

Package ‘edwards97’

October 13, 2022

Title Langmuir Semi-Empirical Coagulation Model

Version 0.1.1

Maintainer Dewey Dunnington <dewey@fishandwhistle.net>

Description Implements the Edwards (1997) <[doi:10.1002/j.1551-8833.1997.tb08229.x](https://doi.org/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 7.2.1

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 (>= 3.0.0), covr

Config/testthat/edition 3

NeedsCompilation no

Author Dewey Dunnington [aut, cre] (<<https://orcid.org/0000-0002-9415-4582>>),
Benjamin Trueman [aut] (<<https://orcid.org/0000-0002-1539-3092>>),
William Raseman [aut] (<<https://orcid.org/0000-0001-5946-8888>>),
Marc Edwards [ctb],
Tai Tseng [ctb]

Repository CRAN

Date/Publication 2022-09-01 02:20:06 UTC

R topics documented:

coagulate	2
dose_of_diminishing_returns	3
edwards_coefs	4
edwards_jar_tests	5
fit_edwards_optim	5

Index	8
--------------	----------

coagulate	<i>Low-level langmuir coagulation calculations</i>
-----------	--

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 <code>edwards_coefs()</code> 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 metal concentration (Al ³⁺ or Fe ³⁺) in 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](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](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 metal concentration (Al ³⁺ or Fe ³⁺) in mmol/L. |
| DOC_final | The final DOC concentration, probably modeled using <code>fit_edwards_optim()</code> or <code>fit_edwards()</code> and <code>coagulate_grid()</code> . |
| molar_mass | The molar 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("A1"),  
  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 <code>coagulate()</code> for more information.
optim_params	Additional arguments to be passed to <code>stats::optim()</code> .
coefs, initial_coefs	A set of initial coefficients from which to start the optimisation. Most usefully one of the coefficient sets returned by <code>edwards_coefs()</code> .
object, x	A fit object created with <code>fit_edwards_optim()</code> .
...	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 metal concentration (Al ³⁺ or Fe ³⁺) in 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\(\)](#).

Index

- * **datasets**
 - edwards_jar_tests, 5
- coagulate, 2
- coagulate(), 4, 6
- coagulate_base (coagulate), 2
- coagulate_grid (fit_edwards_optim), 5
- coagulate_grid(), 3
- coef.edwards_fit_coefs
 - (fit_edwards_optim), 5
- coef.edwards_fit_optim
 - (fit_edwards_optim), 5
- dose_for_criterion
 - (dose_of_diminishing_returns), 3
- dose_of_diminishing_returns, 3
- edwards_coefs, 4
- edwards_coefs(), 2, 5, 6
- edwards_data (edwards_coefs), 4
- edwards_jar_tests, 5
- fit_edwards (edwards_coefs), 4
- fit_edwards(), 3
- fit_edwards_coefs (fit_edwards_optim), 5
- fit_edwards_optim, 5
- fit_edwards_optim(), 3, 4, 6
- fitted.edwards_fit_base
 - (fit_edwards_optim), 5
- glance.edwards_fit_base
 - (fit_edwards_optim), 5
- plot.edwards_fit_base
 - (fit_edwards_optim), 5
- predict.edwards_fit_base
 - (fit_edwards_optim), 5
- print.edwards_fit_base
 - (fit_edwards_optim), 5
- residuals.edwards_fit_base
 - (fit_edwards_optim), 5
- stats::optim(), 6, 7
- tidy.edwards_fit_base
 - (fit_edwards_optim), 5