Package 'edwards97'

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Title Langmuir Semi-Empirical Coagulation Model

Version 0.1.0

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Description Implements the Edwards (1997) <doi:10.1002/j.1551-8833.1997.tb08229.x> Langmuir-based semi-empirical coagulation model, which predicts the concentration of organic carbon remaining in water after treatment with an Al- or Fe-based coagulant. Data and methods are provided to optimise empirical coefficients.

Depends R (>= 3.6.0)

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 7.0.2

URL https://paleolimbot.github.io/edwards97/, https://github.com/paleolimbot/edwards97

BugReports https://github.com/paleolimbot/edwards97/issues

Imports rlang, tibble, broom, cli, withr, glue

Suggests testthat (>= 2.1.0), covr

NeedsCompilation no

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R topics documented:

`coagulate` *Low-level langmuir coagulation calculations*

Description

The Edwards (1997) model is a Langmuir-based semiempirical model designed to predict OC removal during alum coagulation. The model is on a non-linear function derived from physical relationships, primarily the process of Langmuir sorptive removal (Tipping 1981, Jekyl 1986).

Usage

```
coagulate(data, coefs)

coagulate_base(DOC, dose, pH, UV254, K1, K2, x1, x2, x3, b, root = -1)
```

Arguments

`data`	A data frame containing columns `DOC`, `dose`, `pH`, and `UV254`.
`coefs`	The output of `edwards_coefs()` or a similar named vector containing elements `K1`, `K2`, `x1`, `x2`, `x3`, `b` and `root`.
`DOC`	The initial DOC concentration (mg/L).
`dose`	The coagulant dose (mmol/L).
`pH`	The pH of coagulation.
`UV254`	The absorbance of UV254 (1/cm). With `DOC`, used to calculate SUVA.
`K1, K2`	Empirical fitting coefficients relating to SUVA.
`x1, x2, x3`	Empirical fitting coefficients relating to pH.
`b`	The Langmuir term.
`root`	The solution to the equation presented in Edwards (1997) is a quadratic with two roots. `root` can be 1 or -1 to account for these roots, however we see no evidence that anything except -1 here results in realistic predictions.

Value

A vector of predicted organic carbon concentrations (in mg/L) following coagulation.

References

Edwards, M. 1997. Predicting DOC removal during enhanced coagulation. Journal - American Water Works Association, 89: 78–89. https://doi.org/10.1002/j.1551-8833.1997.tb08229.x

Jekel, M.R. 1986. Interactions of humic acids and aluminum salts in the flocculation process. Water Research, 20: 1535-1542. https://doi.org/10.1016/0043-1354(86)90118-1

Tipping, E. 1981. The adsorption of aquatic humic substances by iron oxides. Geochimica et Cosmochimica Acta, 45: 191-199. https://doi.org/10.1016/0016-7037(81)90162-9

Examples

```
alum_jar_tests <- edwards_data("Al")
alum_jar_tests$DOC_final_model <- coagulate(alum_jar_tests, edwards_coefs("Al"))
plot(DOC_final_model ~ DOC_final, data = alum_jar_tests)
```

`dose_of_diminishing_returns`

Calculate the dose of diminishing return

Description

Calculate the dose of diminishing return

Usage

```
dose_of_diminishing_returns(
  dose,
  DOC_final,
  molar_mass = 297,
  threshold = 0.3/10
)

dose_for_criterion(dose, DOC_final, criterion)
```

Arguments

`dose`	The coagulant dose (mmol/L).
`DOC_final`	The final DOC concentration, probably modeled using `fit_edwards_optim()` or `fit_edwards()` and `coagulate_grid()`.
`molar_mass`	The moalr mass of the coagulant, in grams per mol Al or Fe.
`threshold`	The point of diminishing return threshold, in mg/L DOC per mg/L dose. Often this is taken to be 0.3 mg/L DOC per 10 mg/L dose (Brantby 2016).
`criterion`	A desired final DOC concentration in mg/L

Value

The dose (in mmol/L) of diminishing returns.

