Package 'transmem'

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Title Treatment of Membrane-Transport Data

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Description Treatment and visualization of membrane (selective) transport
data. Transport profiles involving up to three species are produced as
publication-ready plots and several membrane performance parameters
(e.g. separation factors as defined in Koros et al. (1996)
<doi:10.1351/pac199668071479> and non-linear regression parameters
for the equations described in Rodriguez de San Miguel et al. (2014)
<doi:10.1016/j.jhazmat.2014.03.052>) can be obtained. Many widely used
experimental setups (e.g. membrane physical aging) can be easily studied
through the package's graphical representations.

License GPL (>= 2)

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BugReports https://github.com/Crparedes/transmem/issues

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transmem-package *transmem: Treatment of membrane-transport data.*

Description

Treatment and visualization of membrane (selective) transport data. Transport profiles involving up to three species are produced as publication-ready plots and several membrane performance parameters (e.g. separation factors as defined in Koros et al. (1996) <doi:10.1351/pac199668071479> and non-linear regression parameters for the equations described in Rodriguez de San Miguel et al. (2014) <doi:10.1016/j.jhazmat.2014.03.052>) can be obtained. Many widely used experimental setups (e.g. membrane physical aging) can be easily studied through the package's graphical representations.

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

References

C. Paredes, E. Rodriguez de San Miguel, Polymer inclusion membrane for the recovery and concentration of lithium from seawater. Master thesis, Universidad Nacional Autónoma de México, México City, México, 2020.

`calibCurve` *Calculates regression curve for external standard calibration.*

Description

Polinomial regression curves for external standard calibration are calculated to later convert signals into concentration values.

Usage

```
calibCurve(curve, order = 1, badpoint = NULL, intercept = TRUE, plot = TRUE)
```

Arguments

curve	Data frame of numeric vectors named 'Conc' and 'Signal' containing the concentrations and the signals, respectively.
order	Regression curve order. 1 for linear (default) and 2 for quadratic.
badpoint	Numeric vector with the points to be ignored in the regresion. This allows the easy elimination of outliers without losing the stored measurement information.
intercept	Logical. If TRUE, the default, the intercept is calculated normally instead of being forced to 0.
plot	Logical. If TRUE, the default, the calibration data is plotted.

Details

A linear method (i.e `lm()`) is applied to obtain the regression curve.

Value

Model of the calibration curve.

Author(s)

Cristhian Paredes, `<craparedesca@unal.edu.co>`

Eduardo Rodriguez de San Miguel, `<erdsmg@unam.mx>`

See Also

[calibPlane](#) when using more than one explanatory variable.

Examples

```
data(curvelithium)
model1 <- calibCurve(curve = curvelithium, order = 1)
model2 <- calibCurve(curve = curvelithium, order = 2)
summary(model1)
summary(model2)
```

---

calibPlane   *Calculates regression plane for external standard calibration.*

Description

A bivariated regression plane for external standard calibration is calculated to later convert signals into concentration values. It differs from [calibCurve](#) in the number of explanatory variables, 2 in this case. This function is useful when some interference effect is being considered such as the magnification of the interest species signal due to the presence of another (known) species in the same sample.

Usage

```
calibPlane(plane, badpoint = NULL, plot = TRUE, lines = 13, theta = -30,
  phi = 40, xlab = "Species 1", ylab = "Species 2", zlab = "Signal",
  pch = 18, cex = 2)
```

Arguments

plane	Data frame of numeric vectors named 'Conc', 'Conc.S' and 'Signal'. The vectors must contain the concentrations of the main species (the one whose concentration in the samples is to be known) and the secondary species (the interferent), and the standard's signals, respectively.
badpoint	Numeric vector with the points to be ignored in the regresion. This allows the easy elimination of outliers without losing the stored measurement information.
plot	Logical. If TRUE, the default, the calibration data is plotted.
lines	Number of lines to use in the mesh of the plane in the plot.
theta	Azimuthal angle at which the plane is visualized.
phi	Altitude angle at which the plane is visualized.
xlab	Label for X axis (main species concentration).
ylab	Label for Y axis (secondary species concentration).
zlab	Label for Z axis (response).
pch	Plotting symbols available in R.
cex	The size of pch symbols.

