# Package: PUPAK (via r-universe)

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**Type** Package

**Title** Parameter Estimation, and Plot Visualization of Adsorption Kinetic Models

**Version** 0.1.1

**Description** Contains model fitting functions for linear and non-linear adsorption kinetic and diffusion models. Adsorption kinetics is used for characterizing the rate of solute adsorption and the time necessary for the adsorption process. Adsorption kinetics offers vital information on adsorption rate, adsorbent performance in response time, and mass transfer processes. In addition, diffusion models are included in the package as solute diffusion affects the adsorption kinetic experiments. This package consists of 20 adsorption and diffusion models, including Pseudo First Order (PFO), Pseudo Second Order (PSO), Elovich, and Weber-Morris model (commonly called the intraparticle model) stated by Plazinski et al. (2009) <doi:10.1016/j.cis.2009.07.009>. This package also contains a summary function where the statistical errors of each model are ranked for a more straightforward determination of the best fit model.

**License** GPL-2

**Encoding** UTF-8

**Imports** stats, Metrics, ggplot2, utils, nls2, segmented

**RoxygenNote** 7.2.0

**NeedsCompilation** no

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---

`aksummary.l` *Linear Adsorption Kinetic Model Summary*

---

## Description

Summarized results of parameter and error values collected from linear adsorption kinetic models, namely: Elovich, Fractional Power, Pseudo-First-Order, and Pseudo-Second-Order.

## Usage

```
aksummary.l(t, qt, qe, sort.by)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time. This parameter should not be equal to zero to prevent infinite value. Any row(s) that contain(s) value of t equal to zero will be automatically removed to proceed with the calculation. |
| qt | the numerical value for the amount adsorbed at time t. This parameter should not be equal to qe or zero as it will cause an infinite value. Any row(s) that contain(s) value of qt equal to qe or zero will be automatically removed to proceed with the calculation. |
| qe | the numerical value for the amount adsorbed at equilibrium |
| sort.by | the name of the statistical error parameter in which the models are sorted in either increasing or decreasing order. The only accepted arguments are "RMSE" for Relative Mean Square Error, 'MAE' for Mean Absolute Error, 'MSE' for Mean Squared Error, 'RAE' for Relative Absolute Error, 'AIC' for Akaike Information Criterion, 'BIC' for Bayesian Information Criterion, 'R2' for Coefficient of Determination, and 'SE' for Standard Error Estimate. This argument is case-sensitive, and failure to input the correct value will yield a summary of models in alphabetical order. |

## Value

the summarized error and parameter values from adsorption kinetic models.

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## Examples

```
t  <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.8
aksummary.l(t,qt,qe,"R2")
```

---

`aksummary.nl` *Non-Linear Adsorption Kinetic Models Summary*

---

## Description

Summarized results of parameter and error values collected from non-linear adsorption kinetic models, namely: Avrami, Elovich, Fractional Power, Pseudo-First-Order, Pseudo-nth-Order, Pseudo-Second-Order, and Richie's Equation.

## Usage

```
aksummary.nl(t, qt, qe, n, sort.by)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qe | the numerical value for the amount adsorbed at equilibrium |
| n | the numerical value for the richie's equation order of reaction |
| sort.by | the name of the statistical error parameter in which the models are sorted in either increasing or decreasing order. The only accepted arguments are "RMSE" for Relative Mean Square Error, 'MAE' for Mean Absolute Error, 'MSE' for Mean Squared Error, 'RAE' for Relative Absolute Error, 'AIC' for Akaike Information Criterion, 'BIC' for Bayesian Information Criterion, 'R2' for Coefficient of Determination, and 'SE' for Standard Error Estimate. This argument is case-sensitive, and failure to input the correct value will yield a summary of models in alphabetical order. |

## Value

the summarized error and parameter values from non-linear adsorption kinetic models.

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## Examples

```
t <- c(15,30,45,60,75,90,105,120)
qt <- c(3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.68
aksummary.nl(t,qt,qe,n=NULL,"SE")
```

---

# avrami *Non-Linear Avrami Adsorption Kinetic Model*

---

## Description

The Avrami Adsorption Kinetic Model investigates the time-concentration profiles of sorbent-sorbate interactions in adsorption-based water treatment. This equation was developed with the experimentally supported assumptions that the new phase is nucleated by germ nuclei that already exist in the old phase, and whose number can be altered by previous treatment (Oladoja, 2016).

