate the example scenario
lemna(focusr3)
```

---

hommen212	*Observed frond numbers reported by Hommen* et al. *(2015)*

Description

The data consists of observed frond numbers from experimental studies for various time points and exposure concentrations. The *Lemna* population was exposed to constant concentrations of *metsulfuron-methyl* for two days, followed by twelve days of recovery.

Usage

```
hommen212
```

Format

An object of class `tbl_df` (inherits from `tbl`, `data.frame`) with 25 rows and 3 columns.

Details

The dataset was presented in Hommen *et al.* (2015)], cf. Figure 3, and was included in this package by courtesy of the authors.

References

Hommen U., Schmitt W., Heine S., Brock Theo C.M., Duquesne S., Manson P., Meregalli G., Ochoa-Acuña H., van Vliet P., Arts G., 2015: How TK-TD and Population Models for Aquatic Macrophytes Could Support the Risk Assessment for Plant Protection Products. Integr Environ Assess Manag 12(1), pp. 82-95. doi: 10.1002/ieam.1715

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lemna   *Simulate a Lemna scenario*

Description

The function numerically integrates the Lemna model using the supplied parameters, environmental factor time series, output time points, and other settings. Numerical integration is handled by deSolve::lsoda() by default which is well suited to handle stiff and non-stiff numerical problems.

Usage

```
lemna(...)

## Default S3 method:
lemna(
  init = c(BM = 0, M_int = 0),
  times,
  param,
  envir,
  ode_mode = c("r", "c"),
  nout = 2,
  ...
)

