Package ‘PUPAIM’

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Type Package

Title A Collection of Physical and Chemical Adsorption Isotherm Models

Version 0.3.1

Description The PUPAIM R package can generally fit any adsorption experimental data to any of the 55 available adsorption isotherm models - 32 nonlinear models and 23 linear models. This package provides parameter estimation, model accuracy analysis, model error analysis, and adsorption plot created using the package ‘ggplot2’. This package will help the users for a much easier way of adsorption model data fitting.

License GPL-2

Encoding UTF-8

Imports Metrics, ggplot2, nls2

RoxygenNote 7.1.2

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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aranovichanalysis

Aranovich Isotherm Non-Linear Analysis

Description

The Aranovich isotherm (Aranovich, 1992) is a three-parameter isotherm model that is a modified version of the BET isotherm. This isotherm model is theoretically corrected by polymolecular adsorption isotherm and is applicable to modeling adsorption with a wide range concentration of the adsorbate molecules.

Usage

aranovichanalysis(Ce, Qe)

Arguments

Ce       the numerical value for the equilibrium capacity
Qe       the numerical value for the adsorbed capacity

Value

the nonlinear regression, parameters for Aranovich isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocarís

References


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)
aranovichanalysis(Ce, Qe)
**Description**

Baudu is a reduced form of Langmuir isotherm since it was observed that the estimation of Langmuir coefficients b and qm by tangent measurements at different equilibrium constants are not constants in the broad concentration range. This can be used if the ranges are \((1+x+y) < 1\) and \((1+x) < 1\).

**Usage**

```r
bauduanalysis(Ce, Qe)
```

**Arguments**

- `Ce` the numerical value for the equilibrium capacity
- `Qe` the numerical value for the adsorbed capacity

**Value**

the nonlinear regression, parameters for Baudu isotherm, and model error analysis

**Author(s)**

Jemimah Christine L. Mesias
Chester C. Deocaris

**References**


**Examples**

```r
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)
bauduanalysis(Ce,Qe)
```
Description

BET was particularly formulated to describe the multilayer adsorption process in gas systems, but can also be employed to an aqueous solution that relates the binding between layers because of the molecular charge among them.

Usage

\[ \text{BET.LM}(C_e, Q_e) \]

Arguments

- \( C_e \): the numerical value for the equilibrium capacity
- \( Q_e \): the numerical value for the adsorbed capacity

Value

the linear regression, parameters for BET isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarís

References


Examples

\[
\begin{align*}
Q_e & \leftarrow c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607) \\
C_e & \leftarrow c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223) \\
\text{BET.LM}(C_e, Q_e) & \\
\end{align*}
\]
Description

BET was particularly formulated to describe the multilayer adsorption process in gas systems, but can also be employed to an aqueous solution that relates the binding between layers because of the molecular charge among them.

Usage

BETanalysis(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the nonlinear regression, parameters for BET isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarís

References


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)
BETanalysis(Ce,Qe)
Dubinin-Radushkevich Isotherm Non-Linear Analysis

dubininradushkevichanalysis

Description
Dubinin-Radushkevich isotherm model is being utilized to define adsorption energy mechanisms with Gaussian distribution onto heterogeneous surfaces. Specifically, this model works well with an intermediate range of adsorbate concentrations because it shows abnormal asymptotic behavior and is unable to forecast Henry’s Law at low pressure.

Usage
dubininradushkevichanalysis(Ce, Qe, Temp)

Arguments
Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity
Temp temperature

Value
the nonlinear regression, parameters for Dubinin-Radushkevich isotherm, and model error analysis

Author(s)
Jemimah Christine L. Mesias
Chester C. Deocaris

References

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
dubininradushkevichanalysis(Ce, Qe, Temp)
Dubinin-Radushkevich Isotherm Linear Analysis

Description

Dubinin-Radushkevich isotherm model is being utilized to define adsorption energy mechanisms with Gaussian distribution onto heterogeneous surfaces. Specifically, this model works well with an intermediate range of adsorbate concentrations because it shows abnormal asymptotic behavior and is unable to forecast Henry’s Law at low pressure.

Usage

dubininradushkevich.LM(Ce, Qe, Temp)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity
Temp temperature

Value

the linear regression, parameters for Dubinin-Radushkevich isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarisi

References


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

dubininradushkevich.LM(Ce,Qe,Temp)
**Description**

Elovich isotherm model is based on kinetic principle which assumes that the adsorption sites would exponentially increase with chemical reactions responsible for adsorption. It is suited for describing the behavior of adsorption concurring with the nature of chemisorption.

