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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R topics documented:

`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. Deocaris

References

Aranovich, G. L. (1992) <doi:10.1021/la00038a071> The Theory of Polymolecular Adsorption. Langmuir, 8(2), 736-739.

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)
```

`bauduanalysis` *Baudu Isotherm Non-Linear Analysis*

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

```
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

Baudu, M. (1990). Etude des interactions solutes-fibres de charbon actif: applications et regeneration (Doctoral dissertation, Rennes 1). from https://www.theses.fr/1990REN10039

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
bauduanalysis(Ce,Qe)
```

BET.LM *Brunauer-Emett-Teller (BET) Isotherm Linear Analysis*

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

```
BET.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 BET isotherm, and model error analysis

Author(s)

Jemimah Christine L. Mesias

Chester C. Deocaris

References

Brunauer, S., Emmett, P.H. and Teller, E. (1938) <doi:10.1021/ja01269a023> Adsorption of Gases in Multimolecular Layers. Journal of the American Chemical Society, 60, 309-319.

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

`BETanalysis` *Brunauer-Emett-Teller (BET) Isotherm Non-Linear Analysis*

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. Deocaris

References

Brunauer, S., Emmett, P.H. and Teller, E. (1938) <doi:10.1021/ja01269a023> Adsorption of Gases in Multimolecular Layers. Journal of the American Chemical Society, 60, 309-319.

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)
```

dubininradushkevichanalysis *Dubinin-Radushkevich Isotherm Non-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

```
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

Dubinin, M.M. and Radushkevich, L.V. (1947) The Equation of the Characteristic Curve of Activated Charcoal. Proceedings of the Academy of Sciences, Physical Chemistry Section, 55, 331.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
```

dubininraduskevich.LM *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. Deocaris

References

Dubinin, M.M. and Radushkevich, L.V. (1947) The Equation of the Characteristic Curve of Activated Charcoal. Proceedings of the Academy of Sciences, Physical Chemistry Section, 55, 331.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
```

elovich.LM *Elovich Isotherm Linear Analysis*

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

Zeldowitsch, J. (1934). "Uber Den Mechanismus der Katalytischen Oxidation Von CO a MnO2," URSS, Acta Physiochim, Vol. 1, No. 2, 1934, pp. 364-449.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
```

`elovichanalysis` *Elovich Isotherm Non-Linear Analysis*

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

Zeldowitsch, J. (1934). "Uber Den Mechanismus der Katalytischen Oxidation Von CO a MnO2," URSS, Acta Physiochim, Vol. 1, No. 2, 1934, pp. 364-449.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
```

`floryhuggins.LM` *Flory-Huggins Isotherm 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

```
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. Deocaris

References

Flory, P. J. (1971). Principles of polymer chemistry. Cornell Univ.Pr.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
```

`floryhugginsanalysis` *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

Flory, P. J. (1971). Principles of polymer chemistry. Cornell Univ.Pr.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
```

`fowlerguggenheim.LM` *Fowler-Guggenheim Isotherm Linear Analysis*

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

```
fowlerguggenheim.LM(Ce, theta, Temp)
```

Arguments

`Ce`	is equal to the numerical value for the equilibrium capacity
`theta`	is the fractional surface coverage
`Temp`	temperature

Value

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

Author(s)

Jemimah Christine L. Mesias

Chester C. Deocaris

References

Fowler, R. H. and Guggenheim, E. A. (1939) Statistical Thermodynamics, Cambridge University Press, London, England.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
Temp <- 298
fowlerguggenheim.LM(Ce, theta, Temp)
```

`fowlerguggenheimanalysis` *Fowler-Guggenheim Isotherm Non-Linear Analysis*

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. Deocaris

References

Fowler, R. H. and Guggenheim, E. A. (1939) Statistical Thermodynamics, Cambridge University Press, London, England.

