

Package ‘bioinactivation’

November 3, 2025

Type Package

Title Mathematical Modelling of (Dynamic) Microbial Inactivation

Version 1.3.1

Description Functions for modelling microbial inactivation under isothermal or dynamic conditions. The calculations are based on several mathematical models broadly used by the scientific community and industry. Functions enable to make predictions for cases where the kinetic parameters are known. It also implements functions for parameter estimation for isothermal and dynamic conditions. The model fitting capabilities include an Adaptive Monte Carlo method for a Bayesian approach to parameter estimation.

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LazyData TRUE

Imports dplyr (>= 1.0.2), deSolve (>= 1.11), FME (>= 1.3.2), lazyeval (>= 0.1.10), ggplot2 (>= 3.3.2), MASS (>= 7.3-39), graphics (>= 3.1.3), stats (>= 3.1.3), rlang (>= 0.1.2), purrr (>= 0.3.4)

Suggests knitr (>= 1.30), testthat (>= 0.9.1), rmarkdown (>= 2.5), tidyr (>= 1.3.0)

VignetteBuilder knitr

RoxygenNote 7.2.3

Depends R (>= 2.10)

NeedsCompilation no

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Repository CRAN

Date/Publication 2025-11-03 18:10:02 UTC

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<i>Arrhenius_iso</i>	<i>Isothermal Arrhenius model</i>
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Description

Returns the predicted logarithmic reduction in microbial count according to Arrhenius model for the time, temperature and model parameters given.

Usage

Arrhenius_iso(time, temp, k_ref, temp_ref, Ea)

Arguments

- time numeric indicating the time at which the prediction is taken.
- temp numeric indicating the temperature of the treatment.
- k_ref numeric indicating the inactivation rate at the reference temperature.
- temp_ref numeric indicating the reference temperature.
- Ea numeric indicating the activation energy.

Value

A numeric with the predicted logarithmic reduction ($\log_{10}(N/N_0)$).

<i>Bigelow_iso</i>	<i>Isothermal Bigelow's Model</i>
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Description

Returns the predicted logarithmic reduction in microbial count according to Bigelow's model for the time, temperature and model parameters given.

Usage

Bigelow_iso(time, temp, z, D_R, temp_ref)

Arguments

- time numeric indicating the time at which the prediction is taken.
- temp numeric indicating the temperature of the treatment.
- z numeric defining the z-value.
- D_R numeric defining the D-value at the reference temperature.
- temp_ref numeric defining the reference temperature.

Value

A numeric with the predicted logarithmic reduction ($\log_{10}(N/N_0)$).

build_temperature_interpolator

Continuum Interpolation of Discrete Temperatures Values

Description

Builds an interpolator of the temperature at each time and its first derivative. First derivatives are approximated using forward finite differences ([approxfun](#)). It is assumed that temperature is 0 and constant outside the time interval provided.

Usage

```
build_temperature_interpolator(temperature_data)
```

Arguments

temperature_data

data frame with the values of the temperatures at each value of time. It need to have 2 columns, named time and temperature.

Value

a list with with two elements:

- temp, the interpolator of the temperature and
- dtemp, the interpolator of its first derivative

See Also

[approxfun](#)

check_model_params

Correctness Check of Model Parameters

Description

Makes 3 checks of compatibility between the input parameters for the adjustment and the DOF of the inactivation model selected.

- Check of equal length of model DOF and input DOF. Raises a warning if failed.
- Check that every single one of the input DOF is a model DOF. Raises a warning if failed.
- Check that every single one of the model DOF are defined as an input DOF.

Usage

```

check_model_params(
  simulation_model,
  known_params,
  starting_points,
  adjust_vars
)

```

Arguments

simulation_model	character with a valid model key.
known_params	named vector or list with the dof of the model known.
starting_points	named vector or list with the dof of the model to be adjusted.
adjust_vars	logical specifying whether the model variables need to be included in the check (not used for isothermal fit)

dArrhenius_model	<i>First derivative of the Arrhenius model</i>
------------------	--

Description

Calculates the first derivative of the Arrhenius model with log-linear inactivation for dynamic problems at a given time for the model parameters provided and the environmental conditions given.

Usage

```
dArrhenius_model(t, x, parms, temp_profile)
```

Arguments

t	numeric vector indicating the time of the experiment.
x	list with the value of N at t.
parms	parameters for the secondary model. No explicit check of their validity is performed.
temp_profile	a function that provides the temperature at a given time.

Details

This function is compatible with the function [predict_inactivation](#).

Value

The value of the first derivative of N at time t as a list.

Model Equation

$$\frac{dN}{dt} = -k * N$$

Model parameters

- temp_ref: Reference temperature for the calculation,
- k_ref: inactivation rate at the ref. temp.
- Ea: Activation energy.

See Also

[predict_inactivation](#)

dBigelow_model

First Derivate of the Linear Bigelow Model

Description

Calculates the first derivative of the linearized version of Bigelow's model for dynamic problems at a given time for the model parameters provided and the environmental conditions given.

Usage

```
dBigelow_model(t, x, parms, temp_profile)
```

Arguments

t	numeric vector indicating the time of the experiment.
x	list with the value of N at t.
parms	parameters for the secondary model. No explicit check of their validity is performed.
temp_profile	a function that provides the temperature at a given time.