**Usage**

```
elovich.LM(Ce, Qe)
```

**Arguments**

- **Ce**  
  the numerical value for the equilibrium capacity
- **Qe**  
  the numerical value for the adsorbed capacity

**Value**

the linear regression, parameters for Elovich isotherm, and model error analysis

**Author(s)**

Jemimah Christine L. Mesias
Chester C. Deocaris

**References**


**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)
elovich.LM(Ce, Qe)
```
Description
Elovich isotherm model is based on kinetic principle which assumes that the adsorption sites would exponentially increase with chemical reactions responsible for adsorption. It is suited for describing the behavior of adsorption concurring with the nature of chemisorption.

Usage
elovichanalysis(Ce, Qe)

Arguments
Ce       the numerical value for equilibrium concentration
Qe       the numerical value for adsorbed capacity

Value
the nonlinear regression, parameters for Elovich isotherm, and model error analysis

Author(s)
Jemimah Christine L. Mesias
Chester C. Deocaris

References


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

Flory-Huggins isotherm model describes the degree of surface coverage characteristics of the adsorbate on the adsorbent. It describes the nature of the adsorption process regarding the feasibility and spontaneity of the process. The theory of the Flory-Huggins provides the mathematical model for the polymer blends’ thermodynamics.

Usage

floryhuggins.LM(Ce, theta)

Arguments

Ce the numerical value for the equilibrium capacity
theta is theta fractional surface coverage

Value

the linear regression, parameters for Flory-Huggins isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarlis

References


Examples

Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
theta <- c(0.1972984, 0.3487013, 0.6147560, 0.7432401, 0.8854408, 0.8900708, 0.9106746, 0.9106746, 0.9611422)
floryhuggins.LM (Ce, theta)
Flory-Huggins Isotherm Non-Linear Analysis

Description

Flory-Huggins isotherm model describes the degree of surface coverage characteristics of the adsorbate on the adsorbent. It describes the nature of the adsorption process regarding the feasibility and spontaneity of the process. The theory of the Flory-Huggins provides the mathematical model for the polymer blends’ thermodynamics.

Usage

floryhugginsanalysis(Ce, theta)

Arguments

Ce is equal to Co which is the numeric value for the initial concentration
theta is the fractional surface coverage

Value

the nonlinear regression, parameters for Flory-Huggins isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocaris

References


Examples

theta <- c(0.19729, 0.34870, 0.61475, 0.74324, 0.88544, 0.89007, 0.91067, 0.91067, 0.96114)
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
floryhugginsanalysis(Ce, theta)
Description

In Fowler-Guggenheim isotherm model, the lateral interaction of the adsorbed molecules is taken into consideration. This is formulated on the basis that the heat adsorption process may vary positively or negatively with loading.

Usage

\texttt{fowlerguggenheim.LM(Ce, theta, Temp)}

Arguments

\begin{itemize}
  \item \texttt{Ce} is equal to the numerical value for the equilibrium capacity
  \item \texttt{theta} is the fractional surface coverage
  \item \texttt{Temp} temperature
\end{itemize}

Value

the linear regression, parameters for Fowler-Guggenheim isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarís

References


Examples

\begin{verbatim}
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607,
       0.80435, 1.10327, 1.58223)
theta <- c(0.1972984, 0.3487013, 0.6147560, 0.7432401, 0.8854408,
          0.8900708, 0.9106746, 0.9106746, 0.9611422)
Temp <- 298
fowlerguggenheim.LM(Ce, theta, Temp)
\end{verbatim}
Description

In Fowler-Guggenheim isotherm model, the lateral interaction of the adsorbed molecules is taken into consideration. This is formulated on the basis that the heat adsorption process may vary positively or negatively with loading.

Usage

fowlerguggenheimanalysis(Ce, theta, Temp)

Arguments

Ce is equal to Co which is the numeric value for the initial concentration
theta is the fractional surface coverage
Temp temperature

Value

the nonlinear regression, parameters for Fowler-Guggenheim isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarisis

References


Examples

theta <- c(0.19729, 0.34870, 0.61475, 0.74324, 0.88544, 0.89007, 0.91067, 0.91067, 0.96114)
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Temp <- 298
fowlerguggenheimanalysis(Ce, theta, Temp)
Freundlich Isotherm Linear Analysis

Description

This isotherm model is an empirical model applicable to diluted solutions adsorption processes. Furthermore, this model gives an equation which defines the surface heterogeneity and the exponential distribution of active sites.

Usage

freundlich.LM(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the linear regression, parameters for Freundlich isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarís

References


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)
freundlich.LM(Ce, Qe)
**freundlichanalysis**  
*Freundlich Isotherm Non-Linear Analysis*

**Description**

This isotherm model is an empirical model applicable to diluted solutions adsorption processes. Furthermore, this model gives an equation which defines the surface heterogeneity and the exponential distribution of active sites.

**Usage**

`freundlichanalysis(Ce, Qe)`

**Arguments**

- `Ce`: the numerical value for the equilibrium capacity  
- `Qe`: the numerical value for the adsorbed capacity

**Value**

the nonlinear regression, parameters for Freundlich isotherm, and model error analysis

**Author(s)**

Jemimah Christine L. Mesias  
Chester C. Deocarís

**References**


**Examples**

```r
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, 0.15739, 0.15735, 0.15735, 0.16607)  
freundlichanalysis(Ce,Qe)
```
Description

The Fritz-Schlunder isotherm model is an empirical expression that can fit over an extensive range of experimental results as a result of the huge number of coefficients in their adsorption isotherm.

Usage

FS3analysis(Ce, Qe)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ce</td>
<td>the numerical value for equilibrium capacity</td>
</tr>
<tr>
<td>Qe</td>
<td>the numerical value for the adsorbed capacity</td>
</tr>
</tbody>
</table>

Value

the nonlinear regression, parameters for Fritz-Schlunder three Parameter isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocaris

References


Examples