References

Bratby, J. 2016. Coagulation and Flocculation in Water and Wastewater Treatment. IWA Publishing. https://books.google.ca/books?id=PabQDAAAQBAJ

Examples

```
dose_curve <- coagulate_grid(fit_edwards("Low DOC"), DOC = 4, UV254 = 0.2, pH = 5.5)
dose_of_diminishing_returns(dose_curve$dose, dose_curve$DOC_final)
dose_for_criterion(dose_curve$dose, dose_curve$DOC_final, criterion = 3)
```

---

edwards_coefs *Coagulation coefficients*

Description

These are coefficients intended for general use. Use `fit_edwards_optim()` to optimise these coefficients for a specific source water.

Usage

```
edwards_coefs(type)

edwards_data(type)

fit_edwards(type)
```

Arguments

type	One of "Low DOC", "Fe", "Al", "General-Fe", "General-Al", or "empty".

Value

A named vector of empirical coefficients to be used in `coagulate()`.

References

Edwards, M. 1997. Predicting DOC removal during enhanced coagulation. Journal - American Water Works Association, 89: 78–89. https://doi.org/10.1002/j.1551-8833.1997.tb08229.x

Examples

```
edwards_coefs("Low DOC")
```

edwards_jar_tests *Example Jar Tests*

Description

Example Jar Tests

Usage

```
edwards_jar_tests
```

Format

An object of class `tbl_df` (inherits from `tbl`, `data.frame`) with 1372 rows and 7 columns.

Author(s)

Marc Edwards and Tai Tseng

References

Edwards, M. 1997. Predicting DOC removal during enhanced coagulation. Journal - American Water Works Association, 89: 78–89. https://doi.org/10.1002/j.1551-8833.1997.tb08229.x

fit_edwards_optim *Fit Empirical Coefficients*

Description

The coefficients calculated by Edwards (1997) and returned by `edwards_coefs()` were designed to produce reasonable results for several general cases, however each source water will have a set of empirical coefficients that produce more accurate predictions than the general case. This function calculates the optimal coefficients given a test set of known initial values (DOC)

Usage

```
fit_edwards_optim(
  data,
  initial_coefs = edwards_coefs("Al"),
  optim_params = list()
)

fit_edwards_coefs(coefs, data = edwards_data("empty"))

## S3 method for class 'edwards_fit_optim'
coef(object, ...)
```

```
## S3 method for class 'edwards_fit_coefs'
coef(object, ...)

## S3 method for class 'edwards_fit_base'
predict(object, newdata = NULL, ...)

coagulate_grid(
  object,
  DOC,
  UV254,
  dose = seq(0.01, 2, length.out = 50),
  pH = seq(5, 8, length.out = 50)
)

## S3 method for class 'edwards_fit_base'
fitted(object, ...)

## S3 method for class 'edwards_fit_base'
residuals(object, ...)

## S3 method for class 'edwards_fit_base'
tidy(x, ...)

## S3 method for class 'edwards_fit_base'
glance(x, ...)

## S3 method for class 'edwards_fit_base'
print(x, ...)

## S3 method for class 'edwards_fit_base'
plot(x, ...)
```

Arguments

`data`	A data frame with columns `DOC` (mg/L), `dose` (mmol/L), `pH` (pH units), `UV254` (1/cm), and `DOC_final` (mg/L). See `coagulate()` for more information.
`optim_params`	Additional arguments to be passed to `stats::optim()`.
`coefs, initial_coefs`	A set of initial coefficients from which to start the optimisation. Most usefully one of the coefficient sets returned by `edwards_coefs()`.
`object, x`	A fit objected created with `fit_edwards_optim()`.
`...`	Not used.
`newdata`	A data frame with columns `DOC` (mg/L), `dose` (mmol/L), `pH` (pH units), and `UV254` (1/cm). If omitted, the data used to fit the model is used.
`DOC`	The initial DOC concentration (mg/L).
`UV254`	The absorbance of UV254 (1/cm). With `DOC`, used to calculate SUVA.

`dose`	The coagulant dose (mmol/L).
`pH`	The pH of coagulation.

Value

An S3 of type "edwards_fit_optim" with components:

data, initial_coefs, optim_params References to inputs.

fit_optim The fit object returned by `stats::optim()`.

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