Details

The model is developed from the isothermal Bigelow's model assuming during the derivation process that D_T is time independent.

This function is compatible with the function [predict_inactivation](#).

Value

The value of the first derivative of N at time t as a list.

Model Equation

$$\frac{dN}{dt} = -N \frac{\ln(10)}{D_T(T)}$$

Model parameters

- temp_ref: Reference temperature for the calculation,
- D_R: D-value at the reference temperature,
- z: z value.

See Also

[predict_inactivation](#)

dGeeraerd_model

First Derivate of Geeraerd's Model

Description

Calculates the first derivative of the Geeraerd's model at a given time for the model parameters provided and the environmental conditions given.

Usage

```
dGeeraerd_model(t, x, parms, temp_profile)
```

Arguments

- | | |
|--------------|--|
| t | numeric vector indicating the time of the experiment. |
| x | list with the values of the variables at time <i>t</i> . |
| parms | parameters for the secondary model. No explicit check of their validity is performed (see section Model Parameters). |
| temp_profile | a function that provides the temperature at a given time. |

Details

This function is compatible with the function [predict_inactivation](#).

Value

A list with the value of the first derivatives of N and C_c at time t.

Model Equation

$$\frac{dN}{dt} = -N \cdot k_{max} \cdot \alpha \cdot \gamma$$

$$\frac{dC_c}{dt} = -C_c \cdot k_{max}$$

$$\alpha = \frac{1}{1+C_c}$$

$$\gamma = 1 - \frac{N_{res}}{N}$$

$$k_{max} = \frac{1}{D_T}$$

$$\log_{10} D_T = \log_{10} D_R + \frac{T_R - T}{z}$$

Model Parameters

- temp_ref: Reference temperature for the calculation,
- D_R: D-value at the reference temperature,
- z: z value,
- N_min: Minimum value of N (defines the tail).

Notes

To define the Geeraerd model without tail, assign $N_{min} = 0$. For the model without shoulder, assign $C_0 = 0$

See Also

[predict_inactivation](#)

dMafart_model

First Derivate of the Weibull-Mafart Model

Description

Calculates the first derivative of Weibull-Mafart model at a given time for the model parameters provided and the environmental conditions given.

Usage

dMafart_model(t, x, parms, temp_profile)

Arguments

t	numeric vector indicating the time of the experiment.
x	list with the value of N at t.
parms	parameters for the secondary model. No explicit check of their validity is performed (see section Model Parameters).
temp_profile	a function that provides the temperature at a given time.

Details

The model is developed from the isothermal Weibull-Mafart model without taking into account in the derivation the time dependence of δ_T for non-isothermal temperature profiles.

This function is compatible with the function [predict_inactivation](#).

Value

The value of the first derivative of N at time t as a list.

Model Equation

$$\frac{dN}{dt} = -N \cdot p \cdot (1/\delta)^p \cdot t^{p-1}$$

$$\delta(T) = \delta_{ref} \cdot 10^{-(T-T_{ref})/z}$$

Model Parameters

- temp_ref: Reference temperature for the calculation.
- delta_ref: Value of the scale factor at the reference temperature.
- z: z-value.
- p: shape factor of the Weibull distribution.

Note

For t=0, dN = 0 unless n=1. Hence, a small shift needs to be introduced to t.

See Also

[predict_inactivation](#)

dMetselaar_model *First Derivate of the Metselaar Model*

Description

Calculates the first derivative of Metselaar model at a given time for the model parameters provided and the environmental conditions given.

Usage

```
dMetselaar_model(t, x, parms, temp_profile)
```

Arguments

t	numeric vector indicating the time of the experiment.
x	list with the value of N at t.
parms	parameters for the secondary model. No explicit check of their validity is performed (see section Model Parameters).
temp_profile	a function that provides the temperature at a given time.

Details

The model is developed from the isothermal Metselaar model without taking into account in the derivation the time dependence of δ_T for non-isothermal temperature profiles.

This function is compatible with the function [predict_inactivation](#).

Value

The value of the first derivative of N at time t as a list.

Model Equation

$$\frac{dN}{dt} = -N \cdot p \cdot (1/D)^p \cdot (t/\Delta)^{p-1}$$

$$D(T) = D_{ref} \cdot 10^{- (T-T_{ref})/z}$$

$$D(T) = D_R \cdot 10^{- (T-T_{ref})/z}$$

Model Parameters

- temp_ref: Reference temperature for the calculation.
- D_R: D-value at the reference temperature.
- z: z-value.
- p: shape factor of the Weibull distribution.
- Delta: Scaling parameter

Note

For $t=0$, $dN = 0$ unless $n=1$. Hence, a small shift needs to be introduced to t .

See Also

[predict_inactivation](#)

dPeleg_model

First Derivate of the Weibull-Peleg Model

Description

Calculates the first derivative of Weibull-Peleg model at a given time for the model parameters provided and the environmental conditions given.

Usage

```
dPeleg_model(t, x, parms, temp_profile)
```

Arguments

t	numeric vector indicating the time of the experiment.
x	list with the value of $\log S$ at t .
parms	parameters for the secondary model. No explicit check of their validity is performed (see section Model Parameters).
temp_profile	a function that provides the temperature at a given time.

Details

The model is developed from the isothermal Weibull model without taking into account in the derivation the time dependence of b for non-isothermal temperature profiles.