```r
Ce <- c(0.9613, 1.0895, 1.5378, 1.9862, 3.3314, 7.8153, 11.4024, 15.8862)
Qe <- c(2.5546, 4.4150, 5.8558, 7.1387, 8.8092, 13.1921, 15.7966, 18.4483)
FS3analysis(Ce,Qe)
```
**FS4analysis**  
*Fritz-Schlunder Four Parameter Isotherm Non-Linear Analysis*

**Description**
An empirical equation of Langmuir-Freundlich isotherm which can fit a wide range of experimental results because of the large number of coefficients in the isotherm.

**Usage**

FS4analysis(Ce, Qe)

**Arguments**

- **Ce**  
  the numerical value for equilibrium capacity
- **Qe**  
  the numerical value for the adsorbed capacity

**Value**

the nonlinear regression, parameters for the Fritz-Schlunder Four Parameter isotherm, and model error analysis

**Author(s)**

- Paul Angelo C. Manlapaz
- Chester C. Deocaris

**References**


**Examples**

```r
## Not run:
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)
FS4analysis(Ce, Qe)
## End(Not run)
```
halsey.LM  

\textit{Halsey Isotherm Linear Analysis}

\textbf{Description}

A multilayer adsorption isotherm model which is suited for adsorption of adsorbate ions at a distance that is relatively large from the surface.

\textbf{Usage}

\begin{verbatim}
halsey.LM(Ce, Qe)
\end{verbatim}

\textbf{Arguments}

\begin{verbatim}
Ce      the numerical value for the equilibrium capacity  
Qe      the numerical value for the adsorbed capacity
\end{verbatim}

\textbf{Value}

the linear regression, parameters for the Halsey isotherm, and model error analysis

\textbf{Author(s)}

Paul Angelo C. Manlapaz  
Chester C. Deocarís

\textbf{References}


\textbf{Examples}

\begin{verbatim}
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)  
halsey.LM(Ce, Qe)
\end{verbatim}
**halseyanalysis**  
*Halsey Isotherm Non-Linear Analysis*

**Description**

A multilayer adsorption isotherm model which is suited for adsorption of adsorbate ions at a distance that is relatively large from the surface.

**Usage**

```r
halseyanalysis(Ce, Qe)
```

**Arguments**

- **Ce**  
  the numerical value for the equilibrium capacity
- **Qe**  
  the numerical value for the adsorbed capacity

**Value**

the nonlinear regression, parameters for the Halsey isotherm, and model error analysis

**Author(s)**

Paul Angelo C. Manlapaz  
Chester C. Deocaris

**References**


**Examples**

```r
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)  
halseyanalysis(Ce, Qe)
```
harkinsjura.LM

HarkinsJura Isotherm Linear Analysis

Description

A model that assumes the possibility of multilayer adsorption on the surface of absorbents having heterogeneous pore distribution.

Usage

harkinsjura.LM(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the linear regression, parameters for the HarkinsJura isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocaris

References

Harkins, W. D., and Jura, G. (1944) <doi:10.1021/ja01236a048> Surfaces of solids. XIII. A vapor adsorption method for the determination of the area of a solid without the assumption of a molecular area, and the areas occupied by nitrogen and other molecules on the surface of a solid. Journal of the American Chemical Society, 66(8), 1366-1373.

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)
harkinsjura.LM(Ce, Qe)
harkinsjuraanalysis

Harkins-Jura Isotherm Non-Linear Analysis

Description

A model that assumes the possibility of multilayer adsorption on the surface of absorbents having heterogenous pore distribution

Usage

harkinsjuraanalysis(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the nonlinear regression, parameters for the Harkins-Jura isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocaris

References

Harkins, W. D., and Jura, G. (1944) <doi:10.1021/ja01236a048> Surfaces of solids. XIII. A vapor adsorption method for the determination of the area of a solid without the assumption of a molecular area, and the areas occupied by nitrogen and other molecules on the surface of a solid. Journal of the American Chemical Society, 66(8), 1366-1373.

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)
harkinsjuraanalysis(Ce, Qe)
Description

It describes the appropriate fit to the adsorption of adsorbate at relatively low concentrations such that all adsorbate molecules are secluded from their nearest neighbours.

Usage

henryanalysis(Ce, Qe)

Arguments

Ce
the numerical value for the equilibrium capacity

Qe
the numerical value for the adsorbed capacity

Value

the linear regression, parameters for the Henry isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocarins

References


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)
henryanalysis(Ce, Qe)
Description

Hill isotherm model shows the connection of different species being adsorbed on to the homogeneous surfaces. This isotherm model supposes that adsorption is a cooperative phenomenon which means the adsorbates having the capability to bind at one specific site on the adsorbent affecting other binding sites on the same adsorbent.

Usage

hill.LM(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the linear regression, parameters for the Hill isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocarís

References


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)
hill.LM(Ce, Qe)
Hill Isotherm Non-Linear Analysis

Description

Hill isotherm model shows the connection of different species being adsorbed on to the homogeneous surfaces. This isotherm model supposes that adsorption is a cooperative phenomenon which means the adsorbates having the capability to bind at one specific site on the adsorbent affecting other binding sites on the same adsorbent.

Usage

hillanalysis(Ce, Qe)

Arguments

Ce  the numerical value for the equilibrium capacity
Qe  the numerical value for the adsorbed capacity

Value

the nonlinear regression, parameters for the Hill isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocariz

References


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)
hillanalysis(Ce, Qe)
Hill-Deboer Isotherm Linear Analysis

Description

Hill-Deboer isotherm model describes as a case where there is mobile adsorption as well as lateral interaction among molecules. The increased or decreased affinity depends on the kind of force among the adsorption molecules. If there is an attraction between adsorbed molecules, there is an increase in affinity. On the other hand, decreased affinity happens when there is repulsion among the adsorbed molecules.

Usage

hilldeboer.LM(Ce, theta, Temp)

Arguments

- **Ce**: the numerical value for the equilibrium capacity
- **theta**: is the fractional surface coverage
- **Temp**: temperature

Value

the linear regression, parameters for the Hill-Deboer isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocarís

References


Examples