Details

A linear method (i.e lm()) is applied to obtain the regression equation. The user must verify model assumptions such as normal distribution of residuals.

Value

Model of the calibration plane

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

Examples

```
data(planelithium)
planeModel <- calibPlane(plane = planelithium)
summary(planeModel$model)
```

---

conc2frac   *Creates a data frame as a complete self-contained transport data set*

Description

The function transforms the data contained in concentration vectors of feed and strip phases to a data frame that contains the complete data of a transport process. This new data frame can be used by several functions inside the package. The output data frame may contain normalized fractions remaining in the feed and already transported to the strip phase, or the original data provided in concentration units.

Usage

```
conc2frac(feed, strip, time = NULL, correct.strip = FALSE, normalize = TRUE)
```

Arguments

feed	Numeric vector with concentrations in the feed phase.
strip	Numeric vector with concentrations in the strip phase.
time	Numeric vector with time at which the aliquots were sampled. It is an optional parameter. If not provided, regular unitary time intervals are assumed.
correct.strip	Logical. If FALSE, the default, the information about the amount transported to the strip phase is used as received but if it is set to TRUE, the initial concentration in the strip phase is substracted to all concentrations in the same phase. This is particularly useful when the blank signal is significative or there is background noise.
normalize	Logical. If TRUE, the default, all concentrations are divided by the initial concentration in the feed phase to give results in fraction units.

Details

The change in concentration of species in the feed and strip phases as a function of time are the main magnitudes being measured in processes involving transport across membranes. The best form to deal with such data is inside a dataframe containing the information about the concentration of given species in both phases and the time transcurred.

Usually, this function is required after using signal2conc wich convert instrumental signals to concentrations.

Value

Data frame with the transport proccess information

Author(s)

Cristhian Paredes, `<craparedesca@unal.edu.co>`

Eduardo Rodriguez de San Miguel, `<erdsmg@unam.mx>`

Examples

```
transData <- conc2frac(feed = c(0.200, 0.169, 0.152, 0.141, 0.138),
                       strip = c(0.000, 0.035, 0.045, 0.062, 0.069),
                       time = c(0, 2, 4, 6, 8))
print(transData)
```

---

concentrationcycles   *Lithium concentration results using a membrane*

Description

A list of 5 datasets, each of one with the transport data of each cycle in a concentration experiment of lithium using a polymer inclusion membrane.

Usage

```
concentrationcycles
```

Format

A list of 5 data frames with 10 rows and 3 variables:

Time Time in hours of each aliquot taken during the experiment

Phase Phase of corresponding aliquot, Feed or Strip

Fraction Remaining lithium concentration in the feed solution or transported lithium concentration to the strip solution

Source

Paredes, C. and Rodríguez de San Miguel, E., Selective lithium extraction and concentration from diluted alkaline aqueous media by a polymer inclusion membrane and application to seawater, Desalination, Volume 487, 2020, 114500, https://doi.org/10.1016/j.desal.2020.114500.

| curvelithium | *External standard calibration curve for lithium in water.* |

Description

A dataset containing the concentrations and emission signals of aqueous lithium standards measured by Flame Atomic Emission Spectrometry (FAES) at a Perkin-Elmer 3100 Atomic Absorption Spectrometer.