Foo, K. Y., and; Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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.LM` *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. Deocaris

References

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

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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. Deocaris

References

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

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
freundlichanalysis(Ce,Qe)
```

`FS3analysis` *Fritz-Schlunder Three Parameter Non-Linear Analysis*

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

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

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

Fritz, W., and Schluender, E. U. (1974) <doi:z10.1016/0009-2509(74)80128-4> Simultaneous adsorption equilibria of organic solutes in dilute aqueous solutions on activated carbon. Chemical Engineering Science, 29(5), 1279-1282.

Examples

```
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

Fritz, W., and Schluender, E. U. (1974) <doi:10.1016/0009-2509(74)80128-4> Simultaneous adsorption equilibria of organic solutes in dilute aqueous solutions on activated carbon. Chemical Engineering Science, 29(5), 1279-1282.

Examples

```
## 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 *Halsey Isotherm 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

```
halsey.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 Halsey isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz

Chester C. Deocaris

References

Halsey, G., and Taylor, H. S. (1947) <doi:10.1063/1.1746618> The adsorption of hydrogen on tungsten powders. The Journal of Chemical Physics, 15(9), 624-630.

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

`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

```
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

Halsey, G., and Taylor, H. S. (1947) <doi:10.1063/1.1746618> The adsorption of hydrogen on tungsten powders. The Journal of Chemical Physics, 15(9), 624-630.

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)
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 heterogenous 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 withoutthe 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)
```

henryanalysis *Henry Isotherm Linear Analysis*

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. Deocaris

References

Deocaris, C., and Osio, L. (2020). Fitting Henry's Adsorption Isotherm model in R using PUPAIM package.

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)
```

`hill.LM` *Hill Isotherm 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

```
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. Deocaris

References

Hill, T. L. (1946). <doi:10.1063/1.1724129> "Statistical mechanics of multimolecular adsorption II. Localized and mobile adsorption and absorption," The Journal of Chemical Physics, vol. 14, no. 7, pp. 441-453.

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)
```

`hillanalysis` *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. Deocaris

References

Hill, T. L. (1946) <doi:10.1063/1.1724129> "Statistical mechanics of multimolecular adsorption II. Localized and mobile adsorption and absorption," The Journal of Chemical Physics, vol. 14, no. 7, pp. 441-453.

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)
```

`hilldeboer.LM` *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. Deocaris

References

De Boer, J. H. (1953). The Dynamical Character of adsorption, Oxford University Press, Oxford, England.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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)
Temp <- 298.15
hilldeboer.LM(Ce,theta, Temp)
```

`hilldeboeranalysis` *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

```
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

De Boer, J. H. (1953). The Dynamical Character of adsorption, Oxford University Press, Oxford, England.

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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
hilldeboeranalysis(Ce,theta, Temp)
```

`jossens.LM` *Jossens Isotherm Linear Analysis*

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

```
jossens.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 Jossens isotherm, and model error analysis

Author(s)

Paul Angelo C. Manlapaz

Chester C. Deocaris

References

Jossens, L., Prausnitz, J. M., Fritz, W., Schlunder, E. U., and Myers, A. L. (1978) <doi:10.1016/0009-2509(78)85015-5> Thermodynamics of multi-solute adsorption from dilute aqueous solutions. Chemical Engineering Science, 33(8), 1097-1106.

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

`jossensanalysis` *Jossens Isotherm Non-Linear Analysis*

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

```
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

Jossens, L., Prausnitz, J. M., Fritz, W., Schlunder, E. U., and Myers, A. L. (1978) <doi:10.1016/0009-2509(78)85015-5> Thermodynamics of multi-solute adsorption from dilute aqueous solutions. Chemical Engineering Science, 33(8), 1097-1106.

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)
jossensanalysis(Ce, Qe)
```

`jovanovic.LM` *Jovanovic Isotherm Linear Analysis*

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

Jovanovic, D.S. (1969) <doi:10.1007/BF01542531> Physical adsorption of gases. Kolloid-Z.u.Z.Polymere 235, 1214-1225.