```r
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
theta <- c(0.1972984, 0.3487013, 0.6147560, 0.7432401, 0.8854408, 0.8900708, 0.9106746, 0.9106746, 0.9611422)
Temp <- 298.15
hilldeboer.LM(Ce, theta, Temp)
```
**Hill-Deboer Isotherm Non-Linear Analysis**

**Description**

Hill-Deboer isotherm model describes as a case where there is mobile adsorption as well as lateral interaction among molecules. The increased or decreased affinity depends on the kind of force among the adsorption molecules. If there is an attraction between adsorbed molecules, there is an increase in affinity. On the other hand, decreased affinity happens when there is repulsion among the adsorbed molecules.

**Usage**

```r
hilldeboeranalysis(Ce, theta, Temp)
```

**Arguments**

- **Ce**: the numerical value for the equilibrium capacity
- **theta**: is the fractional surface coverage
- **Temp**: the temperature of the adsorption experimentation in Kelvin

**Value**

the nonlinear regression, parameters for the Hill-Deboer isotherm, and model error analysis

**Author(s)**

Paul Angelo C. Manlapaz
Chester C. Deocaris

**References**


**Examples**

```r
theta <- c(0.19729, 0.34870, 0.61475, 0.74324, 0.89007, 0.89007, 0.91067, 0.91067, 0.96114)
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Temp <- 298
hilldeboeranalysis(Ce, theta, Temp)
```
Describes the Jossens isotherm model which predicts a simple equation based on the energy distribution of adsorbate-adsorbent interactions at adsorption sites. This model assumes that the adsorbent has heterogeneous surface with respect to the interactions it has with the adsorbate.

Usage

\[ \text{jossens.LM}(C_e, Q_e) \]

Arguments

- \( C_e \): the numerical value for the equilibrium capacity
- \( Q_e \): the numerical value for the adsorbed capacity

Value

the linear regression, parameters for the Jossens isotherm, and model error analysis

Authors

Paul Angelo C. Manlapaz
Chester C. Deocaris

References


Examples

\[ C_e \leftarrow c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223) \]
\[ Q_e \leftarrow c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607) \]
\[ \text{jossens.LM}(C_e, Q_e) \]
**Description**

The Jossens isotherm model predicts a simple equation based on the energy distribution of adsorbate-adsorbent interactions at adsorption sites. This model assumes that the adsorbent has heterogeneous surface with respect to the interactions it has with the adsorbate.

**Usage**

```r
jossensanalysis(Ce, Qe)
```

**Arguments**

- `Ce` the numerical value for the equilibrium capacity
- `Qe` the numerical value for the adsorbed capacity

**Value**

the nonlinear regression, parameters for the Jossens isotherm, and model error analysis

**Author(s)**

Paul Angelo C. Manlapaz
Chester C. Deocaris

**References**


**Examples**