## S3 method for class 'lemna_scenario'
lemna(x, init, times, param, envir, ...)
```

Arguments

`...`	additional parameters passed on to `deSolve::ode()`
`init`	initial state of the model variables
`times`	numeric vector, output times for which model results are returned
`param`	named list, Lemna model parameters
`envir`	named list, contains time series data for each of the five environmental variables
`ode_mode`	character, switch controls if ODE functions implemented in R or C are used, defaults to R
`nout`	numeric, controls the number of additional output variables of the model, such as `C_int` (internal concentration) or `FrondNo` (the number of fronds), see e.g. `deSolve::lsoda()` for details. Defaults to 2
`x`	a `lemna_scenario` object

Value

`data.frame` with simulation results

Methods (by class)

- `default`: All scenario parameters supplied as arguments

- `lemna_scenario`: Scenario parameters supplied as a `lemna_scenario` object

State variables

The model has two state variables:

- `BM`, Biomass (g dw m-2)

- `M_int`, Mass of toxicant in plant population (mass per m2, e.g. ug m-2)

Output times

The function will only return results for the requested time points. The solver may make additional time steps which are not returned, depending on the solver settings such as numerical tolerance. The number of output times and the distance between them can have influence on the numerical precision of results. Please refer to the manual of the deSolve package for more information on that topic.

Parameters

The list of available model parameters, their units, and suggested default values is documented in `param_defaults()`.

Environmental variables

The model requires a time series for each of the five environmental variables For ease of use, a time series can be represented by either a constant numeric value, a `data.frame` containing a time series, a character string with a path to a CSV file containing a time series, or a function returning a value for a certain time point.

The five environmental variables are as follows:

- `conc`, Exposure concentration (mass per volume, e.g ug L-1)

- `tmp`, Temperature (deg C)

- `irr`, Irradiance (kJ m-2 d-1)

- `P`, Phosphorus concentration (mg P L-1)

- `N`, Nitrogen concentration (mg N L-1)

A `data.frame` containing a time series must consist of exactly two columns: The first column contains the time in days, the second column the environmental factor in question. The `data.frame` must contain at least one row. Time points are not required to coincide with the solver's output times but the user should take care that the solver's time step length is sufficiently small so that it can consider the relevant dynamics of the time series. This problem can be avoided by calling the model ODEs implemented in C, see argument `ode_mode`.

If a string is passed as an environmental factor, the function will interpret the string as a file path and will try to load the contents of a CSV file. The same requirements as for a `data.frame` apply to a time series loaded from a file.

When using the pure R code ODE, it is also possible to pass a function as an environmental factor. The function must accept exactly one argument which represents time and must return a single scalar value. Using a function in combination with the compiled code solver will raise an error.

R vs. compiled code

The model can be simulated using pure *R* code (the default) or an implementation that uses the compiled code feature of deSolve. Compiled code is almost always significantly faster than pure *R*. The solver for compiled ODEs also handles environmental variables better than the pure *R* version. For optimal performance, the time series of environmental variables should always be as short as possible and as long as needed.

To use the compiled code feature, set the argument `ode_mode = "c"`.

Simulation output

For reasons of convenience, the return value contains by default two additional variables derived from simulation results: the internal concentration `C_int` as well as the number of fronds `FrondNo`. These can be disabled by setting the argument `nout = 0`.

The compiled code model can return up to 18 additional variables which represent intermediary variables, environmental variables, and derivatives calculated within the model equations. Please refer to the model description of *Klein et al.* for more information on these variables and how they influence model behavior.

The available output levels are as follows:

- `nout >= 1`
  - `C_int`, internal concentration (mass per volume)
- `nout >= 2`
  - `FrondNo`, frond number (-)
- `nout >= 4`
  - `f_loss`, respiration dependency function (-)
  - `f_photo`, photosynthesis dependency function (-)
- `nout >= 10`
  - `fT_photo`, temperature response of photosynthesis (-)
  - `fI_photo`, irradiance response of photosynthesis (-)
  - `fP_photo`, phosphorus response of photosynthesis (-)
  - `fN_photo`, nitrogen response of photosynthesis (-)
  - `fBM_photo`, density response of photosynthesis (-)
  - `fCint_photo`, concentration response of photosynthesis (-)
- `nout >= 16`
  - `C_int_unb`, unbound internal concentration (mass per volume)
  - `C_ext`, external concentration (mass per volume)
  - `Tmp`, temperature (deg C)
  - `Irr`, irradiance (kJ m-2 d-1)
  - `Phs`, Phosphorus concentration (mg P L-1)
  - `Ntr`, Nitrogen concentration (mg N L-1)
- `nout >= 18`
  - dBM, biomass derivative (g dw m-2 d-1)
  - `dM_int`, mass of toxicant in plants derivative (mass per m2 d-1)

References

Klein J., Cedergreen N., Heine S., Kehrein N., Reichenberger S., Rendal C., Schmitt W., Hommen U., 2022: Refined description of the *Lemna* TKTD growth model based on *Schmitt et al.* (2013) – equation system and default parameters, implementation in R. Report of the working group *Lemna* of the SETAC Europe Interest Group Effect Modeling. Version 1.1, uploaded on 09 May 2022. <https://www.setac.org/group/SEIGEffectModeling>

Examples

```
# Simulate the metsulfuron example scenario
lemna(metsulfuron)

# Create a simple plot of the number of fronds
lemna(metsulfuron) -> result
plot(result$time, result$FrondNo)

# Create a nicer plot using a dedicated plotting routine
plot(result)
```

```
# Simulate the example scenario for a period of 30 days
lemna(metsulfuron, times=0:30) -> result30
plot(result30)

##
## Create a custom Lemna scenario from scratch
##

# Initial state: 12 fronds, no toxicant mass
myinit <- c(BM=0.0012, M_int=0)

# Output times: simulate 7 days with a ~2 hour time step
mytime <- seq(0, 7, 0.1)

# Default model parameters + TKTD parameters of a hypothetical substance
myparam <- param_defaults(list(
  EC50_int = 0.1, # 50% effect level (ug L-1)
  b = 0.7,        # slope parameter (-)
  P = 0.01        # permeability (cm d-1)
))

# Custom environmental variables
myenvir <- list(
  # exposure step function:
  # 3 days no exposure, followed by 4 days of 10 ug L-1
  conc = data.frame(t=c(0,3,4,7), conc=c(0,0,10,10)),
  tmp = 18,    # constant temperature of 18 °C
  irr = 15000, # constant irradiance of 15,000 kJ m-2 d-1
  N = 0.6,     # constant Nitrogen concentration of 0.6 mg L-1
  P = 0.3      # constant Phosphorus concentration of 0.3 mg L-1
)

