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Type Package

Title Master Curve Estimates Corresponding to Time-Temperature Superposition

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Depends R (>= 3.0.1), mgcv, sfsmisc, splines

Description Time-Temperature Superposition analysis is often applied to frequency modulated data obtained by Dynamic Mechanic Analysis (DMA) and Rheometry in the analytical chemistry and physics areas. These techniques provide estimates of material mechanical properties (such as moduli) at different temperatures in a wider range of time. This package provides the Time-Temperature superposition Master Curve at a referred temperature by the three methods: the two wider used methods, Arrhenius based methods and WLF, and the newer methodology based on derivatives procedure. The Master Curve is smoothed by B-splines basis. The package output is composed of plots of experimental data, horizontal and vertical shifts, TTS data, and TTS data fitted using B-splines with bootstrap confidence intervals.

License GPL (>= 2)

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Contents

TTS-package *Estimates of material properties by Time-Temperature Superposition (TTS) analysis*

Description

TTS analysis is often applied to frequency modulated data obtained by Dynamic Mechanic Analysis (DMA) and Rheometry in the analytical chemistry and physics areas. These techniques provide estimates of material mechanical properties (such as moduli) at different temperatures in a wider range of time. This package provides the Time-Temperature superposition Master Curve at a referred temperature by the three methods: the two wider used methods, Arrhenius based methods and WLF, and the newer methodology based on derivatives procedure. The Master Curve is smoothed by B-splines basis. The package output is composed of plots of experimental data, horizontal and vertical shifts, TTS data, and TTS data fitted using B-splines with bootstrap confidence intervals.

Details

Package:	TTS
Type:	Package
Version:	1.1
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The main functions and data frame are `TTS`, `TTS_10`,`PLOT.TTS`, `Epoxy`,`SBS`, and `PC`

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References

Naya, S., Meneses A., Tarrio-Saavedra, J., Artiaga R., Lopez-Beceiro, J. and Gracia-Fernandez C. (2013) New method for estimating shift factors in time-temperatura superposition models. Journal of Thermal Analysis and Calorimetry. ISSN 1388-6150. DOI 10.1007/s10973-013-3193-1.

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Zou, J., You F., Su L., Yang Z., Chen G. and Guo S. (2011). Failure Mechanism of Time-Temperature Superposition for Poly(vinyl chloride)/Dioctylphthalate (100/70) System. DOI 10.1002/app.35113.

Ferry J.D. (1980) Viscoelastic Properties of Polymers, Wiley: New York.

Artiaga R., Garcia A. Fundamentals of DMA. In: 'Thermal analysis. Fundamentals and applications to material characterization' (ed.: Artiaga R.) Publicaciones de la Universidade da Coruna, A Coruna, Spain, 183-206 (2005).

Chartoff R.P., Menczel J.D., Dillman S.H. Dynamic mechanical analysis (DMA). In: 'Thermal analysis of polymers. Fundamentals and applications' (eds.: Menczel J.D., Prime R.B.) Wiley, San Jose, 387-496 (2009).

Epoxy — *Dataset obtained from creep tests of an epoxy based composite by using Dynamic Mechanical Thermal Analysis (DMTA)*

Description

Epoxy is a dataset composed of 273 rows and 3 columns that describes the performance of an epoxy resin based composite in a creep type test. This type of laboratory experimental procedure is defined by the application of a constant stress, σ, and the measuring of the strain, $\varepsilon(t)$, or compliance, $J(t) = \varepsilon(t)/\sigma$ (in the present case) as the response variable. The experimental tests are made by Dynamic Mechanical Thermal Analysis (DMTA) technique, using a 3 point bending configuration with the following features: Clamp, 3-Point Bending; Geometry, Rectangular; Size: length of 20 mm, width of 5.55 mm, and thickness of about 0.85 mm.

Format

This data frame is composed of the following columns:

Log10_time It accounts for 39 different times from 2 s to 3599 s, in logarithmic scale for each one of the 7 studied temperatures (overall 273 observations).

Log10_Compliance It accounts for 39 different values for the compliance, J (MPa-1), for each one of the 7 studied temperatures, in base-ten logarithmic scale.