This function is compatible with the function [predict_inactivation](#).

Value

The value of the first derivative of $\log S$ at time t as a list.

Model Equation

$$\frac{d(\log_{10}(S))}{dt} = -b(T) \cdot n \cdot (-\log_{10}(S)/b(T))^{(n-1)/n}$$

$$\backslash\text{deqn}\{b(T) = \mathrm{ln}(1 + \exp(k_b*(T - T_{\text{crit}})))\}{b(T) = \ln(1 + \exp(k_b*(T - T_{\text{crit}})))}$$

Model Parameters

- temp_crit: Temperature below which there is inactivation.
- k_b: slope of the $b \sim \text{temp}$ line for temperatures above the critical one.
- n: shape factor of the Weibull distribution.

Note

For $\log S=0$, $d\log S = 0$ unless $n=1$. Hence, a small shift needs to be introduced to $\log S$.

See Also

[predict_inactivation](#)

dynamic_inactivation *Example Dynamic Inactivation of a Microorganism*

Description

Example of experimental data of the dynamic inactivation process of a microorganism.

Usage

```
data(dynamic_inactivation)
```

Format

A data frame with 19 rows and 2 variables.

Details

- time: Time in minutes of the measurement.
- N: Number of microorganism.
- temperature: Observed temperature.

 fit_dynamic_inactivation

Fitting of Dynamic Inactivation Models

Description

Fits the parameters of an inactivation model to experimental data. The function `FME::modFit` is used for the fitting.

Usage

```
fit_dynamic_inactivation(
  experiment_data,
  simulation_model,
  temp_profile,
  starting_points,
  upper_bounds,
  lower_bounds,
  known_params,
  ...,
  minimize_log = TRUE,
  tol0 = 1e-05
)
```

Arguments

<code>experiment_data</code>	data frame with the experimental data to be adjusted. It must have a column named “time” and another one named “N”.
<code>simulation_model</code>	character identifying the model to be used.
<code>temp_profile</code>	data frame with discrete values of the temperature for each time. It must have one column named <code>time</code> and another named <code>temperature</code> providing discrete values of the temperature at time points.
<code>starting_points</code>	starting values of the parameters for the adjustment.
<code>upper_bounds</code>	named numerical vector defining the upper bounds of the parameters for the adjustment.
<code>lower_bounds</code>	named numerical vector defining the lower bounds of the parameters for the adjustment.
<code>known_params</code>	named numerical vector with the fixed (i.e., not adjustable) model parameters.
<code>...</code>	further arguments passed to <code>FME::modFit</code>
<code>minimize_log</code>	logical. If TRUE, the adjustment is based on the minimization of the error of the logarithmic count. TRUE by default.
<code>tol0</code>	numeric. Observations at time 0 make Weibull-based models singular. The time for observations taken at time 0 are changed for this value.

Value

A list of class `FitInactivation` with the following items:

- `fit_results`: a list of class `modFit` with the info of the adjustment.
- `best_prediction`: a list of class `SimulInactivation` with prediction made by the adjusted model.
- `data`: a data frame with the data used for the fitting.

Examples

```
## EXAMPLE 1 -----

data(dynamic_inactivation) # The example data set is used.

get_model_data() # Retrieve the valid model keys.

simulation_model <- "Peleg" # Peleg's model will be used

model_data <- get_model_data(simulation_model)
model_data$parameters # Set the model parameters

dummy_temp <- data.frame(time = c(0, 1.25, 2.25, 4.6),
                        temperature = c(70, 105, 105, 70)) # Dummy temp. profile

## Set known parameters and initial points/bounds for unknown ones

known_params = c(temp_crit = 100)

starting_points <- c(n = 1, k_b = 0.25, N0 = 1e+05)
upper_bounds <- c(n = 2, k_b = 1, N0 = Inf)
lower_bounds <- c(n = 0, k_b = 0, N0 = 1e4)

dynamic_fit <- fit_dynamic_inactivation(dynamic_inactivation, simulation_model,
                                       dummy_temp, starting_points,
                                       upper_bounds, lower_bounds,
                                       known_params)

plot(dynamic_fit)
goodness_of_fit(dynamic_fit)

## END EXAMPLE 1 -----
```

fit_inactivation_MCMC *Fitting of dynamic inactivation with MCMC*

Description

Fits the parameters of an inactivation model to experimental using the Markov Chain Monte Carlo fitting algorithm implemented in the function [FME::modMCMC](#).

Usage

```
fit_inactivation_MCMC(
  experiment_data,
  simulation_model,
  temp_profile,
  starting_points,
  upper_bounds,
  lower_bounds,
  known_params,
  ...,
  minimize_log = TRUE,
  tol0 = 1e-05
)
```

Arguments

experiment_data	data frame with the experimental data to be adjusted. It must have a column named “time” and another one named “N”.
simulation_model	character identifying the model to be used.
temp_profile	data frame with discrete values of the temperature for each time. It must have one column named time and another named temperature providing discrete values of the temperature at time points.
starting_points	starting values of the parameters for the adjustment.
upper_bounds	named numerical vector defining the upper bounds of the parameters for the adjustment.
lower_bounds	named numerical vector defining the lower bounds of the parameters for the adjustment.
known_params	named numerical vector with the fixed (i.e., not adjustable) model parameters.
...	other arguments for FME::modMCMC .
minimize_log	logical. If TRUE, the adjustment is based on the minimization of the error of the logarithmic count.
tol0	numeric. Observations at time 0 make Weibull-based models singular. The time for observations taken at time 0 are changed for this value.

