Package ‘SHAKTI’

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Type Package

Title Suite for Heat-Related Adsorption Knowledge and Thermodynamic Inference

Description A comprehensive framework for quantifying the fundamental thermodynamic parameters of adsorption reactions—changes in the standard Gibbs free energy (delta G), enthalpy (delta H), and entropy (delta S)—is essential for understanding the spontaneity, heat effects, and molecular ordering associated with sorption processes. By analysing temperature-dependent equilibrium data, thermodynamic interpretation expands adsorption studies beyond conventional isotherm fitting, offering deeper insight into underlying mechanisms and surface–solute interactions. Such an approach typically involves evaluating equilibrium coefficients across multiple temperatures and non-temperature treatments, deriving thermodynamic parameters using established thermodynamic relationships, and determining delta G as a temperature-specific indicator of adsorption favourability. This analytical pathway is widely applicable across environmental science, soil science, chemistry, materials science, and engineering, where reliable assessment of sorption behaviour is critical for examining contaminant retention, nutrient dynamics, and the behaviour of natural and engineered surfaces. By focusing specifically on thermodynamic inference, this framework complements existing adsorption isotherm-fitting packages such as “AdIsMF” <https://CRAN.R-project.org/package=AdIsMF> <doi:10.32614/CRAN.package.AdIsMF>, and strengthens the scientific basis for interpreting adsorption energetics in both research and applied contexts. Details can be found in Roy et al. (2025) <doi:10.1007/s11270-025-07963-7>.

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Contents

`LnKd` *Dimensionless Distribution Coefficient*

Description

This function computes the natural logarithm of dimensionless distribution coefficient (Kd) from adsorption equilibrium data across temperatures, and non-temperature treatments, if any. This function prepares the foundational input required for thermodynamic parameter analysis.

Usage

```
LnKd(V, m, MW.Ad, M.Ad, Non_T_trt, T_trt, Rep, IGC, Ce)
```

Arguments

`V`	Volumn of water in litre
`m`	Mass of the adsorbent in gram
`MW.Ad`	Molar weight of the adsorbate in gram per mole
`M.Ad`	Molarity of the solvent in mole per litre(55.5 for water)
`Non_T_trt`	Non-temperature treatment
`T_trt`	Temperature treatment
`Rep`	Replication
`IGC`	Initial graded concentrations of the adsorbate in milligram per litre
`Ce`	Equilibrium concentration of the adsorbate in milligram per litre

Value

- qe_i: Absorbed amount in milligram per kg
- Kd_i: Distribution coefficient
- lnKd_i: Natural logarithm of Kd
- Mean_lnkd: Average of lnKd

References

Roy, A., Manjaiah, K. M., Datta, S. P., Rakshit, D., Barman, M., Ray, P., Golui, D., Raza, M. B., Tigga, P., Mondal, S., Vishwanath, Meena, S., & Meena, P. (2025). Effect of Low-Molecular-Weight Organic Acids and Silicon on Arsenic Adsorption and Desorption in a Paddy Soil of Bengal Delta Plain: Insights from Thermodynamics and Equilibrium Modeling. Water, Air, & Soil Pollution, 236(6), 344. https://doi.org/10.1007/s11270-025-07963-7

Examples

```
V <- 0.02  # in litre
m <- 2 # in gram
MW.Ad <- 75
M.Ad <- 55.5
Non_T_trt <- c(0,0,0,0,0,0,1,1,1,1,1,1)
T_trt <- c(1,1,1,2,2,2,1,1,1,2,2,2)
Rep <- c(1,2,3,1,2,3,1,2,3,1,2,3)
IGC <- c(2,4)
Ce2 <- c(0.030, 0.031, 0.032, 0.033, 0.034, 0.035, 0.030, 0.031, 0.032, 0.033, 0.034, 0.035)
Ce4 <- c(0.030, 0.031, 0.032, 0.033, 0.034, 0.035, 0.030, 0.031, 0.032, 0.033, 0.034, 0.035)
Ce <- data.frame(Ce2, Ce4)
my.LnKd<- LnKd(V, m, MW.Ad, M.Ad, Non_T_trt, T_trt, Rep, IGC, Ce)
```

`Slope_Intercept` *Estimation of Slope and Intercept*

Description

Generates slope and intercept values from temperature-dependent lnKd data using linear regression, and the corresponding coefficient of determination (R^2) values. These coefficients form the basis for calculating the thermodynamic parameters, providing a simple and transparent bridge between experimental equilibrium measurements and thermodynamic interpretation.

Usage

```
Slope_Intercept(lnKd, Temp)
```

Arguments

`lnKd`	Natural logarithm of distribution coefficient
`Temp`	Temperature in Kelvin

Value

- Intercept: Intercept of the fitted line
- Slope: Slope of the fitted line
- R_square: Coefficient of determination of the fitted line

References

Gouaich, I., Bestani, B., Bouberka, Z., Srenscek-Nazza, J., Michalkiewicz, B., Benzekri-Benallou, M., Boucherdoud, A., and Benderdouche, N. (2023). Characterization of a low-cost Eucalyptus camaldulensis leaves based activated carbon for pharmaceutical residues removal from aqueous solutions. Desalination and Water Treatment, 296, 19–31. https://doi.org/10.5004/dwt.2023.29602

Examples

```
lnKd <- c(5.01, 5.02)
Temp <- c (298, 303)
my.SI<- Slope_Intercept(lnKd, Temp)
```

Thermo_parameters *Estimation of Thermodynamic Parameters*

Description

Calculates delta H, delta S, and delta G across temperature and non-temperature treatments using regression-derived slope and intercept values, integrating van't Hoff and Gibbs-based relationships. This function assesses spontaneity, energetic favourability, and system randomness, providing a comprehensive thermodynamic profile for interpreting adsorption energetics.

Usage

```
Thermo_parameters(lnKd, Temp, Slope, Intercept)
```

Arguments

`lnKd`	Natural logarithm of distribution coefficient corresponding to each initial graded concentrations
`Temp`	Temperature in Kelvin
`Slope`	Estimated slope of the fitted line
`Intercept`	Estimated intercept of the fitted line

Value

- Delta_H: Change in the standard enthalpy
- Delta_S: Change in the standard entropy
- Delta_G: Change in the standard Gibbs free energy
- Descriptive: Mean and standard error of the thermodynamic parameters

References

- Roy, A., Manjaiah, K. M., Datta, S. P., Rakshit, D., Barman, M., Ray, P., Golui, D., Raza, M. B., Tigga, P., Mondal, S., Vishwanath, Meena, S., & Meena, P. (2025). Effect of Low-Molecular-Weight Organic Acids and Silicon on Arsenic Adsorption and Desorption in a Paddy Soil of Bengal Delta Plain: Insights from Thermodynamics and Equilibrium Modeling. Water, Air, & Soil Pollution, 236(6), 344. https://doi.org/10.1007/s11270-025-07963-7
- Yi, Z., Yao, J., Zhu, M., Chen, H., Wang, F., & Liu, X. (2016). Kinetics, equilibrium, and thermodynamics investigation on the adsorption of lead (II) by coal-based activated carbon. SpringerPlus, 5(1), 1160. https://doi.org/10.1186/s40064-016-2839-4

Examples

```
lnKd <- c(7,8)
Temp <- 298
Slope <- c(-180, -200)
Intercept <- c(5, 6)
my.tp <- Thermo_parameters(lnKd, Temp, Slope, Intercept)
```

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