## Usage

```
avrami(t, qt, qe)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qe | the numerical value for the amount adsorbed at equilibrium. If qe is not defined, the value for qe will be equal to the maximum qt. |

## Value

the non-linear regression and the parameter estimation for the Avrami adsorption kinetic model analysis

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Lopes, E. C. N., dos Anjos, F. S. C., Vieira, E. F. S., &; Cestari, A. R. (2003) <doi:10.1016/S0021-9797(03)00326-6> An alternative Avrami equation to evaluate kinetic parameters of the interaction of Hg(II) with thin chitosan membranes. Journal of Colloid and Interface Science, 263(2), 542-547.

Oladoja, N. A. (2016) <doi:10.1080/19443994.2015.1076355> A critical review of the applicability of Avrami fractional kinetic equation in adsorption-based water treatment studies. Desalination and Water Treatment, 57(34), 15813-15825.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.68
avrami(t,qt,qe)
```

bed *Non-Linear Boyd External Diffusion Model*

## Description

The Boyd External Diffusion Model is frequently applied to adsorption kinetic data to calculate the rate constant, assuming that film diffusion is the rate-limiting step in the first few minutes of the adsorption process. The film diffusion has a strong dependency on agitation. Boyd's diffusion models are used in numerous adsorption studies mostly to determine the rate-controlling step (Viegas, Campinas, Costa, and Rosa, 2014).

## Usage

```
bed(t, qt, qinf)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qinf | the numerical value for the amount adsorbed at infinite time. If this parameter is not defined, it will be estimated. |

## Value

the non-linear regression and the parameter estimation for the Boyd External Diffusion model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Boyd, G. E., Adamson, A. W., & Myers, L. S. (1947) <doi:10.1021/ja01203a066> The Exchange Adsorption of Ions from Aqueous Solutions by Organic Zeolites. II. Kinetics1. Journal of the American Chemical Society, 69(11), 2836-2848.

Viegas, R. M. C., Campinas, M., Costa, H., &; Rosa, M. J. (2014) <doi:10.1007/s10450-014-9617-9> How do the HSDM and Boyd's model compare for estimating intraparticle diffusion coefficients in adsorption processes. Adsorption, 20(5-6), 737-746.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qinf <- 4.68
bed(t,qt,qinf)
bed(t,qt)
```

---

`bed.lm` *Linear Boyd External Diffusion Model*

---

## Description

The Boyd External Diffusion Model is frequently applied to adsorption kinetic data to calculate the rate constant, assuming that film diffusion is the rate-limiting step in the first few minutes of the adsorption process. The film diffusion has a strong dependency on agitation. Boyd's diffusion models are used in numerous adsorption studies mostly to determine the rate-controlling step (Viegas, Campinas, Costa, and Rosa, 2014).

## Usage

```
bed.lm(t, qt, qinf)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `qt` | the numerical value for the amount adsorbed at time t. |
| `qinf` | the numerical value for the amount adsorbed at infinite time. If the value for qinf is not given, the highest qt value will be considered as the qinf. |

## Value

the linear regression and the parameter estimation for the Boyd External Diffusion Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Boyd, G. E., Adamson, A. W., & Myers, L. S. (1947) <doi:10.1021/ja01203a066> The Exchange Adsorption of Ions from Aqueous Solutions by Organic Zeolites. II. Kinetics1. Journal of the American Chemical Society, 69(11), 2836-2848.

Viegas, R. M. C., Campinas, M., Costa, H., &; Rosa, M. J. (2014) <doi:10.1007/s10450-014-9617-9> How do the HSDM and Boyd's model compare for estimating intraparticle diffusion coefficients in adsorption processes. Adsorption, 20(5-6), 737-746.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <-c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qinf <- 4.68
bed.lm(t,qt,qinf)
```

---

`bid.lm` *Linear Boyd Intraparticle Diffusion Model*

---

## Description

The Boyd Intraparticle Diffusion Model is frequently applied to analyze if intraparticle diffusion governs the experimental kinetic data. This model assumes that the boundary layer surrounding the adsorbent has a greater effect on the diffusion of solute (Viegas, Campinas, Costa, and Rosa, 2014).

## Usage

```
bid.lm(t, qt, qinf)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `qt` | the numerical value for the amount adsorbed at time t |
| `qinf` | the numerical value for the amount adsorbed at infinite time |

## Value

the linear regression and the parameter estimation for the Boyd Intraparticle Diffusion model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Boyd, G. E., Adamson, A. W., & Myers, L. S. (1947) <doi:10.1021/ja01203a066> The Exchange Adsorption of Ions from Aqueous Solutions by Organic Zeolites. II. Kinetics1. Journal of the American Chemical Society, 69(11), 2836-2848.

Viegas, R. M. C., Campinas, M., Costa, H., &; Rosa, M. J. (2014) <doi:10.1007/s10450-014-9617-9> How do the HSDM and Boyd's model compare for estimating intraparticle diffusion coefficients in adsorption processes. Adsorption, 20(5-6), 737-746.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <-c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qinf <- 4.8
bid.lm(t,qt,qinf)
```

---

# crank *Non-Linear Crank Diffusion Model*

---

## Description

The Crank Diffusion Model is an equation for homogeneous adsorbate diffusion in a sphere-shaped adsorbent with constant surface diffusivity throughout the particle. It's an exact solution for the "infinite bath" case, in which the sphere starts out empty and the solute concentration at the surface remains constant. Due to the constant surface concentration, external film resistance may be ignored (Qiu, Lv, Pan, Zhang, Zhang, and Zhang, 2009).