```r
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, 0.15735, 0.15735, 0.15735, 0.16607)
jossensanalysis(Ce, Qe)
```
Description

The Jovanovic isotherm model was built upon the assumptions based on the Langmuir isotherm model with few possible inclusions of mechanical contact among the desorbing and adsorbing molecules. The adjustment of the adsorption surface from this model made the equation less effective in the physical adsorption but can be applied to adsorption with both mobile and localized monolayer without lateral interaction. Moreover, the equation of the Jovanovic isotherm model is able to reach the limit of saturation when there is high concentration, while it reduces to Henry’s Law at low concentration.

Usage

jovanovic.LM(Ce, Qe)

Arguments

Ce  the numerical value for the equilibrium capacity
Qe  the numerical value for the adsorbed capacity

Value

the linear regression, parameters for the Jovanovic isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocaris

References


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)
jovanovic.LM(Ce, Qe)
**Description**

The Jovanovic isotherm model was built upon the assumptions based on the Langmuir isotherm model with few possible inclusions of mechanical contact among the desorbing and adsorbing molecules. The adjustment of the adsorption surface from this model made the equation less effective in the physical adsorption but can be applied to adsorption with both mobile and localized monolayer without lateral interaction. Moreover, the equation of the Jovanovic isotherm model is able to reach the limit of saturation when there is high concentration, while it reduces to Henry’s Law at low concentration.

**Usage**

\[ \text{jovanovicanalysis}(C_e, Q_e) \]

**Arguments**

- \( C_e \)  
  the numerical value for the equilibrium capacity
- \( Q_e \)  
  the numerical value for the adsorbed capacity

**Value**

the nonlinear regression, parameters for the Jovanovic isotherm, and model error analysis

**Author(s)**

Paul Angelo C. Manlapaz  
Chester C. Deocaris

**References**


**Examples**

\[ C_e \leftarrow c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223) \]
\[ Q_e \leftarrow c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607) \]
\[ \text{jovanovicanalysis}(C_e, Q_e) \]


**kahnanalysis**  

*Kahn Isotherm Non-Linear Analysis*

**Description**

A generalized model recommended for pure solutions, in which both extremes, Langmuir and Freundlich, can be represented. This isotherm was developed to cater to both the single- and multi-component adsorption systems.

**Usage**

kahnanalysis(Ce, Qe)

**Arguments**

Ce  
the numerical value for the equilibrium capacity

Qe  
the numerical value the absorbed capacity

**Value**

the nonlinear regression, parameters for the Kahn isotherm, and model error analysis

**Author(s)**

Paul Angelo C. Manlapaz  
Chester C. Deocaris

**References**


**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)  
kahnanalysis(Ce, Qe)
**Description**

It is also known as localized monomolecular layer model and is only valid for surface coverage \( \theta > 0.68 \).

**Usage**

```r
kiselev.LM(Ce, theta)
```

**Arguments**

- `Ce` the numerical value for equilibrium capacity
- `theta` is the fractional surface coverage

**Value**

the linear regression, parameters for the Kiselev isotherm, and model error analysis

**Author(s)**

Paul Angelo C. Manlapaz  
Chester C. Deocaris

**References**


**Examples**

```r
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
theta <- c(0.1972984, 0.3487013, 0.6147560, 0.7432401, 0.8854408, 0.8900708, 0.9106746, 0.9106746, 0.9611422)
kiselev.LM(Ce, theta)
```
Description

It is also known as localized monomolecular layer model and is only valid for surface coverage \( \theta > 0.68 \).

Usage

\[
\text{kiselevanalysis}(C_e, \theta)
\]

Arguments

- \( C_e \) the numerical value for equilibrium capacity
- \( \theta \) is the fractional surface coverage

Value

the nonlinear regression, parameters for the Kiselev isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocaris

References


Examples

\[
\theta <- \text{c}(0.19729, 0.34870, 0.61475, 0.74324, 0.88544, 0.89007, 0.91067, 0.91067, 0.96114)
\]

\[
C_e <- \text{c}(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
\]

\[
\text{kiselevanalysis}(C_e, \theta)
\]
**Description**

It is three-parameter isotherm model equation that incorporates both Freundlich and Langmuir isotherms for representing equilibrium adsorption data. Koble-Carrigan isotherm model appeared to have advantages over both the Langmuir and Freundlich equations in that it expresses adsorption data over very wide ranges of pressures and temperatures.

**Usage**

```r
koblecarrigan.LM(Ce, Qe)
```

**Arguments**

- **Ce**
  the numerical value for the equilibrium capacity
- **Qe**
  the numerical value for the adsorbed capacity

**Value**

the linear regression, parameters for Koble-Carrigan isotherm, and model error analysis

**Author(s)**

Keith T. Ostan
Chester C. Deocarís

**References**


**Examples**

```r
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)
koblecarrigan.LM(Ce, Qe)
```
Description

It is three-parameter isotherm model equation that incorporates both Freundlich and Langmuir isotherms for representing equilibrium adsorption data. Koble-Corrigan isotherm model appeared to have advantages over both the Langmuir and Freundlich equations in that it expresses adsorption data over very wide ranges of pressures and temperatures.

Usage

koblecarrigananalysis(Ce, Qe)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ce</td>
<td>the numerical value for the equilibrium capacity</td>
</tr>
<tr>
<td>Qe</td>
<td>the numerical value for the adsorbed capacity</td>
</tr>
</tbody>
</table>

Value

the nonlinear regression, parameters for Koble-Carrigan isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocaris

References


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)
koblecarrigananalysis(Ce, Qe)
**Langmuir Isotherm First Linear Form Analysis**

**Description**

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.

**Usage**

```
langmuir1.LM(Ce, Qe)
```

**Arguments**

- `Ce`: the numerical value for the equilibrium capacity
- `Qe`: the numerical value for the adsorbed capacity

**Value**

the parameters for the Langmuir isotherm (first form), model error analysis, and linear regression analysis

**Author(s)**

Keith T. Ostan
Chester C. Deocarís

**References**


**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)
langmuir1.LM(Ce,Qe)
```
Langmuir Isotherm Second Linear Form Analysis

Description

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.