Temperature It is the variable that shows the temperature at which the measurements of compliance are experimentally obtained, namely 30, 40, 50, 60, 70, 80, and 90 Celsius degrees.

Details

The dataset includes the measurements of the compliance property depending on the time and corresponding to different specimens of an epoxy resin based composite. All the observations were obtained by the application of the DMTA experimental technique. The application of the TTS principle to creep tests is becoming more and more common. Creep test provides information about the deformation of a material subjected to a constant load. This test is in accordance with many real applications such as the performance of shoe insoles, structural materials, asphalt, etc. In this framework, TTS provides the degree of the deformation of the material at an extended range of times, when this material is subjected to a constant load. Therefore, TTS is becoming increasingly useful in studies of material degradation and lifetime estimation. The use of the TTS principle with creep tests usually provides smoother master curves since each curve is usually defined by a larger number of experimental observations than, for example, modulus curves as a function of frequency.

Source

Janeiro-Arocas, J., Tarrío-Saavedra, J., López-Beceiro, J., Naya, S., López-Canosa, A., Heredia-García, N., and Artiaga, R. (2016). Creep analysis of silicone for podiatry applications. Journal of the Mechanical Behavior of Biomedical Materials, 63, 456-469. DOI 10.1016/j.jmbbm.2016.07.014.

Naya, S., Meneses A,. Tarrio-Saavedra, J,. Artiaga R., Lopez-Beceiro, J. and Gracia-Fernandez C. (2013) New method for estimating shift factors in time-temperatura superposition models. Journal of Thermal Analysis and Calorimetry. ISSN 1388-6150. DOI 10.1007/s10973-013-3193-1.

Examples

```
data(Epoxy)
```

`PC` *Dataset obtained from polycarbonate (polymer) tests using Dynamic Mechanical Analysis (DMA)*

Description

PC contains 49 rows and 3 columns.

Format

This data frame is composed of the following columns:

A data frame with 49 observations on the following 3 variables:

log10.frequency It accounts for seven different frequencies (rad/s) in logarithmic scale for each temperature (overall 49).

log10.module It accounts for seven different storage modulus, E' (Pa), in base-ten logarithmic scale for each temperature (overall 49).

temperature Seven different temperatures: 147, 148, 149, 150, 151, 152, 153 degrees celsius, each one with the corresponding seven values of frequency and storage modulus (overall 49).

Details

The dataset corresponds to the storage modulus viscoelastic property of different specimens of polycarbonate (PC) and obtained by DMA using TA Instruments Q800 (Naya et al., 2013).

Source

Naya, S., Meneses A,. Tarrio-Saavedra, J,. Artiaga R., Lopez-Beceiro, J. and Gracia-Fernandez C. (2013) New method for estimating shift factors in time-temperatura superposition models. Journal of Thermal Analysis and Calorimetry. ISSN 1388-6150. DOI 10.1007/s10973-013-3193-1.

Examples

```
data(PC)
```

PLOT.TTS *Time-Temperature Superposition (TTS) plots*

Description

Plots of TTS results: experimental data, horizontal and vertical shifts, TTS data, TTS Master Curve fitting with B-Splines and bootstrap confidence intervals are deployed.

Usage

```
PLOT.TTS(x)
```

Arguments

`x`	TTS object.

Details

TTS plots are performed from the outputs of TTS function: data, aT, bT, TTS.data, TTS.gam y residuals.

Value

The following values are returned:

`PLOT.data()`	Generic function to plot the experimental data. By default log10.module versus log10.frequency.
`PLOT.aT()`	Generic plot of the horizontal shifts corresponding to each curve (modulus versus frequency) obtained on temperature.
`PLOT.bT()`	Generic plot of the vertical shifts corresponding to each curve (modulus versus frequency) obtained on temperature.

`PLOT.TTS.data()`
: Generic plot of the experimental data horizontally and vertically shifted with respect to a the curve corresponding to the reference temperature.

`PLOT.TTS.gam()`
: Generic plot of the Master Curve B-splines estimation with bootstrap confidence intervals at 95 per cent.

`PLOT.res()`
: Generic plot of the residuals of Master Curve B-splines fitting.