## Usage

```
crank(t, qt, qinf)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qinf | the numerical value for the amount adsorbed at infinite time. If this argument is not defined, it will be estimated. |

## Value

the non-linear regression and the parameter estimation for the Crank Adsorption Kinetic Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Crank, J. (1979) <ISBN, 0198534116, 9780198534112>The mathematics of diffusion. Oxford university press.

Qiu, H., Lv, L., Pan, B. C., Zhang, Q. J., Zhang, W. M., &; Zhang, Q. X. (2009) <doi:10.1631/jzus.A0820524> Critical review in adsorption kinetic models. In Journal of Zhejiang University: Science A (Vol. 10, Issue 5, pp. 716-724).

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qinf <- 4.68
crank(t,qt,qinf)
```

---

`edsummary.l` *Linear External Diffusion Models Summary*

---

## Description

Summarized results of parameter and error values collected from external diffusion models, namely: Boyd External Diffusion, Furusawa and Smith, and Matthews and Weber.

## Usage

```
edsummary.l(t, qt, Ct, qinf, Co, m, V, b, sort.by)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `qt` | the numerical value for the amount adsorbed at time t |
| `Ct` | the numerical value for the concentration of the adsorbent at time t |
| `qinf` | the numerical value for the amount adsorbed at infinite time |
| `Co` | the numerical value for the initial concentration of the adsorbent |
| `m` | the numerical value for mass of adsorbent |
| `V` | the numerical value for volume of solution |
| `b` | the numerical value or the Langmuir isotherm constant |
| `sort.by` | the name of the statistical error parameter in which the models are sorted in either increasing or decreasing order. The only accepted arguments are "RMSE" for Relative Mean Square Error, 'MAE' for Mean Absolute Error, 'MSE' for Mean Squared Error, 'RAE' for Relative Absolute Error, 'AIC' for Akaike Information Criterion, 'BIC' for Bayesian Information Criterion, 'R2' for Coefficient of Determination, and 'SE' for Standard Error Estimate. This argument is case-sensitive, and failure to input the correct value will yield a summary of models in alphabetical order. |

## Value

the summarized error and parameter values from external diffusion models.

### Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

### Examples

```
t  <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
Ct <- c(10.000,8.141,8.056,7.949,7.863,7.799,7.778,7.756,7.692)
edsummary.l(t,qt,Ct,qinf=4.8,Co=10,m=0.05,V=0.1,b=1.3,"SE")
```

---

## edsummary.nl *Non-Linear External Diffusion Models Summary*

---

### Description

Summarized results of parameter and error values collected from external diffusion models, namely: Boyd External Diffusion, Furusawa and Smith, and Matthews and Weber.

### Usage

```
edsummary.nl(t, qt, Ct, qinf, Co, m, V, b, sort.by)
```

### Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| Ct | the numerical value for the concentration of the adsorbent at time t |
| qinf | the numerical value for the amount adsorbed at infinite time |
| Co | the numerical value for the initial concentration of the adsorbent |
| m | the numerical value for mass of adsorbent |
| V | the numerical value for volume of solution |
| b | the numerical value or the Langmuir isotherm constant |
| sort.by | the name of the statistical error parameter in which the models are sorted in either increasing or decreasing order. The only accepted arguments are "RMSE" for Relative Mean Square Error, 'MAE' for Mean Absolute Error, 'MSE' for Mean Squared Error, 'RAE' for Relative Absolute Error, 'AIC' for Akaike Information Criterion, 'BIC' for Bayesian Information Criterion, 'R2' for Coefficient of Determination, and 'SE' for Standard Error Estimate. This argument is case-sensitive, and failure to input the correct value will yield a summary of models in alphabetical order. |

## Value

the summarized error and parameter values from external diffusion models.

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## Examples

```
t  <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
Ct <- c(10.000,8.141,8.056,7.949,7.863,7.799,7.778,7.756,7.692)
edsummary.nl(t,qt,Ct,qinf=4.8,Co=10,m=0.05,V=0.1,b=1.3,"SE")
```

---

# elovich *Non-Linear Elovich Adsorption Kinetic Model*

---

## Description

The Elovich Adsorption Kinetic Model is an empirical rate equation that states the adsorption energy rises in a linear relationship with surface coverage. The model assumes that adsorption occurs on localized sites, the interaction between adsorbed ions is present, and the concentration of adsorbate is considered to be constant. It is applicable in gas adsorptions as well as wastewater processes (Largitte and Pasquier, 2016).

## Usage