Value

A list of class `FitInactivationMCMC` with the following items:

- `modMCMC`: a list of class `modMCMC` with the information of the adjustment process.
- `best_prediction`: a list of class `SimulInactivation` with the prediction generated by the best predictor.
- `data`: a data frame with the data used for the fitting.

Examples

```

## EXAMPLE 1 -----
data(dynamic_inactivation) # The example data set is used.

get_model_data() # Retrieve the valid model keys.

simulation_model <- "Peleg" # Peleg's model will be used

model_data <- get_model_data(simulation_model)
model_data$parameters # Set the model parameters

dummy_temp <- data.frame(time = c(0, 1.25, 2.25, 4.6),
                          temperature = c(70, 105, 105, 70)) # Dummy temp. profile

## Set known parameters and initial points/bounds for unknown ones

known_params = c(temp_crit = 100)

starting_points <- c(n = 1, k_b = 0.25, N0 = 1e+05)
upper_bounds <- c(n = 2, k_b = 1, N0 = 1e6)
lower_bounds <- c(n = 0.5, k_b = 0.1, N0 = 1e4)

MCMC_fit <- fit_inactivation_MCMC(dynamic_inactivation, simulation_model,
                                dummy_temp, starting_points,
                                upper_bounds, lower_bounds,
                                known_params,
                                niter = 100)
                                # It is recommended to increase niter

plot(MCMC_fit)
goodness_of_fit(MCMC_fit)

## END EXAMPLE 1 -----

```

```

fit_isothermal_inactivation
Fit of Isothermal Experiments

```

Description

Fits the parameters of the model chosen to a set of isothermal experiments using nonlinear regression through the function `nls`.

Usage

```

fit_isothermal_inactivation(
  model_name,
  death_data,

```



```

    starting_point,
    known_params,
    adjust_log = TRUE
  )

```

Arguments

model_name	character specifying the model to adjust.
death_data	data frame with the experiment data where each row is one observation. It must have the following columns: <ul style="list-style-type: none"> • log_diff: Number of logarithmic reductions at each data point. • temp: Temperature of the data point. • time: Time of the data point.
starting_point	List with the initial values of the parameters for the adjustment.
known_params	List of the parameters of the model known.
adjust_log	logical. If TRUE, the adjustment is based on the minimization of the error of the logarithmic microbial count. If FALSE, it is based on the minimization of the error of the microbial count. TRUE by default.

Value

An instance of class `IsoFitInactivation` with the results. This list has four entries:

- nls: The object of class `nls` with the results of the adjustment.
- parameters: a list with the values of the model parameters, both fixed and adjusted.
- model: a string with the key identifying the model used.
- data: the inactivation data used for the fit.

See Also

[nls](#)

Examples

```

## EXAMPLE 1 -----

data("isothermal_inactivation") # data set used for the example.

get_isothermal_model_data() # retrieve valid model keys.
model_name <- "Bigelow" # Bigelow's model will be used for the adjustment.

model_data <- get_isothermal_model_data(model_name)
model_data$params # Get the parameters of the model

## Define the input arguments

known_params = list(temp_ref = 100)
starting_point <- c(z = 10, D_R = 1)

```

```
## Call the fitting function
iso_fit <- fit_isothermal_inactivation(model_name,
                                     isothermal_inactivation, starting_point,
                                     known_params)

## Output of the results

plot(iso_fit, make_gg = TRUE)
goodness_of_fit(iso_fit)

## END EXAMPLE 1 -----
```

Geeraerd_iso

Isothermal Geeraerd Model

Description

Returns the predicted logarithmic reduction in microbial cont according to Geeraerd's model. The isothermal prediction is calculated by analytical integration of the ode for constant temperature

Usage

```
Geeraerd_iso(time, temp, logC0, a, z)
```

Arguments

time	numeric vector with the treatment time
temp	numeric vector with the treatment temperature
logC0	model parameter describing the shoulder length
a	model parameter describing the intercept of the relation
z	z-value

get_isothermal_model_data

Isothermal Model Data

Description

Provides information of the models implemented for fitting of isothermal data. This models are valid only for isothermal adjustment with the function [fit_isothermal_inactivation](#). To make predictions with the function [predict_inactivation](#) or adjust dynamic experiments with [fit_dynamic_inactivation](#), use [get_model_data](#).

Usage

```
get_isothermal_model_data(model_name = "valids")
```

Arguments

model_name Optional string with the key of the model to use.

Value

If model_name is missing, a list of the valid model keys. If model_name is not a valid key, NULL is returned. Otherwise, a list with the parameters of the model selected and its formula for the nonlinear adjustment.

get_model_data	<i>Mapping of Simulation Model Functions</i>
----------------	--

Description

Provides information about the function for dynamic predictions associated to a valid simulation_model key. If simulation_model is missing or NULL, a character vector of valid model keys is provided. This function is designed as an assistant for using the functions [predict_inactivation](#) and [fit_dynamic_inactivation](#). For the adjustment of isothermal experiments with the function [fit_isothermal_inactivation](#), use the function [get_isothermal_model_data](#).

