# Package: transmem (via r-universe)

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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)

**URL** https://CRAN.R-project.org/package=transmem

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

**Encoding** UTF-8

**LazyData** true

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**Depends** R (>= 3.5.0)

**Imports** cmna, ggformula, ggplot2, plot3D

**Suggests** knitr, rmarkdown

**Repository** https://crparedes.r-universe.dev

**RemoteUrl** https://github.com/crparedes/transmem

**RemoteRef** HEAD

**RemoteSha** 3d97a86e27b108b01d3e78c97e6d27a34642210f

# Contents

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.

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| 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](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* |
|---|---|

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## 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)

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

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 tertiary 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 repeateability. 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](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](conc2frac). This is the only non-optional parameter. |
| trend | List of Non-linear regression models of the main species transport profil. Generated using [transTrend](transTrend). |
| secondary | List of secondary species transport data frame (see [conc2frac](conc2frac)). |
| tertiary | List of tertiary species transport data frame (see [conc2frac](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)

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)
# 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 ($\gamma$) 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 ($\Phi$) 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 $\alpha$ and $\beta$ relates the maximum fraction transported at long pertraction times and the steepness of the concentration change, respectively. $\gamma$ 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 $\alpha$ and $\beta$ 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 $\gamma$ 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 $\alpha$ and $\beta$ parameters with asocciated uncertainty for the Paredes model.

### Author(s)

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

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

### 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.

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.

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