```
elovich(t, qt)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |

## Value

the non-linear regression and the parameter estimation for the Elovich Adsorption Kinetic Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Elovich, S. Y., & Larinov, O. G. (1962) Theory of adsorption from solutions of non electrolytes on solid (I) equation adsorption from solutions and the analysis of its simplest form,(II) verification of the equation of adsorption isotherm from solutions. Izvestiya Akademii Nauk, 2(2), 209–216.

Largitte, L., &; Pasquier, R. (2016) <doi:10.1016/j.cherd.2016.02.006> A review of the kinetics adsorption models and their application to the adsorption of lead by an activated carbon. Chemical Engineering Research and Design, 109, 495-504.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
elovich(t,qt)
```

---

`elovich.lm` *Linear Elovich Adsorption Kinetic Model*

---

## Description

The Elovich Adsorption Kinetic Model is an empirical rate equation that states the adsorption energy rises in a linear relationship with surface coverage. The model assumes that adsorption occurs on localized sites, the interaction between adsorbed ions is present, and the concentration of adsorbate is considered to be constant. It is applicable in gas adsorptions as well as wastewater processes (Largitte and Pasquier, 2016).

## Usage

```
elovich.lm(t, qt)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time. This parameter should not be equal to zero to prevent infinite value. Any row(s) that contain(s) value of t equal to zero will be automatically removed to proceed with the calculation. |
| `qt` | the numerical value for the amount adsorbed at time t |

## Value

the linear regression and the parameter estimation for the Elovich Adsorption Kinetic Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Elovich, S. Y., & Larinov, O. G. (1962) Theory of adsorption from solutions of non electrolytes on solid (I) equation adsorption from solutions and the analysis of its simplest form,(II) verification of the equation of adsorption isotherm from solutions. Izvestiya Akademii Nauk, 2(2), 209–216.

Largitte, L., &; Pasquier, R. (2016) <doi:10.1016/j.cherd.2016.02.006> A review of the kinetics adsorption models and their application to the adsorption of lead by an activated carbon. Chemical Engineering Research and Design, 109, 495-504.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <-c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
elovich.lm(t,qt)
```

---

# fas *Non-Linear Furusawa and Smith Diffusion Model*

---

## Description

The Furusawa and Smith Diffusion Model is known to describe the rate of adsorption assuming that only external diffusion resistance was predominant during the initial sorption period and controlled the sorption rate. The diffusion model relates the change in fluid phase concentration and time with the fluid phase concentration at the external surface and an external mass transfer coefficient (Furusawa & Smith, 1974).

## Usage

```
fas(t, Ct, m, V, b, Co)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| Ct | the numerical value for the concentration of the adsorbent at time t |
| m | the numerical value for mass of adsorbent |
| V | the numerical value for volume of solution |
| b | the numerical value for the Langmuir isotherm constant |
| Co | the numerical value for the initial concentration of the adsorbent. If this parameter is not defined, it will be estimated. |

## Value

the non-linear regression and the parameter estimation for the Furusawa and Smith Diffusion Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Furusawa, T., & Smith, J. M. (1974) <doi:10.1002/aic.690200111> Intraparticle mass transport in slurries by dynamic adsorption studies. AIChE Journal, 20(1), 88–93.

Yakub, E., Agarry, S. E., Omoruwou, F., &; Owabor, C. N. (2020) <doi:10.1080/02726351.2019.1616862> Comparative study of the batch adsorption kinetics and mass transfer in phenol-sand and phenol-clay adsorption systems. Particulate Science and Technology, 38(7), 801-811.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
Ct <- c(10.000,8.141,8.056,7.949,7.863,7.799,7.778,7.756,7.692)
m <- 0.05
V <- 0.1
b <- 1.3
Co <- 10
fas(t,Ct,m,V,b,Co)
```

---

`fas.lm` *Linear Furusawa and Smith Diffusion Model*

---

## Description

The Furusawa and Smith Diffusion Model is known to describe the rate of adsorption, assuming that only external diffusion resistance was predominant during the initial adsorption period and controlled the adsorption rate. The diffusion model relates the change in fluid phase concentration and time with the fluid phase concentration at the external surface and an external mass transfer coefficient (Furusawa & Smith, 1974).

## Usage

```
fas.lm(t, Ct, m, V, b, Co)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `Ct` | the numerical value for the concentration of the adsorbent at time t. This parameter should not contain a value equal to zero. Any row(s) that contain(s) value of Ct equal to zero will be automatically removed to proceed with the calculation. |
| `m` | the numerical value for mass of adsorbent |

| | |
|---|---|
| V | the numerical value for volume of solution |
| b | the numerical value for the Langmuir isotherm constant |
| Co | the numerical value for the initial concentration of the adsorbent |

## Value

the linear regression and the parameter estimation for the Furusawa and Smith Diffusion Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Furusawa, T., & Smith, J. M. (1974) <doi:10.1002/aic.690200111> Intraparticle mass transport in slurries by dynamic adsorption studies. AIChE Journal, 20(1), 88–93.