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References

Naya, S., Meneses A., Tarrio-Saavedra, J., Artiaga R., Lopez-Beceiro, J. and Gracia-Fernandez C. (2013) New method for estimating shift factors in time-temperatura superposition models. Journal of Thermal Analysis and Calorimetry. ISSN 1388-6150. DOI 10.1007/s10973-013-3193-1.

Williams, M. L. (1964) Structural analysis of Viscoelastic materials. AIAA Journal, 785-808.

Artiaga R., Garcia A. Fundamentals of DMA. In: 'Thermal analysis. Fundamentals and applications to material characterization' (ed.: Artiaga R.) Publicaciones de la Universidade da Coruna, A Coruna, Spain, 183-206 (2005).

Examples

```
## TTS object applied to PC dataset.
data(PC)
Derive <- TTS(PC)
x <- Derive
## Generic plots for TTS analysis
PLOT <- PLOT.TTS(x)
names(PLOT)
##[1] "PLOT.data"     "PLOT.aT"       "PLOT.bT"       "PLOT.TTS.data"
##[5] "PLOT.TTS.gam"  "PLOT.res"
## Generic plots of: data, aT, bT, TTS.data, TTS.gam and res
PLOT$PLOT.data(main="PLOT: Data",xlab="log10.Frequency (rad/s)",ylab="log10.E'(Pa)")
PLOT$PLOT.aT(main="PLOT: horizontal translation factors", xlab="Temperature", ylab="aT")
PLOT$PLOT.bT(main="PLOT: vertical translation factors", xlab="Temperature",ylab="bT")
PLOT$PLOT.TTS.data(xlab="log10.Frequency (rad/s)",ylab="log10.E'(Pa)")
PLOT$PLOT.TTS.gam( xlab="log10.Frequency (rad/s)", ylab = "log10.E'(Pa)",
main = "Fitted gam, Bootstrap confidence intervals",
sub = "Reference temperature = 150 degrees celsius")
PLOT$PLOT.res(main="TTS: gam residual", xlab="Fitted", ylab="Standardized residuals")
```

SBS — *Dataset obtained from creep tests of styrene-butadiene-styrene (SBS) composite by using Dynamic Mechanical Thermal Analysis (DMTA)*

Description

SBS is a dataset composed of 195 rows and 3 columns that describes the performance in the framework of a creep test of a styrene-butadiene-styrene (SBS) composite. The creep tests are defined by the application of a constant stress, σ, and the measuring of the strain, $\varepsilon(t)$, or compliance, $J(t) = \varepsilon(t)/\sigma$ (in the present case), as the response variable. The experimental tests are made by Dynamic Mechanical Thermal Analysis (DMTA) technique, using a 3 point bending configuration with the following features: Clamp, 3-Point Bending; Geometry, Rectangular; Size: length of 20 mm, width of 5.54 mm, and thickness of about 3.87 mmm.

Format

This data frame is composed of the following columns:

Log10_time It accounts for 39 different times from 2 s to 3600 s, in logarithmic scale for each one of the 5 studied temperatures (overall 195 observations).

Log10_Compliance It accounts for 39 different values for the compliance, J (MPa-1), for each one of the 5 studied temperatures, in base-ten logarithmic scale.

Temperature It is the variable that shows the temperature at which the measurements of compliance are experimentally obtained, namely 40, 50, 60, 70, and 80 Celsius degrees.

Details

The dataset corresponds to the measure of the compliance property (with respect to the time) of different specimens of a SBS composite. The measurements were obtained by DMTA experimental technique.

The application of the TTS principle to creep tests is becoming more and more common. Creep test provides information about the deformation of a material subjected to a constant load. This test is in accordance with many real applications such as the performance of shoe insoles, structural materials, asphalt, etc. In this framework, TTS provides the degree of the deformation of the material at an extended range of times, when this material is subjected to a constant load. Therefore, TTS is becoming increasingly useful in studies of material degradation and lifetime estimation. The use of the TTS principle with creep tests usually provides smoother master curves since each curve is usually defined by a larger number of experimental observations than, for example, modulus curves as a function of frequency.