Usage

```
curvelithium
```

Format

A data frame with 8 rows and 2 variables:

Conc lithium concentration in the standards, in mg/kg

Signal emission signal of lithium at 670.8 nm, in arbitrary units

Source

Paredes, C. and Rodríguez de San Miguel, E., Selective lithium extraction and concentration from diluted alkaline aqueous media by a polymer inclusion membrane and application to seawater, Desalination, Volume 487, 2020, 114500, https://doi.org/10.1016/j.desal.2020.114500.

| cyclesPlot | *Plots transport profiles for processes involving several cycles* |

Description

Given the data (data frames) of a transport process that was carried in several cycles (e.g. membrane reuse or metal concentration studies), plots the transport profiles like in a continuous experiment indicating the end of each cycle

Usage

```
cyclesPlot(trans, xlab = "Time (h)", ylab = expression(Phi), xlim = NULL,
  ylim = NULL, xbreaks = NULL, ybreaks = NULL, size = 1.8,
  legend = FALSE)
```

Arguments

`trans`	List containing the (ordered) transport data of each cycle. Each data frame must be generated using [conc2frac](#).
`xlab`	Label to be used for x axis. Text and expression allowed.
`ylab`	Label to be used for y axis. Text and expression allowed.
`xlim`	Numeric vector of limits for X-axis.
`ylim`	Numeric vector of limits for X-axis.
`xbreaks`	Numeric vector of x-axis breaks.
`ybreaks`	Numeric vector of x-axis breaks.
`size`	Size used for points in the plot.
`legend`	Logical. If `FALSE`, the default, the legend is not included.

Details

If a concentration experiment has been made through the cycles, it is recommended the y-axis to be in concentration scale instead of fractions. To get the transport data frame in concentration units use conc2frac(..., normalize = FALSE). For more details see [conc2frac](#).

Most `transmem` graphical representations are made using the package `ggplot2` so the function returns a ggplot2 object that can be assigned to a variable for further modification.

Value

Plot of the transport process carried in several cycles

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

References

Wickham H (2016). ggplot2: Elegant Graphics for Data Analysis. Springer-Verlag New York. ISBN 978-3-319-24277-4, <https://ggplot2.tidyverse.org>.

---

fixSecondary	*Interpolates secondary species concentration at missing time values*

Description

If the secondary species concentration is determined in just a fraction of the aliquots and for some reason, the concentration in all the aliquots is required or desired, the function fits a polynomial trend line to the existing data and interpolates the concentration in missing aliquots.

Usage

```
fixSecondary(conc, time, compTime, order = 2)
```

Arguments

conc	Species concentration original vector.
time	Times at which given concentrations were determined.
compTime	Times at which the given species concentration must be interpolated.
order	Order of the polynomial to be fitted to data (1 or 2). Default to 2.

Value

Vector of interpolated concentrations at times provided in compTime.

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

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multiPlotSP	*Plots several single-phase transport profiles overlayed*

Description

Given a list of several complete transport data, the function overlays the transport profiles in a defined phase. The function is useful in membrane reuse experiments as transport profile deterioration is easily visualized.

Usage

```
multiPlotSP(trans, phase = "strip", trend = NULL, legend = FALSE,
  xlab = "Time (h)", ylab = expression(Phi), xlim = NULL, ylim = NULL,
  xbreaks = NULL, ybreaks = NULL, size = 3, plot = TRUE, shape = 15,
  bw = FALSE, arw = FALSE, arw.pos = NULL, arw.txt = NULL,
  txt.pos = NULL, txt.size = NULL)
```

Arguments

trans	List of data frames with the complete transport information of interest species. Must be generated using [conc2frac](). This is the only non-optional parameter.
phase	Phase to be represented in the plot: 'strip', the default, or 'feed'.
trend	List of Non-linear regression models of the main species transport profil. Generated using [transTrend]().
legend	Logical. If FALSE, the default, the legend is not included.
xlab	Label to be used for x axis. Text and expression allowed.