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)
```

jovanovicanalysis *Jovanovic Isotherm Non-Linear Analysis*

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

```
jovanovicanalysis(Ce, Qe)
```

Arguments

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

Value

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

Author(s)

Paul Angelo C. Manlapaz

Chester C. Deocaris

References

: Saadi, R., Saadi, Z., Fazaeli, R., Fard, N. E. (2015) <DOI: 10.1007/s11814-015-0053-7> Monolayer and multilayer adsorption isotherm models for sorption from aqueous media. Korean J. Chem. Eng., 32(5), 787-799 (2015)

: Vargas, A., Cazetta, A., Kunita, M., Silva, T., Almeida V. (2011) <DOI:10.1016/j.cej.2011.01.067> Adsorption of methylene blue on activated carbon produced from Flamboyant pods (Delonix regia): Study of adsorption isotherms and kinetic models. Chemical Engineering Journal 168 (2011) 722-730

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)
jovanovicanalysis(Ce, Qe)
```

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

Khan, A. R., Al-Waheab, I. R., and Al-Haddad, A. (1996) <doi:10.1080/09593331708616356> A generalized equation for adsorption isotherms for multi-component organic pollutants in dilute aqueous solution. Environmental Technology (United Kingdom), 17(1), 13-23.

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)
```

kiselev.LM *Kiselev Isotherm Linear Analysis*

Description

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

Usage

```
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

Kiselev, A. V. (1958). "Vapor adsorption in the formation of adsorbate molecule complexes on the surface," Kolloid Zhur, vol. 20, pp. 338-348.

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

`kiselevanalysis` *Kiselev Isotherm Non linear Analysis*

Description

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

Usage

```
kiselevanalysis(Ce, theta)
```

Arguments

`Ce`	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

Kiselev, A. V. (1958). "Vapor adsorption in the formation of adsorbate molecule complexes on the surface," Kolloid Zhur, vol. 20, pp. 338-348.

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)
kiselevanalysis(Ce, theta)
```

koblecarrigan.LM *Koble-Carrigan Isotherm Linear Analysis*

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

```
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. Deocaris

References

Corrigan, T. E., and Koble, R. A.(1952) <doi:10.1021/ie50506a049> Adsorption isotherms for pure hydrocarbons Ind. Eng. Chem. 44 383-387.

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

`koblecarrigananalysis` *Koble-Carrigan Isotherm Nonlinear Analysis*

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

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

Value

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

Author(s)

Keith T. Ostan

Chester C. Deocaris

References

Corrigan, T. E., and Koble, R. A.(1952) <doi:10.1021/ie50506a049> Adsorption isotherms for pure hydrocarbons Ind. Eng. Chem. 44 383-387.

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)
```

`langmuir1.LM` *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. 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.

Chen, X. (2015) <doi:/10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14-22.

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)
```

`langmuir2.LM` *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

```
langmuir2.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 (second form), model error analysis, and linear regression 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.

Chen, X. (2015) <doi:/10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14-22.

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)
langmuir2.LM(Ce,Qe)
```

`langmuir3.LM` *Langmuir Isotherm Third Linear Form Analysis*

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. 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.

Chen, X. (2015) <doi:/10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14-22.

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)
```

`langmuir4.LM` *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. 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.

Chen, X. (2015) <doi:/10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14-22.

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)
```

`langmuiranalysis` *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

```
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

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)
langmuiranalysis(Ce,Qe)
```

marckzewskijaroniecanalysis
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

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

Value

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

Author(s)

Keith T. Ostan

Chester C. Deocaris

References

Marczewski, A. W., Derylo-Marczewska, A., and Jaroniec, M. (1986) <doi:10.1016/0021-9797(86)90309-7M> Energetic heterogeneity and molecular size effects in physical adsorption on solid surfaces. Journal of Colloid And Interface Science, 109(2), 310-324.

