Package 'adsoRptionCMF'

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Type Package

Title Classical Model Fitting of Adsorption Isotherms

Version 0.1.1

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Description

Provides tools for classical parameter estimation of adsorption isotherm models, including both linear and nonlinear forms of the Freundlich, Langmuir, and Temkin isotherms. This package allows
users to fit these models to experimental data, providing parameter estimates along with fit statistics
such as Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC). Error metrics are
computed to evaluate model performance, and the package produces model fit plots with bootstrapped 95%
confidence intervals. Additionally, it generates residual plots for diagnostic assessment of the models.
Researchers and engineers in material science, environmental engineering, and chemical engineering can
rigorously analyze adsorption behavior in their systems using this straightforward, non-Bayesian approach.
For more details, see Harding (1907) <doi:10.2307/2987516>.

License GPL-3

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Imports nls2, stats, Metrics, ggplot2, boot

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Contents

`fit_freundlichLM` *Freundlich Isotherm Linear Analysis*

Description

Performs linear modeling for the Freundlich adsorption isotherm using log-transformed data.

Arguments

`Ce`	numeric vector for equilibrium concentration
`Qe`	numeric vector for adsorbed amount
`verbose`	logical; if TRUE (default), prints summary and messages

Value

A list containing the results of the linear Freundlich model fitting, including:

- **Parameter estimates** for the Freundlich model (KF and n).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Freundlich, H. 1907. Ueber die adsorption in loesungen. Z. Phys. Chem.57:385-470

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fit_freundlichLM(Ce, Qe, verbose = TRUE)
fit_freundlichLM(Ce, Qe)
```

---

fit_freundlichNLM *Freundlich Isotherm Non-Linear Analysis*

Description

Performs non-linear modeling for the Freundlich adsorption isotherm.

Arguments

Ce	numeric vector for equilibrium concentration
Qe	numeric vector for adsorbed amount

Value

A list containing the results of the non-linear Freundlich model fitting, including:

- **Parameter estimates** for the Freundlich model (KF and n).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Freundlich, H. 1907. Ueber die adsorption in loesungen. Z. Phys. Chem.57:385-470

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fit_freundlichNLM(Ce,Qe)
```

`fit_langmuirLM1` *Langmuir Isotherm Linear (Form 1) Analysis*

Description

Performs linear modeling for the Langmuir adsorption isotherm using the linearized form Ce/Qe = (1/Qmax·b) + (Ce/Qmax).

Arguments

`Ce`	numeric vector for equilibrium concentration
`Qe`	numeric vector for adsorbed amount
`verbose`	logical; if TRUE (default), prints summary and messages

Value

A list containing the results of the linear Langmuir (Form 1) model fitting, including:

- **Parameter estimates** for the Langmuir model (Qmax and Kl).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Langmuir, I. (1918) <doi:10.1021/ja01269a066> The adsorption of gases on plane surfaces of glass, mics and platinum. Journal of the American Chemical Society, 1361-1403.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fit_langmuirLM1(Ce, Qe, verbose = TRUE)
fit_langmuirLM1(Ce, Qe)
```

`fit_langmuirLM2` *Langmuir Isotherm Linear (Form 2) Analysis*

Description

Performs linear modeling for the Langmuir adsorption isotherm using the linearized form 1/Qe = (1/Qmax·b)(1/Ce) + (1/Qmax).

Arguments

`Ce`	numeric vector for equilibrium concentration
`Qe`	numeric vector for adsorbed amount
`verbose`	logical; if TRUE (default), prints summary and messages

Value

A list containing the results of the linear Langmuir (Form 2) model fitting, including:

- **Parameter estimates** for the Langmuir model (Qmax and Kl).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Langmuir, I. (1918) <doi:10.1021/ja01269a066> The adsorption of gases on plane surfaces of glass, mics and platinum. Journal of the American Chemical Society, 1361-1403.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fit_langmuirLM2(Ce, Qe, verbose = TRUE)
fit_langmuirLM2(Ce, Qe)
```

`fit_langmuirLM3` *Langmuir Isotherm Linear (Form 3) Analysis*

Description

Performs linear modeling for the Langmuir adsorption isotherm using the linearized form Qe = Qmax - (1/b)(Qe/Ce).