Usage

```
get_model_data(simulation_model = NULL)
```

Arguments

simulation_model
(optional) character with a valid model key or NULL.

Value

If simulation_model is NULL or missing, a character vector of possible names. Otherwise, a list including information of the relevant function:

- ode: Pointer to the function defining the model ode.
- cost: Pointer to the function calculating the error of the approximation.
- dtemp: logical defining whether the function requires the definition of the first derivative of temperature.
- variables: a character vector defining which entry variables are needed by the model.
- variables_priv: for internal use only.
- parameters: character vector with the parameters needed by the model.

See Also

[predict_inactivation](#), [fit_dynamic_inactivation](#)

get_prediction_cost *Error of the Prediction of Microbial Inactivation*

Description

Calculates the error of the prediction of microbial inactivation for the chosen inactivation model and the given parameters with respect to the experimental data provided. This function is compatible with the function [fit_dynamic_inactivation](#).

Usage

```
get_prediction_cost(  
  data_for_fit,  
  temp_profile,  
  simulation_model,  
  P,  
  known_params  
)
```

Arguments

data_for_fit	A data frame with the experimental data to fit. It must contain a column named “time” and another one named “N”.
temp_profile	data.frame defining the temperature profile. It must have a column named “time” and another named “temperature”.
simulation_model	character key defining the inactivation model.
P	list with the unknown parameters of the model to be adjusted.
known_params	list with the parameters of the model fixed (i.e., not adjusted)

Value

An instance of [FME::modCost](#) with the error of the prediction.

goodness_dyna	<i>Goodness of fit for Dynamic fits</i>
---------------	---

Description

Goodness of fit for Dynamic fits

Usage

```
goodness_dyna(object)
```

Arguments

object	An instance of FitInactivation
--------	--------------------------------

goodness_iso	<i>Goodness of fit for Isothermal fits</i>
--------------	--

Description

Goodness of fit for Isothermal fits

Usage

```
goodness_iso(object)
```

Arguments

object	An object of class IsoFitInactivation.
--------	--

goodness_MCMC	<i>Goodness of fit for MCMC fits</i>
---------------	--------------------------------------

Description

Goodness of fit for MCMC fits

Usage

```
goodness_MCMC(object)
```

Arguments

object	An instance of FitInactivationMCMC
--------	------------------------------------

goodness_of_fit *Goodness of fit for microbial inactivation models*

Description

Generates a table with several statistical indexes describing the quality of the model fit:

- ME: Mean Error.
- RMSE: Root Mean Squared Error.
- loglik: log-likelihood.
- AIC: Akaike Information Criterion.
- AICc: Akaike Information Criterion with correction for finite sample size.
- BIC: Bayesian Information Criterion.
- Af: Accuracy factor.
- Bf: Bias factor.

Usage

```
goodness_of_fit(object)
```

Arguments

object A model fit generated by bioinactivation

is.FitInactivation *Test of FitInactivation object*

Description

Tests if an object is of class FitInactivation.

Usage

```
is.FitInactivation(x)
```

Arguments

x object to be checked.

Value

A logic specifying whether x is of class FitInactivation

is.FitInactivationMCMC

Test of FitInactivationMCMC object

Description

Tests if an object is of class FitInactivationMCMC.

Usage

is.FitInactivationMCMC(x)

Arguments

x object to be checked.

Value

A logic specifying whether x is of class FitInactivationMCMC

is.IsoFitInactivation *Test of IsoFitInactivation object*

Description

Tests if an object is of class IsoFitInactivation.

Usage

is.IsoFitInactivation(x)

Arguments

x object to be checked.

Value

A logic specifying whether x is of class IsoFitInactivation

is.PredInactivationMCMC

Test of PredInactivationMCMC object

Description

Tests if an object is of class PredInactivationMCMC.

Usage

is.PredInactivationMCMC(x)

Arguments

x object to be checked.

Value

A logic specifying whether x is of class PredInactivationMCMC

is.SimulInactivation *Test of SimulInactivation object*

Description

Tests if an object is of class SimulInactivation.

Usage

is.SimulInactivation(x)

Arguments

x object to be checked.

Value

A logic specifying whether x is of class SimulInactivation

`isothermal_inactivation`*Example Isothermal Inactivation of a Microorganism*

Description

Example of experimental data for an isothermal process of a microorganism.

Usage

```
data(isothermal_inactivation)
```

Format

A data frame with 36 rows and 3 variables.

Details

- time: Time in minutes of the measurement.
- temp: Temperature at which the experiment was made.
- log_diff: Logarithmic difference.

`laterosporus_dyna`*Example Dynamic Inactivation of a Laterosporus*

Description

Example of experimental data of the dynamic inactivation process of Laterosporus

Usage

```
data(laterosporus_dyna)
```

Format

A data frame with 20 rows and 3 variables.

Details

- time: Time in minutes of the measurement.
- temp: observed temperature.
- logN: recorded number of microorganism.

laterosporus_iso	<i>Example Isothermal Inactivation of a Laterosporus</i>
------------------	--

Description

Example of experimental data for an isothermal process of Laterosporus.

Usage

```
data(laterosporus_iso)
```

Format

A data frame with 52 rows and 3 variables.

Details

- time: Time in minutes of the measurement.
- temp: Temperature at which the experiment was made.
- log_diff: Logarithmic difference.