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)
```

radkeprausnitzanalysis *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

Radke, C. J. and Prausnitz, J. M. (1972) <doi:10.1021/i160044a003> Adsorption of organic solutions from dilute aqueous solution on activated carbon, Ind. Eng. Chem. Fund. 11 (1972) 445-451.

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)
```

radkepraustnitz.LM *Radke-Prausnitz Isotherm Linear 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

```
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

Radke, C. J. and Prausnitz, J. M. (1972) <doi:10.1021/i160044a003> Adsorption of organic solutions from dilute aqueous solution on activated carbon, Ind. Eng. Chem. Fund. 11 (1972) 445-451.

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

`redlichpeterson.LM` *Redlich-Peterson Isotherm Linear 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

```
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. Deocaris

References

Peterson, D. L. and Redlich, O.(1959) <doi:10.1021/j150576a611> A useful adsorption isotherm. J PhysChem US;63(6):1024. Research, vol. 6, no. 1, pp. 265-276, 2012.

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

`redlichpetersonanalysis` *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. Deocaris

References

Peterson, D. L. and Redlich, O.(1959) <doi:10.1021/j150576a611> A useful adsorption isotherm. J PhysChem US;63(6):1024. Research, vol. 6, no. 1, pp. 265-276, 2012.

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. Deocaris

References

Sips, R. (1948) <doi:10.1063/1.1746922> On the structure of a catalyst surface. The Journal of Chemical Physics, 16(5), 490-495.

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` *Sips Isotherm Nonlinear 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

```
sipsanalysis(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 Sips isotherm, and model error analysis

Author(s)

Keith T. Ostan

Chester C. Deocaris

References

Sips, R. (1948) <doi:10.1063/1.1746922> On the structure of a catalyst surface. The Journal of Chemical Physics, 16(5), 490-495.

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)
sipsanalysis(Ce,Qe)
```

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. 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.

Chen, X. (2015) <doi:10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14–22.

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

Value

initial starting values for parameters based on Langmuir second linear model

Author(s)

Paul Angelo C. Manlapaz

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.

Chen, X. (2015) <doi:10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14–22.

`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

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)
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. 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.

Chen, X. (2015) <doi:10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14–22.

`SSLangmuir3analysis` *Langmuir Isotherm Nonlinear Analysis via selfStart and Langmuir Third 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

```
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

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)
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

```
SSLangmuir4(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 fourth linear model

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.

Chen, X. (2015) <doi:10.3390/info6010014> Modeling of Experimental Adsorption Isotherm Data. 14–22.

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.

Usage

```
SSLangmuir4analysis(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 fourth 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)
SSLangmuir4analysis(Ce,Qe)
```

---

temkin.LM *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

```
temkin.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 Temkin isotherm, and model error analysis

Author(s)

Keith T. Ostan

Chester C. Deocaris

References

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

Foo, K. Y., and Hameed, B. H. (2009, September 13). <doi:10.1016/j.cej.2009.09.013> Insights into the modeling of adsorption isotherm systems. Chemical Engineering Journal.

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

Author(s)

Keith T. Ostan

Chester C. Deocaris

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
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

Toth, J. (1971). State equations of the solid gas interface layer. Acta Chem. Acad. Hung. 69:311-317

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)
tothanalysis(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

```
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

Volmer, M. (1925) <doi:10.1515/zpch-1925-11519> Thermodynamische folgerungen aus der zustandsgleichung fur adsorbierte stoffe. Z. Phys. Chem. 115, 253-261.

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)
volmeranalysis(Ce,Qe)
```

webervanvlietanalysis *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

```
webervanvlietanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	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. Deocaris

References

Van Vliet, B.M., Weber Jr., Hozumi, H.. (1979) <doi:10.1016/0043-1354(80)90107-4> Modeling and prediction of specific compound adsorption by activated carbon and synthetic adsorbents. Water Research Vol.14, pp. 1719 to 1728.

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)
webervanvlietanalysis(Ce,Qe)
```

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