Yakub, E., Agarry, S. E., Omoruwou, F., &; Owabor, C. N. (2020) <doi:10.1080/02726351.2019.1616862> Comparative study of the batch adsorption kinetics and mass transfer in phenol-sand and phenol-clay adsorption systems. Particulate Science and Technology, 38(7).

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
Ct <- c(10.000,8.141,8.056,7.949,7.863,7.799,7.778,7.756,7.692)
m <- 0.05
V <- 0.1
b <- 1.3
Co <- 10
fas.lm(t,Ct,m,V,b,Co)
```

---

# fp *Non-Linear Fractional Power Adsorption Kinetic Model*

---

## Description

The Fractional Power Adsorption Kinetic Model is an empirical rate equation in which the specific adsorption rate at a unit time can be estimated using its product's constant.(Netzahuatl-Munoz, Del Carmen Cristiani-Urbina, and Cristiani-Urbina, 2015)

## Usage

```
fp(t, qt, qe)
```

### Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qe | the numerical value for the amount adsorbed at equilibrium. If this parameter is not defined, it will be estimated. |

### Value

the non-linear regression and the parameter estimation for the Fractional Power Adsorption Kinetic Model

### Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

### References

Dalai, R. C. (1974) <doi:10.1080/00103627409366531> Desorption of soil phosphate by anion-exchange resin. Communications in Soil Science and Plant Analysis, 5(6), 531-538.

Netzahuatl-Munoz, A. R., del Carmen Cristiani-Urbina, M., &; Cristiani-Urbina, E. (2015) <doi:10.1371/journal.pone.01370
Chromium biosorption from Cr(VI) aqueous solutions by Cupressus lusitanica bark: Kinetics, equilibrium and thermodynamic studies. PLoS ONE, 10(9).

### Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.68
fp(t,qt,qe)
```

---

## fp.lm *Linear Fractional Power Adsorption Kinetic Model*

---

### Description

The Fractional Power Adsorption Kinetic Model is an empirical rate equation in which the specific adsorption rate at a unit time can be estimated using its product's constant. The model was first used to explain the adsorption kinetics of phosphate in soils by anion exchange resin. It is also called the modified Freundlich equation (Netzahuatl-Muñoz, Del Carmen Cristiani-Urbina, and Cristiani-Urbina, 2015).

## Usage

```
fp.lm(t, qt, qe)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time. This parameter should not contain a value equal to zero to prevent infinite value. Any row(s) that contain(s) value of t equal to zero will be automatically removed to proceed with the calculation. |
| qt | the numerical value for the amount adsorbed at time t. This parameter should not contain a value equal to zero to prevent incalculable value. Any row(s) that contain(s) value of qt equal to zero will be automatically removed to proceed with the calculation. |
| qe | the numerical value for the amount adsorbed at equilibrium |

## Value

the linear regression and the parameter estimation for the Fractional Power model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Dalai, R. C. (1974) <doi: 10.1080/00103627409366531> Desorption of soil phosphate by anion-exchange resin. Communications in Soil Science and Plant Analysis, 5(6), 531-538.

Netzahuatl-Munoz, A. R., del Carmen Cristiani-Urbina, M., &; Cristiani-Urbina, E. (2015) <doi:10.1371/journal.pone.01370
Chromium Biosorption from Cr(VI) aqueous solutions by Cupressus lusitanica bark: Kinetics, equilibrium and thermodynamic studies. PLoS ONE, 10(9).

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <-c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.8
fp.lm(t,qt,qe)
```

idsummary *Internal Diffusion Models Summary*

## Description

Summarized results of parameter and error values collected from internal diffusion models, namely: Boyd Internal Diffusion, Crank, and Weber and Morris