Metselaar_iso	<i>Isothermal Metselaar model</i>
---------------	-----------------------------------

Description

Returns the predicted logarithmic reduction in microbial count according to Metselaars's model for the time, temperature and model parameters given.

Usage

```
Metselaar_iso(time, temp, D_R, z, p, Delta, temp_ref)
```

Arguments

time	numeric indicating the time at which the prediction is taken.
temp	numeric indicating the temperature of the treatment.
D_R	numeric defining the delta-value at the reference temperature.
z	numeric defining the z-value.
p	numeric defining shape factor of the Weibull distribution.
Delta	numeric reparametrization factor
temp_ref	numeric indicating the reference temperature.

Value

A numeric with the predicted logarithmic reduction ($\log_{10}(N/N_0)$).

plot.FitInactivation *Plot of FitInactivation Object*

Description

Plots a comparison between the experimental data provided and the prediction produced by the model parameters adjusted for an instance of `FitInactivation`.

Usage

```
## S3 method for class 'FitInactivation'
plot(
  x,
  y = NULL,
  ...,
  make_gg = TRUE,
  plot_temp = FALSE,
  label_y1 = "logN",
  label_y2 = "Temperature",
  ylims = NULL
)
```

Arguments

<code>x</code>	the object of class <code>FitInactivation</code> to plot.
<code>y</code>	ignored
<code>...</code>	additional arguments passed to <code>plot</code> .
<code>make_gg</code>	logical. If <code>TRUE</code> , the plot is created using <code>ggplot2</code> . Otherwise, the plot is created with base R. <code>TRUE</code> by default.
<code>plot_temp</code>	logical. Whether the temperature profile will be added to the plot. <code>FALSE</code> by default.
<code>label_y1</code>	Label of the principal y-axis.
<code>label_y2</code>	Label of the secondary y-axis.
<code>ylims</code>	Numeric vector of length 2 with the Limits of the y-axis. <code>NULL</code> by default (0, <code>max_count</code>).

Value

If `make_gg = FALSE`, the plot is created. Otherwise, an instance of `ggplot` is generated, printed and returned.

`plot.FitInactivationMCMC`*Plot of FitInactivationMCMC Object*

Description

Plots a comparison between the experimental data provided and the prediction produced by the model parameters adjusted for an instance of `FitInactivationMCMC`.

Usage

```
## S3 method for class 'FitInactivationMCMC'
plot(
  x,
  y = NULL,
  ...,
  make_gg = TRUE,
  plot_temp = FALSE,
  label_y1 = "logN",
  label_y2 = "Temperature",
  ylims = NULL
)
```

Arguments

<code>x</code>	the object of class <code>FitInactivation</code> to plot.
<code>y</code>	ignored
<code>...</code>	additional arguments passed to <code>plot</code> .
<code>make_gg</code>	logical. If <code>TRUE</code> , the plot is created using <code>ggplot2</code> . Otherwise, the plot is created with base R. <code>TRUE</code> by default.
<code>plot_temp</code>	logical. Whether the temperature profile will be added to the plot. <code>FALSE</code> by default.
<code>label_y1</code>	Label of the principal y-axis.
<code>label_y2</code>	Label of the secondary y-axis.
<code>ylims</code>	Numeric vector of length 2 with the Limits of the y-axis. <code>NULL</code> by default (<code>0</code> , <code>max_count</code>).

Value

If `make_gg = FALSE`, the plot is created. Otherwise, an instance of `ggplot` is generated, printed and returned.

`plot.IsoFitInactivation`*Plot of IsoFitInactivation Object*

Description

For each one of the temperatures studied, plots a comparison between the predicted result and the experimental one for an instance of IsoFitInactivation.

Usage

```
## S3 method for class 'IsoFitInactivation'  
plot(x, y = NULL, ..., make_gg = FALSE)
```

Arguments

x	the object of class IsoFitInactivation to plot.
y	ignored
...	additional arguments passed to plot.
make_gg	logical. If TRUE, the plot is created using ggplot2. Otherwise, the plot is created with base R. FALSE by default.

`plot.PredInactivationMCMC`*Plot of PredInactivationMCMC Object*

Description

Plots the prediction interval generated by [predict_inactivation_MCMC](#).

Usage

```
## S3 method for class 'PredInactivationMCMC'  
plot(x, y = NULL, ..., make_gg = TRUE)
```

Arguments

x	the object of class PredInactivationMCMC to plot.
y	ignored
...	additional arguments passed to plot.
make_gg	logical. If TRUE, the plot is created using ggplot2. Otherwise, the plot is created with base R. TRUE by default.

Details

The plot generated in ggplot (default) generates a dashed line with the mean of the MC simulations. Moreover, a ribbon with the 2 first quantiles (i.e. columns 3 and 4) is generated.

The plot generated with base R (make_gg = FALSE) generates a solid line with the mean of the MC simulations. Each one of the other quantiles included in the data frame are added with different

Value

If make_gg = FALSE, the plot is created. Otherwise, an an instance of ggplot is generated, printed and returned.

plot.SimulInactivation

Plot of SimulInactivation Object

Description

Plots the predicted evolution of the logarithmic count with time for an instance of SimulInactivation.