# Simulate the custom scenario and plot results
lemna(init=myinit, times=mytime, param=myparam, envir=myenvir) -> result_custom
plot(result_custom)

# Simulate again, forcing the solver to use smaller time steps of hmax=0.001.
# The resulting curves are almost identical for this example.
lemna(init=myinit, times=mytime, param=myparam, envir=myenvir, hmax=0.001) -> result_custom2
library(ggplot2)
ggplot(result_custom, aes(time, FrondNo)) +
  geom_line() +
  geom_line(data=result_custom2, color="red", style="dashed")

# Combine all settings into a scenario object and simulate it
scenario <- new_lemna_scenario(
 init = myinit,
 param = myparam,
 times = mytime,
 envir = myenvir
)
lemna(scenario)
```

---

lemna_desolve   *Access to the ODE solver*

Description

This function can be used by external packages to access the ODE implemented in C without the surrounding sanity checks and data loading procedures. All parameters will be passed on to the solver.

Usage

```
lemna_desolve(...)
```

Arguments

...   parameters passed on to deSolve::ode()

Value

result from deSolve::ode()

---

metsulfuron   *A Lemna scenario fitted to metsulfuron-methyl effect data*

Description

The dataset consists of a named list which contains vectors describing initial state, parameters, output times, and environmental variables of the *Lemna* model.

Usage

```
metsulfuron
```

Format

An object of class lemna_scenario of length 4.

Details

The scenario will simulate a period of 14 days with daily outputs, a start population of 12 fronds, unlimited growth conditions, and an exposure pattern represented by a step-function.

The scenario setup was published by Schmitt *et al.* (2013). A mechanistic combined toxicokinetic-toxicodynamic (TK/TD) and growth model for the aquatic macrophytes *Lemna spp.* was parameterized by the authors based on literature data. TK/TD parameters were determined by calibrating the model using substance specific effect data of metsulfuron-methyl.

References

Schmitt W., Bruns E., Dollinger M., Sowig P., 2013: Mechanistic TK/TD-model simulating the effect of growth inhibitors on *Lemna* populations. Ecol Model 255, pp. 1-10. doi: 10.1016/j.ecolmodel.2013.01.017

Examples

```
# Simulate the example scenario
lemna(metsulfuron)

# Simulate a longer time period of 21 days
lemna(metsulfuron, times=0:21)

# Print the scenario's exposure series
metsulfuron$envir$conc

# Print all environmental variables
metsulfuron$envir
```

---

new_lemna_scenario   *Lemna scenario constructor*

Description

Lemna scenario constructor

Usage

```
new_lemna_scenario(
  init = c(BM = 0, M_int = 0),
  times = c(),
  param = list(),
  envir = list()
)
```

Arguments

init	initial state of the model variables
times	numeric vector, output times for which model results are returned
param	named list, Lemna model parameters
envir	named list, contains time series data for each of the five environmental variables

Value

a `lemna_scenario` object

param_defaults	*Default parameters*

Description

Returns the default Lemna model parameters as reported by Klein *et al.* (2022).

Usage

```
param_defaults(values)