Usage

\[ \text{langmuir2.LM}(C_e, Q_e) \]

Arguments

- \( C_e \): the numerical value for the equilibrium capacity
- \( Q_e \): the numerical value for the adsorbed capacity

Value

the parameters for the Langmuir isotherm (second form), model error analysis, and linear regression analysis

Author(s)

Keith T. Ostan
Chester C. Deocarís

References


Examples

\[
\begin{align*}
C_e & \leftarrow \text{c}(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223) \\
Q_e & \leftarrow \text{c}(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607) \\
\text{langmuir2.LM}(C_e, Q_e)
\end{align*}
\]
Description

The Langmuir adsorption isotherm is used to describe the equilibrium between adsorbate and adsorbent system, where the adsorbate adsorption is limited to one molecular layer at or before a relative pressure of unity is reached.

Usage

langmuir3.LM(Ce, Qe)

Arguments

Ce  
the numerical value for the equilibrium capacity

Qe  
the numerical value for the adsorbed capacity

Value

the parameters for the Langmuir isotherm (third form), model error analysis, and linear regression analysis

Author(s)

Keith T. Ostan
Chester C. Deocarisi

References


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)  
langmuir3.LM(Ce,Qe)
Langmuir Isotherm Fourth Linear Form Analysis

Description

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.

Usage

`langmuir4.LM(Ce, Qe)`

Arguments

- **Ce**: the numerical value for the equilibrium capacity
- **Qe**: the numerical value for the adsorbed capacity

Value

the parameters for the Langmuir isotherm (fourth form), model error analysis, and linear regression analysis

Author(s)

Keith T. Ostan
Chester C. Deocarис

References


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)
langmuir4.LM(Ce, Qe)
```
**Langmuir Isotherm Nonlinear Analysis**

### Description

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.

### Usage

```r
langmuiranalysis(Ce, Qe)
```

### Arguments

- **Ce**: the numerical value for the equilibrium capacity
- **Qe**: the numerical value for the adsorbed capacity

### Value

the nonlinear regression, parameters for Langmuir isotherm, and model error analysis

### Author(s)

Keith T. Ostan  
Chester C. Deocaris

### References


### Examples

```r
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, 0.10662, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)  
langmuiranalysis(Ce, Qe)
```
Marckzewski-Jaroniec Isotherm Nonlinear Analysis

Description

The Marczewski-Jaroniec Isotherm model has a resemblance to Langmuir Isotherm model. It is developed on the basis of the supposition of local Langmuir isotherm and adsorption energies distribution in the active sites on adsorbent. This equation comprises all isotherm equations being an extension of simple Langmuir Isotherm to single solute adsorption on heterogeneous solids.

Usage

marckzewskijaroniecanalysis(Ce, Qe)

Arguments

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ce</td>
<td>the numerical value for the equilibrium capacity</td>
</tr>
<tr>
<td>Qe</td>
<td>the numerical value for the absorbed capacity</td>
</tr>
</tbody>
</table>

Value

the nonlinear regression, parameters for Marckzewski-Jaroniec isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocarís

References


Examples

Qe <- c(0.19729, 0.34870, 0.61475, 0.74324, 0.88544, 0.89007, 0.91067, 0.91067, 0.96114)
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
marckzewskijaroniecanalysis(Ce,Qe)
Radke-Prausnitz Isotherm Nonlinear Analysis

Description

The Radke-Prausnitz isotherm model has several important properties which provides a good fit over a wide range of adsorbate concentrations but more preferred in most adsorption systems at low adsorbate concentration.

Usage

radkeprausnitzanalysis(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the nonlinear regression, parameters for Radke-Prausnitz isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocaris

References


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)  
radkeprausnitzanalysis(Ce,Qe)
### Description

The Radke-Prausnitz isotherm model has several important properties which provide a good fit over a wide range of adsorbate concentrations but more preferred in most adsorption systems at low adsorbate concentration.

### Usage

```r
radkepraustnitz.LM(Ce, Qe)
```

### Arguments

- **Ce**
  - the numerical value for the equilibrium capacity
- **Qe**
  - the numerical value for the adsorbed capacity

### Value

- the linear regression, parameters for Radke-Prausnitz isotherm, and model error analysis

### Author(s)

Keith T. Ostan
Chester C. Deocaris

### References


### Examples

```r
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)
radkepraustnitz.LM(Ce, Qe)
```
Description

Redlich-Peterson isotherm model has an exponential function which can be found in the denominator and in the numerator, it has a linear dependence on the concentration denoting the adsorption equilibrium depending on a wide range of concentration.

Usage

```r
redlichpeterson.LM(Ce, Qe)
```

Arguments

- `Ce` the numerical value for the equilibrium capacity
- `Qe` the numerical value for the adsorbed capacity

Value

the linear regression, parameters for Redlich-Peterson isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocarís

References


Examples