Usage

```
## S3 method for class 'SimulInactivation'
plot(
  x,
  y = NULL,
  ...,
  make_gg = TRUE,
  plot_temp = FALSE,
  label_y1 = "logN",
  label_y2 = "Temperature",
  ylims = NULL
)
```

Arguments

x	The object of class SimulInactivation to plot.
y	ignored
...	additional arguments passed to plot.
make_gg	logical. If TRUE, the plot is created using ggplot2. Otherwise, the plot is crated with base R. TRUE by default.
plot_temp	logical. Whether the temperature profile will be added to the plot. FALSE by default.
label_y1	Label of the principal y-axis.
label_y2	Label of the secondary y-axis.
ylims	Numeric vector of length 2 with the Limits of the y-axis. NULL by default (0, max_count).

Value

If `make_gg = FALSE`, the plot is created. Otherwise, an an instance of `ggplot` is generated, printed and returned.

predict_inactivation *Prediction of Dynamic Inactivation*

Description

Predicts the inactivation of a microorganism under isothermal or non-isothermal temperature conditions. The thermal resistance of the microorganism are defined with the input arguments.

Usage

```
predict_inactivation(
  simulation_model,
  times,
  parms,
  temp_profile,
  ...,
  tol0 = 1e-05
)
```

Arguments

<code>simulation_model</code>	character identifying the model to be used.
<code>times</code>	numeric vector of output times.
<code>parms</code>	list of parameters defining the parameters of the model.
<code>temp_profile</code>	data frame with discrete values of the temperature for each time. It must have one column named <code>time</code> and another named <code>temperature</code> providing discrete values of the temperature at time points.
<code>...</code>	Additional arguments passed to <code>deSolve::ode</code> .
<code>tol0</code>	numeric. Observations at time 0 make Weibull-based models singular. The time for observatins taken at time 0 are changed for this value. By default (<code>tol0 = 1e-5</code>)

Details

The value of the temperature is calculated at each value of time by linear interpolation of the values provided by the input argument `temp_profile`. The function `deSolve::ode` is used for the resolution of the differential equation.

Value

A list of class `SimulInactivation` with the results. It has the following entries:

- `model`: character defining the model use for the prediction.
- `model_parameters`: named numeric vector with the values of the model parameters used.
- `temp_approximations`: function used for the interpolation of the temperature. For a numeric value of time given, returns the value of the temperature and its first derivative.
- `simulation`: A data frame with the results calculated. Its first column contains the times at which the solution has been calculated. The following columns the values of the variables of the model. The three last columns provide the values of $\log N$, S and $\log S$.

Examples

```
## EXAMPLE 1 -----

## Retrieve the model keys available for dynamic models.
get_model_data()

## Set the input arguments
example_model <- "Geeraerd" # Geeraerd's model will be used
times <- seq(0, 5, length=100) # values of time for output

model_data <- get_model_data(example_model) # Retrieve the data of the model used
print(model_data$parameters)
print(model_data$variables)
model_parms <- c(D_R = 1,
                z = 10,
                N_min = 100,
                temp_ref = 100,
                N0 = 100000,
                C_c0 = 1000
                )

## Define the temperature profile for the prediction
temperature_profile <- data.frame(time = c(0, 1.25, 2.25, 4.6),
                                temperature = c(70, 105, 105, 70))

## Call the prediction function
prediction_results <- predict_inactivation(example_model, times,
                                         model_parms, temperature_profile)

## Show the results
head(prediction_results$simulation)
plot(prediction_results)
time_to_logreduction(1.5, prediction_results)

## END EXAMPLE 1 -----
```

 predict_inactivation_MCMC

Dynamic Prediction Intervals from a Monte Carlo Adjustment

Description

Given a model adjustment of a dynamic microbial inactivation process performed using any of the functions in bioinactivation calculates probability intervals at each time point using a Monte Carlo method.

Usage

```
predict_inactivation_MCMC(
  fit_object,
  temp_profile,
  n_simulations = 100,
  times = NULL,
  quantiles = c(2.5, 97.5),
  additional_pars = NULL
)
```

Arguments

fit_object	An object of classes FitInactivationMCMC, IsoFitInactivation or FitInactivation.
temp_profile	data frame with discrete values of the temperature for each time. It must have one column named time and another named temperature providing discrete values of the temperature at time points.
n_simulations	a numeric indicating how many Monte Carlo simulations to perform. 100 by default.
times	numeric vector specifying the time points when results are desired. If NULL, the times in MCMC_fit\$best_prediction are used. NULL by default.
quantiles	numeric vector indicating the quantiles to calculate in percentage. By default, it is set to c(2.5, 97.5) which generates a prediction interval with confidence 0.95. If NULL, the quantiles are not calculated and all the simulations are returned.
additional_pars	Additional parameters not included in the adjustment (e.g. the initial number of microorganism in an isothermal fit).

Value

A data frame of class PredInactivationMCMC. On its first column, time at which the calculation has been made is indicated. If quantiles = NULL, the following columns contain the results of each simulation. Otherwise, the second and third columns provide the mean and median of the simulations at the given time point. Following columns contain the quantiles of the results.

sample_dynaFit	<i>Random sample of the parameters of a FitInactivation object</i>
----------------	--

Description

Function to be called by [predict_inactivation_MCMC](#). Produces a random sample of the parameters adjusted from dynamic experiments with non linear regression.