ylab	Label to be used for y axis. Text and expression allowed.
xlim	Numeric vector of limits for X-axis.
ylim	Numeric vector of limits for X-axis.
xbreaks	Numeric vector of x-axis breaks.
ybreaks	Numeric vector of x-axis breaks.
size	Size used for points in the plot.
plot	Logical. If TRUE, the default, the plot is printed in the current graphical device.
shape	Shape to use in the points to be plotted.
bw	Logical, if FALSE, the default, a color version of the plot is given. If a black and white version is required, it must be set to TRUE.
arw	Logical default to FALSE. If TRUE, a vertical arrow is drawn in the plot. Its use is recommended when a trend along the profiles is to be indicated.
arw.pos	Numeric vector of the coordinates of the arrow if arw = TRUE. The format is (x0, x1, y0, y1)
arw.txt	Text to be (optionally) printed alongside the arrow.
txt.pos	Numeric vector of the position of the center of the text provided in arw.txt. The format is (x, y). If not provided, the text is located close to the arrow but a little alignment could be required.
txt.size	Size of the text accompanying the arrow.

Details

Most transmem graphical representations are made using the package ggplot2 so the function returns a ggplot2 object that can be assigned to a variable for further modification.

Value

Plot with the overlayed transport profiles for a single phase

Author(s)

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Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

Examples

```
data(reusecycles)
# First step is to get trend lines for each cycle:
trend <- list()
for (i in 1:length(reusecycles)) {
  trend[[i]] <- transTrend(trans = reusecycles[[i]])
}
# Default plot using colors:
multiPlotSP(trans = reusecycles, trend = trend, legend = TRUE)

# Black and white plot including an arrow:
```

```
multiPlotSP(trans = reusecycles, trend = trend, legend = TRUE, bw = TRUE,
            arw = TRUE, arw.pos = c(6.1, 6.1, 0.8, 0.6),
            arw.txt = 'Cycle', txt.pos = c(6.15, 0.7))
```

---

permcoef   *Calculates permeability coefficients*

Description

Permeability coefficients across a membrane as derived from integrated Fick's law can be obtained from transport data according to the equation

$$\ln\left(\frac{C}{C^0}\right) = -\frac{P\,a}{V}t$$

where P is the permeability coefficient, a is the membrane exposed area, C and C^0 are the species concentrations at any time and at initial time in the feed phase, respectively, and V is solution volume.

Usage

```
permcoef(trans, vol, area, units = c("cm^3", "cm^2", "h"), conc0 = NULL,
  plot = FALSE)
```

Arguments

trans	Data frame with the complete transport information of interest species. Must be generated using conc2frac.
vol	Volume of the feed solution.
area	Membrane exposed area to the feed solution.
units	Units in which volume, area and time are provided. Volume and area are function's parameters while the time is extracted from the trans data frame.
conc0	Initial concentration of the species in the feed solution. The value may be extracted from transport information if the data frame provided in trans is not normalized. See conc2frac for details.
plot	logical default to TRUE. Should the plot be made?

Details

Species concentration units may be arbitrary as long as the permeability coefficient is calculated using the change in concentration ratio which is, as most ratios, adimensional

Value

A numeric vector with the permeability coefficient and it's standard uncertainty from the regression. Units are meters per second.

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

---

planelithium   *Bivariated calibration plane for lithium in prescence of sodium.*

Description

A dataset containing the concentrations of lithium and sodium combined standards and absorbance signals measured by Flame Atomic Absorption Spectrometry (FAAS) at a Perkin-Elmer 3100 Atomic Absorption Spectrometer.

Usage

```
planelithium
```

Format

A data frame with 40 rows and 3 variables:

Conc lithium concentration in the standards, in mg/kg

Signal absorbance signal of lithium at 670.8 nm, in absorbance units

Conc.S sodium concentration in the standards, in mg/kg

Source

Paredes, C. and Rodríguez de San Miguel, E., Selective lithium extraction and concentration from diluted alkaline aqueous media by a polymer inclusion membrane and application to seawater, Desalination, Volume 487, 2020, 114500, https://doi.org/10.1016/j.desal.2020.114500.

---

reusecycles   *Membrane reuse capability to transport lithium*

Description

A list of 10 datasets, each of one with the transport data of each cycle in a reuse capability experiment of a polimeric inclusion membrane selective to lithium ions.