```r
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)
redlichpeterson.LM(Ce, Qe)
```
Redlich-Peterson Isotherm Nonlinear Analysis

Description

Redlich-Peterson isotherm model has an exponential function which can be found in the denominator and in the numerator, it has a linear dependence on the concentration denoting the adsorption equilibrium depending on a wide range of concentration.

Usage

redlichpetersonanalysis(Ce, Qe)

Arguments

Ce  
the numerical value for the equilibrium capacity

Qe  
the numerical value for the adsorbed capacity

Value

the nonlinear regression, parameters for Redlich-Peterson isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocariz

References


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)
redlichpetersonanalysis(Ce,Qe)
sips.LM

Sips Isotherm Linear Analysis

Description

It is the most applicable to use in the monolayer adsorption isotherm model amongst the three-parameter isotherm models and is also valid for the prediction of heterogeneous adsorption systems as well as localized adsorption with no interactions occurring between adsorbates.

Usage

sips.LM(Ce, Qe)

Arguments

Ce  the numerical value for the equilibrium capacity
Qe  the numerical value for the adsorbed capacity

Value

the linear regression, parameters for Sips isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocarís

References


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)
sips.LM(Ce,Qe)
sipsanalysis  
\textit{Sips Isotherm Nonlinear Analysis}

\section*{Description}

It is the most applicable to use in the monolayer adsorption isotherm model amongst the three-
parameter isotherm models and is also valid for the prediction of heterogeneous adsorption systems as well as localized adsorption with no interactions occurring between adsorbates.

\section*{Usage}

\begin{verbatim}
sipsanalysis(Ce, Qe)
\end{verbatim}

\section*{Arguments}

\begin{itemize}
  \item \textbf{Ce} \quad \text{the numerical value for the equilibrium capacity}
  \item \textbf{Qe} \quad \text{the numerical value for the adsorbed capacity}
\end{itemize}

\section*{Value}

\text{the nonlinear regression, parameters for Sips isotherm, and model error analysis}

\section*{Author(s)}

Keith T. Ostan
Chester C. Deocaris

\section*{References}


\section*{Examples}

\begin{verbatim}
  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)
  sipsanalysis(Ce, Qe)
\end{verbatim}
**SSLangmuir1**

**selfStart using Langmuir First Linear Model**

**Description**

It calculates initial estimates for the model parameters from data so `nls` has a greater chance of convergence.

**Usage**

`SSLangmuir1(Ce, Qmax,Kl)`

**Arguments**

- `Ce` the numerical value for the equilibrium capacity
- `Qmax` the maximum adsorption capacity
- `Kl` the numerical value for the adsorbed capacity

**Value**

initial starting values for parameters based on Langmuir first linear model

**Author(s)**

Keith T. Ostan
Chester C. Deocarisa

**References**


**SSLangmuir1analysis**

**Langmuir Isotherm Nonlinear Analysis via selfStart and Langmuir First Linear Model**

**Description**

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.
Usage

SSLangmuir1analysis(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the nonlinear regression via selfStart, initial starting values for parameters based on Langmuir first
linear model, predicted parameter values, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocaris

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)
SSLangmuir1analysis(Ce,Qe)

SSLangmuir2

selfStart using Langmuir Second Linear Model

Description

It calculates initial estimates for the model parameters from data so nls has a greater chance of
convergence.

Usage

SSLangmuir2(Ce, Qmax,Kl)

Arguments

Ce the numerical value for the equilibrium capacity
Qmax the maximum adsorption capacity
Kl the numerical value for the adsorbed capacity
SSLangmuir2analysis

Value

initial starting values for parameters based on Langmuir second linear model

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocaris

References


SSLangmuir2analysis

Langmuir Isotherm Nonlinear Analysis via selfStart and Langmuir Second Linear Model

Description

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.

Usage

SSLangmuir2analysis(Ce, Qe)

Arguments

Ce the numerical value for the equilibrium capacity
Qe the numerical value for the adsorbed capacity

Value

the nonlinear regression via selfStart, initial starting values for parameters based on Langmuir second linear model, predicted parameter values, and model error analysis

Author(s)

Paul Angelo C. Manlapaz
Chester C. Deocaris
References


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)
SSLangmuir2analysis(Ce,Qe)

---

SSLangmuir3

selfStart using Langmuir Third Linear Model

Description

It calculates initial estimates for the model parameters from data so nls has a greater chance of convergence.

Usage

SSLangmuir3(Ce, Qmax,Kl)

Arguments

Ce the numerical value for the equilibrium capacity
Qmax the maximum adsorption capacity
Kl the numerical value for the adsorbed capacity

Value

initial starting values for parameters based on Langmuir third linear model

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocarís

References

Description

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.

Usage

`SSLangmuir3analysis(Ce, Qe)`

Arguments

- **Ce**: the numerical value for the equilibrium capacity
- **Qe**: the numerical value for the adsorbed capacity

Value

the nonlinear regression via `selfStart`, initial starting values for parameters based on Langmuir third linear model, predicted parameter values, and model error analysis

Author(s)

Jemimah Christine L. Mesias
Chester C. Deocaris

References


Examples

