Package ‘bioinactivation’

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Type Package

Title Mathematical Modelling of (Dynamic) Microbial Inactivation

Version 1.3.0

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

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Contents

`Arrhenius_iso` *Isothermal Arrhenius model*

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 ($log10(N/N0)$).

`Bigelow_iso` *Isothermal Bigelow's Model*

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 ($log10(N/N0)$).

`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` *First derivative of the Arrhenius model*

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 independenent.

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 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

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

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

```
\deqn{\frac{dC_c}{dt} = - C_c \cdot k_{max}}{
          dC_c/dt = - C_c * k_max}

\deqn{\alpha = \frac {1}{1+C_c}}{
          \alpha = 1/(1+C_c)}

\deqn{\gamma = 1 - \frac{N_{res}}{N}}{
          \gamma = 1 - N_res/N}

\deqn{k_{max} = \frac{1}{D_T}}{k_max = 1/D_T}

\deqn{log_{10}D_T = log_{10}D_R + \frac{T_R-T}{z}}{
           log(D_T) = log(D_R) + (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

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

\deqn{\delta(T) = \delta_{ref} \cdot 10^{- (T-T_ref)/z} }{
          delta(T) = delta_ref * 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

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

\deqn{D(T) = D_{ref} \cdot 10^{- (T-T_ref)/z} }{
          D(T) = D_R * 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 logS 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 logS at time `t` as a list.

Model Equation

$$\frac{d(\log_{10}(S))}{dt} = -b(T) \cdot n \cdot (-log10(S)/b(T))^{(n-1)/n)}$$

```
\deqn{b(T) = \mathrm{ln}(1 + exp( k_b*(T - T_{crit}) ))}{
          b(T) = ln( 1 + exp( k_b*(T - T_crit) ) )}
```

Model Parameters

- temp_crit: Temperature below which there is inactivation.
- k_b: slope of the b ~ temp line for temperatures above the critical one.
- n: shape factor of the Weibull distribution.

Note

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

See Also

`predict_inactivation`

`dynamic_inactivation` *Example Dynamic Inactivation of a Microorganis*

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

`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.
`...`	further arguments passed to FME::modFit
`minimize_log`	logical. If `TRUE`, the adjustment is based on the minimization of the error of the logarithmic count. `TRUE` by default.
`tol0`	numeric. Observations at time 0 make Weibull-based models singular. The time for observatins 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 observatins 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 specyfing the model to adjust.
`death_data`	data frame with the experiment data where each row is one observation. It must have the following columns: • 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` *Mapping of Simulation Model Functions*

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` *Goodness of fit for Dynamic fits*

Description

Goodness of fit for Dynamic fits

Usage

```
goodness_dyna(object)
```

Arguments

`object`	An instance of FitInactivation

`goodness_iso` *Goodness of fit for Isothermal fits*

Description

Goodness of fit for Isothermal fits

Usage

```
goodness_iso(object)
```

Arguments

`object`	An object of class IsoFitInactivation.

`goodness_MCMC` *Goodness of fit for MCMC fits*

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 Infromation 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 Microorganis*

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` *Example Isothermal Inactivation of a Laterosporus*

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` *Isothermal Metselaar model*

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 ($log10(N/N0)$).

`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

`x`	the object of class `FitInactivation` 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.

`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

`x`	the object of class `FitInactivation` 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.

`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 crated 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 crated 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 wth 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 resistence of the microorganism are defined with the input arguments.

Usage

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

Arguments

`simulation_model`	character identifying the model to be used.
`times`	numeric vector of output times.
`parms`	list of parameters defining the parameters of the model.
`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.
`...`	Additional arguments passed to deSolve::ode.
`tol0`	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 (`tol0 = 1e-5`)

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 `logN`, `S` and `logS`.

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)  # Retrive 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` *Random sample of the parameters of a FitInactivation object*

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 `MCMC_fit$best_prediction` 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` *Random sample of the parameters of a IsoFitInactivation object*

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 `FitInactivationMCMC` as generated by `fit_inactivation_MCMC`.
`times`	numeric vector specifying the time points when results are desired. If `NULL`, 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` *Random sample of the parameters of a FitInactivationMCMC object*

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 `FitInactivationMCMC` as generated by `fit_inactivation_MCMC`.
`times`	numeric vector specifying the time points when results are desired. If `NULL`, the times in `MCMC_fit$best_prediction` 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` *Summary of a FitInactivation object*

Description

Summary of a FitInactivation object

Usage

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

Arguments

`object`	Instance of Fit Inactivation
`...`	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 treatement time is calculated by linear interpolation betweent 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 ($log10(N/N0)$).

`WeibullPeleg_iso` *Isothermal Weibull-Peleg Model*

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 ($log10(N/N0)$).

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