Usage

```
reusecycles
```

Format

A list of 10 data frames with 10 rows and 3 variables:

Time Time in hours of each aliquot taken during the cycle

Phase Phase of corresponding aliquot, Feed or Strip

Fraction Remaining lithium fraction in the feed solution or transported lithium fraction to the strip solution

Source

Paredes, C. and Rodríguez de San Miguel, E., Selective lithium extraction and concentration from diluted alkaline aqueous media by a polymer inclusion membrane and application to seawater, Desalination, Volume 487, 2020, 114500, https://doi.org/10.1016/j.desal.2020.114500.

---

seawaterLiNaK   *Lithium, sodium and potassium transport profiles across a membrane*

Description

A list of 6 datasets containing by duplicate the transport profiles for lithium, sodium, and potassium from a synthetic simplified seawater matrix using a polymer inclusion membrane selective to lithium. Lithium samples were taken every 45 minutes during 4.5 hours while sodium and potassium determinations were made in samples taken every 1.5 hours.

Usage

```
seawaterLiNaK
```

Format

A list of 6 data frames (two for each lithium, sodium, and potassium) with 14 or 8 rows and 3 variables:

Time Time in hours of each aliquot taken during the experiment

Phase Phase of corresponding aliquot, Feed or Strip

Fraction Remaining lithium concentration in the feed solution or transported lithium concentration to the strip solution

Source

Paredes, C. and Rodríguez de San Miguel, E., Selective lithium extraction and concentration from diluted alkaline aqueous media by a polymer inclusion membrane and application to seawater, Desalination, Volume 487, 2020, 114500, https://doi.org/10.1016/j.desal.2020.114500.

---

sepfactor   *Calculates separation factors between two transported species*

Description

Given the transport data frames of two species, the function calculates the separation factors of the main species A against a secondary species B for each sample taken. If the dataset of secondary species is smaller than that of the main species (e.g. if secondary species were determined in only half the aliquots), the transport profile is completed using `fixSecondary` function and a message will be printed.

Usage

```
sepfactor(main, secon, order = 2, mode = "batch", plot = TRUE)
```

Arguments

main	Main species transport data. Must be a data frame generated using `conc2frac`, data normalization is indifferent.
secon	Undesired species transport data. Must be a data frame generated using `conc2frac`, data normalization is indifferent.
order	Gives the polinomia order to be used if the secondary species information needs to be corrected due to missing data.
mode	Operation mode of the membranse system. Only `'batch'` and `'continuous'` allowed. For semicontinuous systems the separation factor is calculated as for continuous systems.
plot	Logical. If `TRUE`, the default, the plot is printed in the current graphical device.

Details

Separation factor for batch systems at any time different from zero is defined as

$$SF_{A/B}(t) = \frac{C_a/C_b}{C_a^0/C_b^0}$$

where C_a and C_b are the concentrations of A and B, respectively, in the strip solution at a time t, and C_a^0 and C_b^0 are the concentrations of A and B, respectively, in the feed phase at $t = 0$ (Chen et al., 2018).

For continuous or semicontinuous systems, the separation factor is calculated according to the equation

$$SF_{A/B}(t) \frac{C_{a,\,s}/C_{b,\,s}}{C_{a,\,f}/C_{b,\,f}}$$

where $C_{a,\,s}$, $C_{b,\,s}$ are A and B concentrations in the strip phase at a time t and $C_{a,\,f}$, $C_{b,\,f}$ are the concentrations of A and B in the feed solution at a time t (Koros and Shimidzu, 1996). Separation factor at $t = 0$ equals 1 indicating that no species separation has occurred yet.

Value

Data frame with two variables: Time in the same units as provided data and SF with the separation factors at each time.

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

References

Q. B. Chen, Z. Y. Ji, J. Liu, Y. Y. Zhao, S. Z. Wang, J. S. Yuan, Development of recovering lithium from brines by selective-electrodialysis: Effect of coexisting cations on the migration of lithium, Journal of Membrane Science 548 (2018) 408-420. doi:10.1016/j.memsci.2017.11.040.505

J. Koros, H. Ma, T. Shimidzu, Terminology for membranes and membrane processes (iupac recommendations 1996), Pure and Applied Chemistry 68 (7) (1996) 1479-1489. doi:10.1351/pac199668071479.