Usage

```
sample_dynaFit(dynamic_fit, times, n_simulations)
```

Arguments

dynamic_fit	An object of class FitInactivationMCMC as generated by fit_inactivation_MCMC .
times	numeric vector specifying the time points when results are desired. If NULL, the times in <code>MCMC_fit\$best_prediction</code> are used.
n_simulations	a numeric indicating how many Monte Carlo simulations to perform.

Details

It is assumed that the parameters follow a Multivariate Normal distribution with the mean the parameters estimated by [FME::modFit](#). The unscaled covariance matrix returned by [FME::modFit](#) is used.

The function produces a random sample.

Value

Returns a list with 4 components.

- `par_sample`: data frame with the parameter sample.
- `simulation_model`: model key for the simulation
- `known_pars`: parameters of the model known
- `times`: points where the calculation is made.

sample_IsoFit	<i>Random sample of the parameters of a IsoFitInactivation object</i>
---------------	---

Description

Function to be called by [predict_inactivation_MCMC](#). Produces a random sample of the parameters adjusted from isothermal experiments.

Usage

```
sample_IsoFit(iso_fit, times, n_simulations)
```

Arguments

iso_fit	An object of class <code>FitInactivationMCMC</code> as generated by fit_inactivation_MCMC .
times	numeric vector specifying the time points when results are desired. If <code>NULL</code> , an equispaced interval between 0 and the maximum time of the observations with length 50 is used.
n_simulations	a numeric indicating how many Monte Carlo simulations to perform.

Details

It is assumed that the parameters follow a Multivariate Normal distribution with the mean and covariance matrix estimated by the adjustment. The function produces a random sample using the function [MASS::mvrnorm](#).

Value

Returns a list with 4 components.

- `par_sample`: data frame with the parameter sample.
- `simulation_model`: model key for the simulation
- `known_pars`: parameters of the model known
- `times`: points where the calculation is made.

sample_MCMCfit	<i>Random sample of the parameters of a FitInactivationMCMC object</i>
----------------	--

Description

Function to be called by `predict_inactivation_MCMC`. Produces a random sample of the parameters calculated on the iterations of the Monte Carlo simulation.

Usage

```
sample_MCMCfit(MCMC_fit, times, n_simulations)
```

Arguments

MCMC_fit	An object of class <code>FitInactivationMCMC</code> as generated by <code>fit_inactivation_MCMC</code> .
times	numeric vector specifying the time points when results are desired. If NULL, the times in <code>MCMC_fit\$best_prediction</code> are used.
n_simulations	a numeric indicating how many Monte Carlo simulations to perform.

Value

Returns a list with 4 components.

- `par_sample`: data frame with the parameter sample.
- `simulation_model`: model key for the simulation
- `known_pars`: parameters of the model known
- `times`: points where the calculation is made.

summary.FitInactivation	<i>Summary of a FitInactivation object</i>
-------------------------	--

Description

Summary of a `FitInactivation` object

Usage

```
## S3 method for class 'FitInactivation'
summary(object, ...)
```

Arguments

object	Instance of <code>Fit Inactivation</code>
...	ignored

summary.FitInactivationMCMC

Summary of a FitInactivationMCMC object

Description

Summary of a FitInactivationMCMC object

Usage

```
## S3 method for class 'FitInactivationMCMC'  
summary(object, ...)
```

Arguments

object	Instance of FitInactivationMCMC
...	ignored

summary.IsoFitInactivation

Summary of a IsoFitInactivation object

Description

Summary of a IsoFitInactivation object

Usage

```
## S3 method for class 'IsoFitInactivation'  
summary(object, ...)
```

Arguments

object	Instance of IsoFitInactivation
...	ignored

time_to_logreduction *Time to reach X log reductions*

Description

Calculates the treatment time required to reach a given number of log reductions.

Usage

```
time_to_logreduction(n_logs, my_prediction)
```

Arguments

n_logs Numeric of length one indicating the number of log recutions
my_prediction An object of class SimulInactivation

Details

The treatment time is calculated by linear interpolation between the two points of the simulation whose logS is closer to n_logs

WeibullMafart_iso *Isothermal Weibull-Mafart Model*

Description

Returns the predicted logarithmic reduction in microbial count according to Weibull-Mafarts's model for the time, temperature and model parameters given.

Usage

```
WeibullMafart_iso(time, temp, delta_ref, z, p, temp_ref)
```

Arguments

time numeric indicating the time at which the prediction is taken.
temp numeric indicating the temperature of the treatment.
delta_ref numeric defining the delta-value at the reference temperature.
z numeric defining the z-value.
p numeric defining shape factor of the Weibull distribution.
temp_ref numeric indicating the reference temperature.

Value

A numeric with the predicted logarithmic reduction ($\log_{10}(N/N_0)$).

WeibullPeleg_iso	<i>Isothermal Weibull-Peleg Model</i>
------------------	---------------------------------------

Description

Returns the predicted logarithmic reduction in microbial count according to Weibull-Peleg's model for the time, temperature and model parameters given.

Usage

```
WeibullPeleg_iso(time, temp, n, k_b, temp_crit)
```

Arguments

time	numeric indicating the time at which the prediction is taken.
temp	numeric indicating the temperature of the treatment.
n	numeric defining shape factor of the Weibull distribution.
k_b	numeric indicating the slope of the b~temp line.
temp_crit	numeric with the value of the critical temperature.

Value

A numeric with the predicted logarithmic reduction ($\log_{10}(N/N_0)$).

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