```r
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)
SSLangmuir3analysis(Ce, Qe)
```
SSLangmuir4

**selfStart using Langmuir Fourth Linear Model**

**Description**

It calculates initial estimates for the model parameters from data so nls has a greater chance of convergence.

**Usage**

```r
SSLangmuir4(Ce, Qmax, K1)
```

**Arguments**

- `Ce`: the numerical value for the equilibrium capacity
- `Qmax`: the maximum adsorption capacity
- `K1`: the numerical value for the adsorbed capacity

**Value**

initial starting values for parameters based on Langmuir fourth linear model

**Author(s)**

Keith T. Ostan
Chester C. Deocaris

**References**


---

SSLangmuir4analysis

**Langmuir Isotherm Nonlinear Analysis via selfStart and Langmuir Fourth Linear Model**

**Description**

The Langmuir isotherm is described to be the most useful and simplest isotherm for both chemical adsorption and physical adsorption. It assumes that there is uniform adsorption energy onto the monolayer surface and that there would be no interaction between the adsorbate and the surface.
temkin.LM

**Usage**

\texttt{SSLangmuir4analysis(Ce, Qe)}

**Arguments**

- \texttt{Ce} the numerical value for the equilibrium capacity
- \texttt{Qe} the numerical value for the adsorbed capacity

**Value**

the nonlinear regression via selfStart, initial starting values for parameters based on Langmuir fourth linear model, predicted parameter values, and model error analysis

**Author(s)**

Keith T. Ostan  
Chester C. Deocaris

**References**


**Examples**

\begin{verbatim}
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)
SSLangmuir4analysis(Ce,Qe)
\end{verbatim}

---

**temkin.LM**

\textit{Temkin Isotherm Linear Analysis}

**Description**

Temkin isotherm is a monolayer adsorption isotherm model which takes into account the effects that the indirect interaction amongst adsorbate molecules could have on the adsorption process.

**Usage**

\texttt{temkin.LM(Ce, Qe, Temp)}

**Arguments**

- \texttt{Ce} the numerical value for the equilibrium capacity
- \texttt{Qe} the numerical value for the adsorbed capacity
- \texttt{Temp} temperature
Value

the linear regression, parameters for Temkin isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocaris

References


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 <- 298.15
temkin.LM(Ce,Qe,Temp)

---

**temkinanalysis**

Temkin Isotherm Nonlinear Analysis

Description

Temkin isotherm is a monolayer adsorption isotherm model which takes into account the effects that the indirect interaction amongst adsorbate molecules could have on the adsorption process.

Usage

`temkinanalysis(Ce, Qe, Temp)`

Arguments

- **Ce**: the numerical value for the equilibrium capacity
- **Qe**: the numerical value for the adsorbed capacity
- **Temp**: temperature

Value

the nonlinear regression, parameters for Temkin isotherm, and model error analysis
tothanalysis

Author(s)

Keith T. Ostan
Chester C. Deocaris

References


Examples

```r
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
temkinanalysis(Ce, Qe, Temp)
```

tothanalysis  Toth Isotherm Nonlinear Analysis

Description

Another empirical modification of the Langmuir equation with the aim of reducing the error between experimental data and predicted value of equilibrium data.

Usage

tothanalysis(Ce, Qe)

Arguments

- **Ce**: the numerical value for the equilibrium capacity
- **Qe**: the numerical value for the fractional coverage

Value

the nonlinear regression, parameters for Toth isotherm, and model error analysis

Author(s)

Keith T. Ostan
Chester C. Deocaris

References

Examples

```r
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)
volmeranalysis(Ce, Qe)
```

---

volmeranalysis  
**Volmer Isotherm Non-Linear Analysis**

Description

The Volmer isotherm describes a distribution of monolayer adsorption processes. This theoretical model has the assumption in which the adsorbate molecules can move toward the surfaces of adsorbents, and the interactions that can be formed between the adsorbates are negligible.

Usage

```r
volmeranalysis(Ce, Qe)
```

Arguments

- `Ce` : the numerical value for the equilibrium capacity
- `Qe` : the numerical value for the adsorbed capacity

Value

the nonlinear regression, parameters for Aranovich isotherm, and model error analysis

Author(s)

Keith T. Ostan  
Chester C. Deocaris

References


Examples

```r
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)
volmeranalysis(Ce, Qe)
```
**Weber-Van Vliet Isotherm Nonlinear Analysis**

**Description**

It provides an excellent description of data patterns for a broad range of systems. This model is suitable for batch rate and fixed-bed modelling procedures as it gives a direct parameter evaluation.

**Usage**

\[
\text{webervanvlietanalysis}(C_e, Q_e)
\]

**Arguments**

- \(C_e\) the numerical value for the equilibrium capacity
- \(Q_e\) the numerical value for the adsorbed capacity

**Value**

the nonlinear regression and the parameters for Weber-Van-Vliet Isotherm Analysis

**Author(s)**

Keith T. Ostan
Chester C. Deocarís

**References**


**Examples**

\[
C_e \leftarrow c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
\]
\[
Q_e \leftarrow c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
\]
\[
\text{webervanvlietanalysis}(C_e, Q_e)
\]
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