Examples

```
data(seawaterLiNaK)
sepfactor(main = seawaterLiNaK$Lithium.1,
          secon = seawaterLiNaK$Sodium.1)
sepfactor(main = seawaterLiNaK$Lithium.1,
          secon = seawaterLiNaK$Potassium.1)
```

---

signal2conc   *Converts signals into concentration by using given model.*

Description

After a calibration model is established (either by using [calibCurve](#) or [calibPlane](#)), the function interpolates the signals of samples to get the associated concentrations.

Usage

```
signal2conc(signal, model, dilution = NULL, planar = FALSE, Conc.S = NULL)
```

Arguments

signal	Numeric vector of signals to be interpolated.
model	Regression model of the calibration. Must be obtained using [calibCurve](#) or [calibPlane](#).
dilution	Numeric vector of dilution factors applied to samples before measurement
planar	Logical, default to FALSE. It must be set to TRUE if more than one explanatory variable is used. A planar calibration model must be provided to model parameter.

Conc.S   Numeric vector of the concentrations of the interferent species to be considered
                when a planar calibration model is provided to model. It is taken into account if
                planar = TRUE.

Value

Numeric vector of species concentrations.

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

Examples

```
# A regression model is needed:
data(curvelithium)
model <- calibCurve(curve = curvelithium, order = 2)

signal <- c(0.395, 0.259, 0.188, 0.141, 0.110, 0.095, 0.084)
(conc <- signal2conc(signal = signal, model = model))
```

---

transPlot   *Plots transport profiles of single run experiments*

Description

Given the transport complete information of the interest species and, optionally, secondary and ter-
tiary species, the function plots transport profiles including (if given) non-linear regression models
that can be obtained using `transTrend`.

Usage

```
transPlot(trans, trend = NULL, secondary = NULL, tertiary = NULL,
  sec.trend = "spline", lin.secon = FALSE, span = 0.75, legend = FALSE,
  xlab = "Time (h)", ylab = expression(Phi), xlim = NULL, ylim = NULL,
  xbreaks = NULL, ybreaks = NULL, size = 2.8, bw = FALSE, srs = NULL,
  plot = TRUE)
```

Arguments

trans	Data frame with the complete transport information of interest species. Must be generated using `conc2frac`. This is the only non-optional parameter.
trend	Non-linear regression model of the main transport profile generated using `transTrend`.
secondary	Secondary species transport data frame (see `conc2frac`).
tertiary	Tertiaty species transport data frame (see `conc2frac`).

sec.trend	Type of trend line to be used for secondary and tertiary species data. Default is `'spline'` but `'linear'`, `'loess'` and `'logarithmic'` are also allowed.
lin.secon	Deprecated. Use `sec.trend = 'linear'` instead.
span	Amount of smoothing when `sec.tred = 'loess'`. Is a value between 0 and 1. Default is 0.75
legend	Logical. If `FALSE`, the default, the legend is not included.
xlab	Label to be used for x axis. Text and expression allowed.
ylab	Label to be used for y axis. Text and expression allowed.
xlim	Numeric vector of limits for X-axis.
ylim	Numeric vector of limits for X-axis.
xbreaks	Numeric vector of x-axis breaks.
ybreaks	Numeric vector of x-axis breaks.
size	Size used for points in the plot.
bw	Logical, if `FALSE`, the default, a color version of the plot is given. If a black and white version is required, it must be set to `TRUE`.
srs	Deprecated.
plot	Logical. If `TRUE`, the default, the plot is printed in the current graphical device.

Details

Most `transmem` graphical representations are made using the package `ggplot2` so the function returns a ggplot2 object that can be assigned to a variable for further modification.