param_new(values)
```

Arguments

values optional named numeric `vector`, values will override any defaults

Details

Model parameters:

Growth model:

- `k_photo_fixed`, Model switch for unlimited growth conditions (TRUE/FALSE)
- `k_photo_max`, Maximum photosynthesis rate (d-1)
- `k_loss`, Reference loss rate (d-1)
- `BM_min`, Threshold density for setting dBM/dt to zero (g dw m-2)

Temperature response of photosynthesis:

- `T_opt`, Optimum growth temperature (deg C)
- `T_min`, Minimum growth temperature (deg C)
- `T_max`, Maximum growth temperature (deg C)

Temperature response of biomass loss rate:

- `Q10`, Temperature coefficient (-)
- `T_ref`, Reference temperature for response=1 (°C)

Irradiance reponse of photosynthesis:

- `alpha`, Slope of irradiance response (m2 d kJ-1)
- `beta`, Intercept of irradiance response (-)

Nutrient response of photosynthesis:

- `N_50`, Half-saturation constant of Nitrogen (mg N L-1)
- `P_50`, Half-saturation constant of Phosphorus (mg P L-1)

Density dependence of photosynthesis:

- `BM_L`, Carrying capacity (g dw m-2)

Concentration response (Toxicodynamics):

- `EC50_int`, Internal concentration resulting in 50% effect (mass per volume)

- E_max, Maximum inhibition (-)
- b, Slope parameter (-)

Internal concentration (Toxicokinetics):

- P, Permeability (cm d-1)
- r_A_DW, Area per dry-weight ratio (cm2 g-1)
- r_FW_DW, Fresh weight per dry weight ratio (-)
- r_FW_V, Fresh weight density (g cm-3)
- r_DW_FN Dry weight per frond ratio (g dw)
- K_pw, Partitioning coefficient plant:water (-)
- k_met, Metabolisation rate (d-1)

Value

named list

Functions

- param_new: A parameter set without default values

References

Klein J., Cedergreen N., Heine S., Kehrein N., Reichenberger S., Rendal C., Schmitt W., Hommen U., 2022: Refined description of the *Lemna* TKTD growth model based on *Schmitt et al.* (2013) – equation system and default parameters, implementation in R. Report of the working group *Lemna* of the SETAC Europe Interest Group Effect Modeling. Version 1.1, uploaded on 09 May 2022. https://www.setac.org/group/SEIGEffectModeling

Examples

```
# Returns default model parameters, some parameters are not defined (NA)
param_defaults()

# Overwrite one of the default parameters
param_defaults(list(k_photo_max = 0.42))

# Provide values for substance specific TKTD parameters
param_defaults(list(
  EC50_int = 23, # 50% effect level (mass per volume)
  b = 1,         # slope parameter (-)
  P = 0.42       # permeability (cm d-1)
))

# Returns a list of required model parameters with all values set to NA
param_new()
```

---

plot.lemna_result *Plot a Lemna scenario result*

Description

Creates up to four plots in a gridded layout depicting

1. Exposure (i.e. external) concentration, as well as damage (internal concentration, `C_int`) if available

2. Internal toxicant mass (`M_int`)

3. Population size as biomass (`BM`)

4. Population size as number of fronds (`FrondNo`) if available

Usage

```
## S3 method for class 'lemna_result'
plot(x, y, munit = "ug/m2", cunit = "ug/L", legend = TRUE, ...)
```

Arguments

x	`lemna_result` object
y	unused parameter
munit	character, unit of internal mass, defaults to ug/m2
cunit	character, unit of exposure, defaults to ug/L
legend	logical, if TRUE then a legend is displayed, set to FALSE to hide legend, defaults to TRUE
...	unused parameter

Value

a gridded plot

Examples

```
# Simulate a sample scenario and plot results
result <- lemna(metsulfuron)
plot(result)

# Hide the legend of the concentration plot
plot(result, legend=FALSE)

# Simulate and plot a scenario with changing environmental conditions
plot(lemna(focusd1))
```

---

schmitt77   *Observed frond numbers reported by Schmitt* et al. *(2013)*

Description

The data consists of observed frond numbers from experimental studies for various time points and exposure concentrations. The *Lemna* population was exposed to constant concentrations of *metsulfuron-methyl* for seven days, followed by seven days of recovery.

Usage

```
schmitt77
```

Format

An object of class `tbl_df` (inherits from `tbl`, `data.frame`) with 49 rows and 3 columns.

Details

The dataset was presented in Schmitt *et al.* (2013), cf. Figure 2, and was included in this package by courtesy of the authors.

References

Schmitt W., Bruns E., Dollinger M., Sowig P., 2013: Mechanistic TK/TD-model simulating the effect of growth inhibitors on *Lemna* populations. Ecol Model 255, pp. 1-10. doi: 10.1016/j.ecolmodel.2013.01.017

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