## Usage

```
idsummary(t, qt, qinf, sort.by)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qinf | the numerical value for the amount adsorbed at infinite time. If this argument is not defined, the maximum qt will be set as qinf. |
| sort.by | the name of the statistical error parameter in which the models are sorted in either increasing or decreasing order. The only accepted arguments are "RMSE" for Relative Mean Square Error, 'MAE' for Mean Absolute Error, 'MSE' for Mean Squared Error, 'RAE' for Relative Absolute Error, 'AIC' for Akaike Information Criterion, 'BIC' for Bayesian Information Criterion, 'R2' for Coefficient of Determination, and 'SE' for Standard Error Estimate. This argument is case-sensitive, and failure to input the correct value will yield a summary of models in alphabetical order. |

## Value

the summarized error and parameter values from internal diffusion models.

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## Examples

```
t  <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
idsummary(t,qt,qinf=4.8,"SE")
```

maw *Non-Linear Matthews and Weber Diffusion Model*

## Description

The Matthews and Weber Diffusion Model is used in determining the rate constant for film diffusion where it assumes that intraparticle diffusion can be neglected at the early period of contact. Derived from Fickien's law application, the solute concentration in the liquid phase in this model is expressed as a function of solute concentration difference in the liquid phase and at the adsorbent surface (Prasad & Srivastava, 2009).

## Usage

```
maw(t, Ct, Co)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| Ct | the numerical value for the concentration of the adsorbent at time t |
| Co | the numerical value for the initial concentration of the adsorbent. If this parameter is not defined, it will be estimated. |

## Value

the non-linear regression and the parameter estimation for the Matthews and Weber diffusion model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Mathews, A. P., &; Weber, W. J. (1984) <doi:10.1080/00986448408940104> Modeling and parameter evaluation for adsorption in slurry reactors. Chemical Engineering Communications, 25(1-6), 157-171.

Krishna Prasad, R., & Srivastava, S. N. (2009) <doi:10.1016/j.cej.2008.05.021> Sorption of distillery spent wash onto fly ash: Kinetics and mass transfer studies. Chemical Engineering Journal, 146(1), 90–97.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
Ct <- c(10.000,8.141,8.056,7.949,7.863,7.799,7.778,7.756,7.692)
Co <- 10
maw(t,Ct,Co)
```

---

`maw.lm` *Linear Matthews and Weber Diffusion Model*

---

## Description

The Matthews and Weber Diffusion Model is used in determining the rate constant for film diffusion where it assumes that intraparticle diffusion can be neglected at the early period of contact. Derived from Fickien's law application, the solute concentration in the liquid phase in this model is expressed as a function of solute concentration difference in the liquid phase and at the adsorbent surface (Prasad & Srivastava, 2009).

## Usage

```
maw.lm(t, Ct, Co)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `Ct` | the numerical value for the concentration of the adsorbent at time t. This parameter should not contain a value equal to zero. Any row(s) that contain(s) value of Ct equal to zero will be automatically removed to proceed with the calculation. |
| `Co` | the numerical value for the initial concentration of the adsorbent |

## Value

the linear regression and the parameter estimation for the Matthews and Weber diffusion model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Mathews, A. P., &; Weber, W. J. (1984) <doi:10.1080/00986448408940104> Modeling and parameter evaluation for adsorption in slurry reactors. Chemical Engineering Communications, 25(1-6), 157-171.

Krishna Prasad, R., & Srivastava, S. N. (2009) <doi:10.1016/j.cej.2008.05.021> Sorption of distillery spent wash onto fly ash: Kinetics and mass transfer studies. Chemical Engineering Journal, 146(1), 90–97.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
Ct <-c(10.000,8.141,8.056,7.949,7.863,7.799,7.778,7.756,7.692)
Co <- 10
maw.lm(t,Ct,Co)
```

---

`pfo` *Non-Linear Pseudo-First-Order Adsorption Kinetic Model*

---

## Description

The Pseudo-First Order Adsorption Kinetic Model follows the Linear Driving Force model (LDF) which states that the rate of mass transfer is equal to the transfer coefficient and the difference between the amount adsorbed and the amount adsorbed in equilibrium. This model is an empirical rate equation known to describe the rate of sorption in liquid-phase systems. The PFO model is not suitable for the whole adsorption reaction since the rate of adsorption decreases until it reaches the maximum adsorption capacity, and thus, the rate is zero at equilibrium (Plazinski, Rudzinski, and Plazinska, 2009).

## Usage

```
pfo(t, qt, qe)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `qt` | the numerical value for the amount adsorbed at time t |
| `qe` | the numerical value for the amount adsorbed at equilibrium. If this parameter is not defined, it will be estimated. |

## Value

the non-linear regression and the parameter estimation for the Pseudo-First-Order Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Lagergren, S. (1898), Zur theorie der sogenannten adsorption gelöster stoffe, Kungliga Svenska Vetenskapsakademiens. Handlingar, 24 (4) : 1-39.

