Package 'AdIsMF'

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Type Package

Title Adsorption Isotherm Model Fitting

Version 0.1.0

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Description The Langmuir and Freundlich adsorption isotherms are pivotal in characterizing adsorption processes, essential across various scientific disciplines. Proper interpretation of adsorption isotherms involves robust fitting of data to the models, accurate estimation of parameters, and efficiency evaluation of the models, both in linear and non-linear forms. For researchers and practitioners in the fields of chemistry, environmental science, soil science, and engineering, a comprehensive package that satisfies all these requirements would be ideal for accurate and efficient analysis of adsorption data, precise model selection and validation for rigorous scientific inquiry and real-world applications. Details can be found in Langmuir (1918) <doi:10.1021/ja02242a004> and Giles (1973) <doi:10.1111/j.1478-4408.1973.tb03158.x>.

Encoding UTF-8

License GPL-3

Imports AICcmodavg, ggplot2, nls2, stats

NeedsCompilation no

RoxygenNote 7.3.1

Repository CRAN

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Contents

FLM *Freundlich Linear Model*

Description

This model will fit the adsorption data to the linear form of the Freundlich equation and will give the estimates of the Freundlich parameters, namely "kf" and "1/n" while evaluating the performance efficiency of the linear model of Freundlich through several error functions.

Usage

```
FLM (ce, qe)
```

Arguments

ce	Equilibrium concentration of the adsorbate in the solution
qe	Amount adsorbed

Value

- Freundlich Isotherm Linear Model: Model summary
- correlation (ce, qe): Correlation between ce and qe
- kf: Freundlich constant
- 1/n: Freundlich exponent related to adsorption intensity
- AIC: Akaike information criterion
- AICc: Corrected Akaike information criterion
- BIC: Bayesian information criterion
- RMSE: Root Mean Squared Error
- MSE: Mean Squared Error
- MAE: Mean Absolute Error
- MAPE: Mean Absolute Percentage Error
- Chi.square: Chi-square value

References

- Giles, C. H. (1973). The history and use of the Freundlich adsorption isotherm. Journal of the Society of Dyers and Colourists, 89(8), 287-291.
- Datta, S. P., Bhadoria, P. B. S., & Kar, S. (1998). Availability of extractable boron in some acid soils, West Bengal, India. Communications in soil science and plant analysis, 29(15-16), 2285-2306.

Examples

```
ce <- c(0.025, 0.04, 0.055, 0.099, 0.139, 0.402, 1.999, 11.336)
qe <- c(17.21, 35.42, 51.238, 72.659, 89.268, 182.21, 345.29, 634.231)
m.fit <- FLM (ce, qe)
```

FNLM *Freundlich Nonlinear Model*

Description

This model will fit the adsorption data to the nonlinear form of the Freundlich equation and will give the estimates of the Freundlich parameters, namely "kf" and "1/n" while evaluating the performance efficiency of the nonlinear model of Freundlich through several error functions.

Usage

```
FNLM (ce, qe)
```

Arguments

ce	Equilibrium concentration of the adsorbate in the solution
qe	Amount adsorbed

Value

- Freundlich Isotherm Nonlinear Model: Model summary
- correlation (ce, qe): Correlation between ce and qe
- kf: Freundlich constant
- 1/n: Freundlich exponent related to adsorption intensity
- AIC: Akaike information criterion
- AICc: Corrected Akaike information criterion
- BIC: Bayesian information criterion
- RMSE: Root Mean Squared Error
- MSE: Mean Squared Error
- MAE: Mean Absolute Error
- MAPE: Mean Absolute Percentage Error
- Chi.square: Chi-square value

References

- Giles, C. H. (1973). The history and use of the Freundlich adsorption isotherm. Journal of the Society of Dyers and Colourists, 89(8), 287-291.
- Datta, S. P., Bhadoria, P. B. S., & Kar, S. (1998). Availability of extractable boron in some acid soils, West Bengal, India. Communications in soil science and plant analysis, 29(15-16), 2285-2306.

Examples

```
ce <- c(0.025, 0.04, 0.055, 0.099, 0.139, 0.402, 1.999, 11.336)
qe <- c(17.21, 35.42, 51.238, 72.659, 89.268, 182.21, 345.29, 634.231)
m.fit <- FNLM (ce, qe)
```

LLM *Langmuir Linear Model*

Description

This model will fit the adsorption data to the linear form of the Langmuir equation and will give the estimates of the Langmuir parameters, namely "b" and "k" while evaluating the performance efficiency of the linear model of Langmuir through several error functions.

Usage

```
LLM(ce, qe)
```

Arguments

ce	Equilibrium concentration of the adsorbate in the solution
qe	Amount adsorbed

Value

- Langmuir Isotherm Linear Model: Model summary
- correlation (ce, qe): Correlation between ce and qe
- b: Adsorption maxima
- k: Langmuir adsorption constant related to bonding energy
- AIC: Akaike information criterion
- AICc: Corrected Akaike information criterion
- BIC: Bayesian information criterion
- RMSE: Root Mean Squared Error
- MSE: Mean Squared Error
- MAE: Mean Absolute Error
- MAPE: Mean Absolute Percentage Error
- Chi.square: Chi-square value

References

- Langmuir, I. (1918). The adsorption of gases on plane surfaces of glass, mica and platinum. Journal of the American Chemical society, 40(9), 1361-1403.
- Datta, S. P., Bhadoria, P. B. S., & Kar, S. (1998). Availability of extractable boron in some acid soils, West Bengal, India. Communications in soil science and plant analysis, 29(15-16), 2285-2306.

Examples

```
ce <- c(0.025, 0.04, 0.055, 0.099, 0.139, 0.402, 1.999, 11.336)
qe <- c(17.21, 35.42, 51.238, 72.659, 89.268, 182.21, 345.29, 634.231)
m.fit <- LLM (ce, qe)
```

LNLM *Langmuir Nonlinear Model*

Description

This model will fit the adsorption data to the nonlinear form of the Langmuir equation and will give the estimates of the Langmuir parameters, namely "b" and "k" while evaluating the performance efficiency of the nonlinear model of Langmuir through several error functions.

Usage

```
LNLM (ce, qe)
```

Arguments

ce	Equilibrium concentration of the adsorbate in the solution
qe	Amount adsorbed

Value

- Langmuir Isotherm Nonlinear Model: Model summary
- correlation (ce, qe): Correlation between ce and qe
- b: Adsorption maxima
- k: Langmuir adsorption constant related to bonding energy
- AIC: Akaike information criterion
- AICc: Corrected Akaike information criterion
- BIC: Bayesian information criterion
- RMSE: Root Mean Squared Error
- MSE: Mean Squared Error
- MAE: Mean Absolute Error
- MAPE: Mean Absolute Percentage Error
- Chi.square: Chi-square value

References

- Langmuir, I. (1918). The adsorption of gases on plane surfaces of glass, mica and platinum. Journal of the American Chemical society, 40(9), 1361-1403.
- Datta, S. P., Bhadoria, P. B. S., & Kar, S. (1998). Availability of extractable boron in some acid soils, West Bengal, India. Communications in soil science and plant analysis, 29(15-16), 2285-2306.

Examples

```
ce <- c(0.025, 0.04, 0.055, 0.099, 0.139, 0.402, 1.999, 11.336)
qe <- c(17.21, 35.42, 51.238, 72.659, 89.268, 182.21, 345.29, 634.231)
m.fit <- LNLM (ce, qe)
```

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