This function has a version that uses replicated experiments and may be useful to illustrate repeate-ability. For more information see `transPlotWR`.

Value

Plot of the transport profile considering all provided species.

Author(s)

Cristhian Paredes, <craparedesca@unal.edu.co>

Eduardo Rodriguez de San Miguel, <erdsmg@unam.mx>

References

Wickham H (2016). ggplot2: Elegant Graphics for Data Analysis. Springer-Verlag New York. ISBN 978-3-319-24277-4, https://ggplot2.tidyverse.org.

Examples

```
data(seawaterLiNaK)
trend <- transTrend(trans = seawaterLiNaK$Lithium.1, model = 'paredes')
transPlot(trans = seawaterLiNaK$Lithium.1, trend = trend,
          secondary = seawaterLiNaK$Sodium.1,
          tertiary = seawaterLiNaK$Potassium.1)
transPlot(trans = seawaterLiNaK$Lithium.1, trend = trend,
          secondary = seawaterLiNaK$Sodium.1,
          tertiary = seawaterLiNaK$Potassium.1, bw = TRUE)
```

---

transPlotWR   *Plots transport profiles of replicated experiments*

Description

The function works the same way as `transPlot` but requires several experimental data sets that
must be concatenated in lists. This allows the process reproducibility to be evaluated in the analysis
of the results.

Usage

```
transPlotWR(trans, trend = NULL, secondary = NULL, tertiary = NULL,
  legend = FALSE, xlab = "Time (h)", ylab = expression(Phi),
  xlim = NULL, ylim = NULL, xbreaks = NULL, ybreaks = NULL,
  lin.secon = FALSE, sec.trend = "spline", span = 0.75,
  explicit = FALSE, size = 3, plot = TRUE, bw = FALSE, srs = NULL)
```

Arguments

trans	List of data frames with the complete transport information of interest species. Must be generated using `conc2frac`. This is the only non-optional parameter.
trend	List of Non-linear regression models of the main species transport profil. Generated using `transTrend`.
secondary	List of secondary species transport data frame (see `conc2frac`).
tertiary	List of tertiary species transport data frame (see `conc2frac`).
legend	Logical. If `FALSE`, the default, the legend is not included.
xlab	Label to be used for x axis. Text and expression allowed.
ylab	Label to be used for y axis. Text and expression allowed.
xlim	Numeric vector of limits for X-axis.
ylim	Numeric vector of limits for X-axis.
xbreaks	Numeric vector of x-axis breaks.
ybreaks	Numeric vector of x-axis breaks.
lin.secon	Deprecated. Use sec.trend = 'linear' instead.

sec.trend	Type of trend line to be used for secondary and tertiary species data. Default is `'spline'` but `'linear'`, `'loess'` and `'logarithmic'` are also allowed.
span	Amount of smoothing when `sec.tred = 'loess'`. Is a value between 0 and 1. Default is 0.75
explicit	Logical, if `FALSE`, the default, transport informations are averaged and plotted using errorbars that with the standard deviation values. If `TRUE`, all provided data is plotted in the same graphic.
size	Size used for points in the plot.
plot	Logical. If `TRUE`, the default, the plot is printed in the current graphical device.
bw	Logical, if `FALSE`, the default, a color version of the plot is given. If a black and white version is required, it must be set to `TRUE`.
srs	Deprecated.

Details

Most `transmem` graphical representations are made using the package `ggplot2` so the function returns a ggplot2 object that can be assigned to a variable for further modification.

Value

Plot of replicated transport profiles including all provided species

Author(s)

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References

Wickham H (2016). ggplot2: Elegant Graphics for Data Analysis. Springer-Verlag New York. ISBN 978-3-319-24277-4, <https://ggplot2.tidyverse.org>.