Arguments

`Ce`	Numeric vector for equilibrium concentrations
`Qe`	Numeric vector for adsorbed amounts
`verbose`	logical; if TRUE (default), prints summary and messages

Value

A list containing the results of the linear Langmuir (Form 3) model fitting, including:

- **Parameter estimates** for the Langmuir model (Qmax and Kl).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Langmuir, I. (1918) <doi:10.1021/ja01269a066> The adsorption of gases on plane surfaces of glass, mics and platinum. Journal of the American Chemical Society, 1361-1403.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fit_langmuirLM3(Ce, Qe, verbose = TRUE)
fit_langmuirLM3(Ce, Qe)
```

`fit_langmuirLM4` *Langmuir Isotherm Linear (Form 4) Analysis*

Description

Performs linear modeling for the Langmuir adsorption isotherm using the linearized form Qe/Ce = bQmax - bQe.

Arguments

`Ce`	Numeric vector for equilibrium concentrations
`Qe`	Numeric vector for adsorbed amounts
`verbose`	logical; if TRUE (default), prints summary and messages

Value

A list containing the results of the linear Langmuir (Form 4) model fitting, including:

- **Parameter estimates** for the Langmuir model (Qmax and Kl).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Langmuir, I. (1918) <doi:10.1021/ja01269a066> The adsorption of gases on plane surfaces of glass, mics and platinum. Journal of the American Chemical Society, 1361-1403.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fit_langmuirLM4(Ce, Qe, verbose = TRUE)
fit_langmuirLM4(Ce, Qe)
```

`fit_langmuirNLM` *Langmuir Isotherm Non-Linear Analysis*

Description

Performs non-linear modeling for the Langmuir adsorption isotherm.

Arguments

`Ce`	numeric vector for equilibrium concentration
`Qe`	numeric vector for adsorbed amount

Value

A list containing the results of the non-linear Langmuir model fitting, including:

- **Parameter estimates** for the Langmuir model (Qmax and Kl).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Langmuir, I. (1918) <doi:10.1021/ja01269a066> The adsorption of gases on plane surfaces of glass, mics and platinum. Journal of the American Chemical Society, 1361-1403.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fit_langmuirNLM(Ce, Qe)
```

`fit_temkinLM` *Temkin Isotherm Linear Analysis*

Description

Performs linear modeling for the Temkin adsorption isotherm.

Arguments

`Ce`	numeric vector for equilibrium concentration
`Qe`	numeric vector for adsorbed amount
`Temp`	numeric value of temperature in Kelvin
`verbose`	logical; if TRUE (default), prints summary and messages

Value

A list containing the results of the linear Temkin model fitting, including:

- **Parameter estimates** for the Temkin model (aT and bT).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Temkin, M.J., and Pyzhev, V. (1940). Kinetics of ammonia synthesis on promoted iron catalyst. Acta Phys. Chim. USSR 12, 327-356.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
Temp <- 298
fit_temkinLM(Ce, Qe, Temp, verbose = TRUE)
fit_temkinLM(Ce, Qe, Temp)
```

`fit_temkinNLM` *Temkin Isotherm Non-Linear Analysis*

Description

Performs non-linear modeling for the Temkin adsorption isotherm.

Arguments

`Ce`	numeric vector for equilibrium concentration
`Qe`	numeric vector for adsorbed amount
`Temp`	numeric value for temperature (in Kelvin)

Value

A list containing the results of the non-linear Temkin model fitting, including:

- **Parameter estimates** for the Temkin model (aT and bT).
- **Fit statistics** such as Akaike Information Criterion (AIC), Bayesian Information Criterion (BIC), and R-squared.
- **Error metrics** including Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Squared Error (MSE), Relative Absolute Error (RAE), and standard error of estimates.
- A **model fit plot** with bootstrapped 95
- A **residual plot** for diagnostic assessment of model performance.

Author(s)

Paul Angelo C. Manlapaz

References

Temkin, M.J., and Pyzhev, V. (1940). Kinetics of ammonia synthesis on promoted iron catalyst. Acta Phys. Chim. USSR 12, 327-356.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
Temp <- 298
fit_temkinNLM(Ce, Qe, Temp)
```

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