Plazinski, W., Rudzinski, W., &; Plazinska, A. (2009) <doi:10.1016/j.cis.2009.07.009> Theoretical models of sorption kinetics including a surface reaction mechanism: A review. In Advances in Colloid and Interface Science (Vol. 152, Issues 1-2, pp. 2-13).

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.68
pfo(t,qt,qe)
```

---

`pfo.lm` *Linear Pseudo-First-Order Adsorption Kinetic Model*

---

## Description

The Pseudo-First-Order Adsorption Kinetic Model follows the Linear Driving Force model (LDF) which states that the rate of mass transfer is equal to the transfer coefficient and the difference between the amount adsorbed and the amount adsorbed in equilibrium. This model is an empirical rate equation known to describe the rate of sorption in liquid-phase systems. The PFO model is not suitable for the whole adsorption reaction since the rate of adsorption decreases until it reaches the maximum adsorption capacity, and thus, the rate is zero at equilibrium (Plazinski, Rudzinski, and Plazinska, 2009).

## Usage

```
pfo.lm(t, qt, qe, est.qe)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `qt` | the numerical value for the amount adsorbed at time t. |
| `qe` | the numerical value for the amount adsorbed at equilibrium. If the value for qe is not given, the highest qt value will be considered as the qe. |
| `est.qe` | option for calculating estimated qe. If the value is FALSE, it will calculate linear regression with fixed intercept. If the value is TRUE, it will calculate the linear regression in form y=mx+b. The default value for est.qe is FALSE. |

## Value

the linear regression and the parameter estimation for the Pseudo First Order Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Lagergren, S. (1898), Zur theorie der sogenannten adsorption gelster stoffe, Kungliga Svenska Vetenskapsakademiens. Handlingar, 24 (4) : 1-39.

Plazinski, W., Rudzinski, W., &; Plazinska, A. (2009) <doi:10.1016/j.cis.2009.07.009> Theoretical models of sorption kinetics including a surface reaction mechanism: A review. In Advances in Colloid and Interface Science</i> (Vol. 152, Issues 1-2, pp. 2-13).

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <-c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.8
pfo.lm(t,qt,qe,est.qe=FALSE)
```

---

pno *Non-Linear Pseudo-nth-Order Adsorption Kinetic Model*

---

## Description

The Pseudo-nth Order Adsorption Kinetic Model is an empirical rate equation known to describe the kinetic analysis of neither order 1 nor 2 kinetic parameters. It will have a significant effect on the calculation of the rate constants as the rate constant is dependent on the order of reaction (Tseng, Wu, Wu, and Juang, 2014).

## Usage

```
pno(t, qt, qe)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qe | the numerical value for the amount adsorbed at equilibrium. If this parameter is not defined, it will be estimated. |

## Value

the non-linear regression and the parameter estimation for the Pseudo-nth-Order Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Ozer, A. (2007) <doi:10.1016/j.jhazmat.2006.07.040> Removal of Pb(II) ions from aqueous solutions by sulphuric acid-treated wheat bran. Journal of Hazardous Materials, 141(3), 753-761.

Tseng, R. L., Wu, P. H., Wu, F. C., &; Juang, R. S. (2014) <doi:10.1016/j.cej.2013.10.013> A convenient method to determine kinetic parameters of adsorption processes by nonlinear regression of pseudo-nth-order equation. Chemical Engineering Journal, 237, 153-161.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.8
pno(t,qt,qe)
```

---

# pso *Non-Linear Pseudo Second-Order Adsorption Kinetic Model*

---

## Description

The Pseudo-Second-Order Adsorption Kinetic Model is an empirical rate equation known to be the simplified second-order expression of the Pseudo-First Order Adsorption Kinetic Model. It is widely applied to adsorption systems, from biomass to nanomaterials as adsorbent and from heavy metals to pharmaceuticals as adsorbate or contaminant (Revellame, Fortela, Sharp, Hernandez, and Zappi, 2020).

## Usage

```
pso(t, qt, qe)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |
| qe | the numerical value for the amount adsorbed at equilibrium. If this parameter is not defined, it will be estimated. |

## Value

the non linear regression and the parameters for the pseudo-second order non-linear model analysis

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Ho, Y. S., &; Mckay, G. (1999) <doi:10.1016/S0032-9592(98)00112-5> Pseudo-second order model for sorption processes. In Process Biochemistry (Vol. 34).