Examples

```
data(seawaterLiNaK)
# Transport data frames and transport NLS regresions must be in lists
lithium   <- list(seawaterLiNaK$Lithium.1, seawaterLiNaK$Lithium.2)
sodium    <- list(seawaterLiNaK$Sodium.1, seawaterLiNaK$Sodium.2)
potassium <- list(seawaterLiNaK$Potassium.1, seawaterLiNaK$Potassium.2)
trend     <- list(transTrend(trans = seawaterLiNaK$Lithium.1),
                  transTrend(trans = seawaterLiNaK$Lithium.2))

transPlotWR(trans = lithium, trend = trend, secondary = sodium,
            tertiary = potassium, bw = TRUE)
```

| transTrend | *Fits trend equations that model transport profiles* |

Description

Given a transport profile dataset, the results may be studied and compared in terms of empirical functions that describe the transport process in terms of regression parameters that can be asociated with the performance of the membrane system. The parameters are obtained by non-linear regression and are independent for each solution at both sides of the membrane. This is particularly useful when performing system optimizations since the parameters can be used as response variables depending on the optimization goal.

Usage

```
transTrend(trans, model = "paredes", eccen = 1)
```

Arguments

trans	Data frame with the complete transport information of interest species. Must be generated using [conc2frac](). This is the only non-optional parameter.
model	Model to be used in the regression. Default to `'paredes'` but `'rodriguez'` also allowed. See details.
eccen	Eccentricity factor (γ) for the model when `model` is set to `'paredes'`.

Details

Two empirical equations have been implemented in the function. In the `'rodriguez'` model (Rodriguez de San Miguel et al., 2014), the fractions (Φ) in feed or strip phases as a function of time (t) are fitted to

$$\Phi(t) = Ae^{-t/d} + y_0$$

where A, d and y_0 are the parameters to be found. In this model, parameter d determines the steepness of the species concentration change in time, y_0 reflects the limiting value to which the profiles tend to at long pertraction times and A is not supposed to play an important role in the transport description. The parameters of each phase are summarized in the functions G_{feed} and G_{strip} for the feed and strip phases:

$$G_{feed} = \frac{1}{y_0 d}, \qquad G_{strip} = \frac{y_0}{d}$$

The bigger each G function, the better the transport process.

In the `'paredes'` model (Paredes and Rodriguez de San Miguel, 2020), the transported fractions to the strip solution and from the feed solution are adjusted to the equations:

$$\Phi_s(t) = \frac{\alpha_s t^\gamma}{\beta_s^{-1} + t^\gamma}$$

$$\Phi_f(t) = 1 - \frac{\alpha_f t^\gamma}{\beta_f^{-1} + t^\gamma}$$

respectively. In those equations, adjustable parameters α and β relates the maximum fraction transported at long pertraction times and the steepness of the concentration change, respectively. γ is an excentricity factor to improve the adjustment and does not need to be changed for systems under similar conditions. The subscripts s and f means strip and feed phases, respectively.

The later model has the disadvantage over the former that the equation to use depends on the phase to be modeled but has the great advantage that if no significant accumulation is presented in the membrane, the parameters α and β should be quite similar for both phases and a consensus value can be obtained in various simple ways, while the other model yields quite diferent parameters for each phase. Paredes parameters are combined by using meta-analysis tools that consider the associated uncertainty of each one due to lack of fit to get summarized, lower-uncertainty results. Besides, once the γ parameter has been chosen, the later model uses only two parameters and while comparing models with similar performance, the simpler the better.

Value

A list of 4 or 5 components (depending on the model chosen) with the regression information for each phase, the eccentricity factor (only in Paredes model), the name of the model used, and the sumarized results of the regression: G_{feed} and G_{strip} values for the Rodriguez model or summarized α and β parameters with asocciated uncertainty for the Paredes model.

Author(s)

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References

E. Rodriguez de San Miguel, X. Vital, J. de Gyves, Cr(vi) transport via a sup ported ionic liquid membrane containing cyphos il101 as carrier: System analysis and optimization through experimental design strategies, Journal of Hazardous Materials 273 (2014) 253 - 262. doi:10.1016/j.jhazmat.2014.03.052.

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