Revellame, E. D., Fortela, D. L., Sharp, W., Hernandez, R., &; Zappi, M. E. (2020) <doi:10.1016/j.clet.2020.100032> Adsorption kinetic modeling using pseudo-first order and pseudo-second order rate laws: A review. In Cleaner Engineering and Technology (Vol. 1). Elsevier Ltd.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.68
pso(t,qt,qe)
```

---

# pso.lm *Linear Pseudo-Second-Order Adsorption Kinetic Model*

---

## Description

The Pseudo-Second-Order Adsorption Kinetic Model is an empirical rate equation known to be the simplified second-order expression of the Pseudo-First Order Adsorption Kinetic Model. It is widely applied to adsorption systems, from biomass to nanomaterials as adsorbent and from heavy metals to pharmaceuticals as adsorbate or contaminant (Revellame, Fortela, Sharp, Hernandez, and Zappi, 2020).

## Usage

```
pso.lm(t, qt, qe)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t. This parameter should not contain a value equal to zero as it will cause an infinite value. Any row(s) that contain(s) value of qt equal to zero will be automatically removed to proceed with the calculation. |
| qe | the numerical value for the amount adsorbed at equilibrium |

## Value

the linear regression and the parameter estimation for the Pseudo-Second-Order Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Ho, Y. S., &; Mckay, G. (1999) <doi:10.1016/S0032-9592(98)00112-5> Pseudo-second order model for sorption processes. In Process Biochemistry (Vol. 34).

Revellame, E. D., Fortela, D. L., Sharp, W., Hernandez, R., &; Zappi, M. E. (2020) <doi:10.1016/j.clet.2020.100032>. Adsorption kinetic modeling using pseudo-first order and pseudo-second order rate laws: A review. In Cleaner Engineering and Technology (Vol. 1). Elsevier Ltd.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <-c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.8
pso.lm(t,qt,qe)
```

---

`richie` *Non-Linear Ritchie's Equation*

---

## Description

The Ritchie's Equation is a well-known empirical rate equation for gas particle adsorption on solid surfaces. Assuming that the rate of adsorption is exclusively determined by the percentage of vacant sites at time t (Kaki, Gögsu, Altindal, Salih, and Bekaroglu, 2020).

## Usage

```
richie(t, qt, qe, n)
```

## Arguments

| | |
|---|---|
| `t` | the numerical value for contact time |
| `qt` | the numerical value for the amount adsorbed at time t |
| `qe` | the numerical value for the amount adsorbed at equilibrium. If this parameter is not defined, it will be estimated. |
| `n` | the Richie's equation order of reaction. If the parameter value n=1, the function will proceed to first-order Richie's equation. If the value n=2, the function will proceed to second-order Richie's equation, and if the n is not defined, the value of n will be estimated. |

## Value

the non-linear regression and the parameters estimation for the Richie adsorption kinetic model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. DelaCruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Ritchie, A. G. (1977) <doi:10.1039/F19777301650> Alternative to the Elovich equation for the kinetics of adsorption of gases on solids. Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases, 73, 1650-1653.

Kaki, E., Gögsu, N., Altindal, A., Salih, B., &; Bekaroglu, Ö. (2020) <doi:10.1142/S1088424619500196> Synthesis, characterization and VOCs adsorption kinetics of diethylstilbestrol-substituted metallophthalocyanines. In Porphyrin Science By Women (In 3 Volumes) (pp. 991-999). World Scientific Publishing Co.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <- c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
qe <- 4.68
richie(t,qt,qe)
richie(t,qt,n=3)
```

---

# wam.pl *Piecewise-Linear Weber and Morris Intraparticle Diffusion Model*

---

## Description

The Weber and Morris Intraparticle Diffusion Model is a multi-linear sorption process in which the intraparticle diffusion process is the limiting factor, where other interaction mechanisms such as adsorption on the external surface and diffusion into the interior may be happening simultaneously (Campos, Barbosa, Rodriguez-Diaz, and Duarte, 2018).

## Usage

```
wam.pl(t, qt)
```

## Arguments

| | |
|---|---|
| t | the numerical value for contact time |
| qt | the numerical value for the amount adsorbed at time t |

## Value

the piecewise-linear regression and the parameter estimation for the Weber and Morris Intraparticle Diffusion Model

## Author(s)

Jeff Ryan S. Magalong

Joshua Z. Dela Cruz

Jeann M. Bumatay

Chester C. Deocaris

## References

Weber, W.J. and Morris, J.C. (1963) Kinetics of Adsorption on Carbon from Solutions. Journal of the Sanitary Engineering Division, American Society of Civil Engineers, 89, 31-60.

Campos, N. F., Barbosa, C. M. B. M., Rodriguez-Diaz, J. M., &; Duarte, M. M. M. B. (2018) <doi:10.1177/0263617418773844> Removal of naphthenic acids using activated charcoal: Kinetic and equilibrium studies. Adsorption Science and Technology, 36(7-8), 1405-1421.

## Examples

```
t <- c(0,15,30,45,60,75,90,105,120)
qt <-c(0.000,3.718,3.888,4.102,4.274,4.402,4.444,4.488,4.616)
wam.pl(t,qt)
```

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