Source

Janeiro-Arocas, J., Tarrío-Saavedra, J., López-Beceiro, J., Naya, S., López-Canosa, A., Heredia-García, N., and Artiaga, R. (2016). Creep analysis of silicone for podiatry applications. Journal of the Mechanical Behavior of Biomedical Materials, 63, 456-469. DOI 10.1016/j.jmbbm.2016.07.014.

Naya, S., Meneses A,. Tarrio-Saavedra, J,. Artiaga R., Lopez-Beceiro, J. and Gracia-Fernandez C. (2013) New method for estimating shift factors in time-temperatura superposition models. Journal of Thermal Analysis and Calorimetry. ISSN 1388-6150. DOI 10.1007/s10973-013-3193-1.

Examples

```
data(SBS)
```

TTS *Time-Temperature Superposition (TTS) analysis*

Description

The Master Curve at a specific temperature is estimated using Time-Temperature Superposition (TTS) procedures. The Master Curve means the variation of a specific viscoelastic property of the selected material depending on time or frequency. TTS procedures provide the viscoelastic property variation at the selected temperature in a wider interval of time or frequency than in the experimental case. The Master Curve is estimated for each selected reference temperaure using TTS procedures. Three TTS methodologies are implemented in this package: the two wider used methods, Arrhenius based methods and WLF, and the newer methodology based on derivatives procedure. The Master Curve is smoothed by B-splines basis.

Usage

```
TTS(
  x,
  reference.temperature = 150,
  n = 100,
  nB = 100,
  method = c("derived", "WLF", "Arrhenius")
)
```

Arguments

`x` Matrix or data frame composed of three columns: a numeric column vector with the experimental frequencies (in logarithmic scale, base-ten), the modulus (E' or G') base-ten logarithm vector and, finally the corresponding temperatures vector.

`reference.temperature` Value of the selected reference temperatura at which the Master Curve of modulus will be obtained, the default value of temperature is 150.

`n` Number of partitions in the frequency domain in order to fit the B-spline basis. The default value is 100.

`nB` Number of bootstrap replicates to estimate confidence intervals of master curve fitting. The default is 100.

`method` A string vector composed of one of the following options: "derived" (by default), "WLF" and "Arrhenius".

Details

El New method for estimating shift factors in time-temperatura superposition models (Naya et al., 2013) opens the possibility to perform the TTS function. The horizontal and vertical shifts are calculated. Namely, the different methods are differenciated due to the expression for estimating the horizontal shifts, aT. The "derivated" method is based on the application of horizontal shifts to the moduli derivatives (depending on the frequency) and thus obtaining the Master Curve at the selected temperature:

(dE')/dx(x+aT) -> (dE')/dx(x)

WLF method is defined by the parametric expression:

Log10(aT)=-C1*(T-To)/(C2+(T-To))

Where C1 and C2 are constants to be estimated, T is the temperature and To the reference temperature.

Arrhenius method is defined by the parametric expression:

Log10(aT)=Ea*((1/T)-(1/To))*log10(2.718282)/R

Where Ea is the activation energy, R = 8.314 J/mol is the universal gas constant, T is the absolute temperature (Kelvin degrees), and To the reference temperature (Celsius degrees).

The vertical shifts, bT, are calculated taking into account the vertical distance between the moduli curves.

Value

The function returns a list composed of the following outputs:

`data`	Input experimental data.
`aT`	Numerical vector of horizontal shifts between the modulus curves.
`bT`	Numerical vector of vertical shifts between the modulus curves.
`TTS.data`	Master Curve Data frame defined by three columns: log10frequency, log10module and temperature.
`ref.temp`	Reference temperature value.
`TTS.gam`	Data frame of the Generalized Additive Model with B-splines (GAM) estimate of the Master Curve. It contains two columns: frequency and Prediction.
`I.lower`	Lower limit of bootstrap confidence interval corresponding to the estimated B-splines Master Curve.
`I.upper`	Upper limit of bootstrap confidence interval corresponding to the estimated B-splines Master Curve.
`residuals`	Residuals corresponding to the GAM with B-splines Master Curve fitting.

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References

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Artiaga R., Garcia A. Fundamentals of DMA. In: 'Thermal analysis. Fundamentals and applications to material characterization' (ed.: Artiaga R.) Publicaciones de la Universidade da Coruna, A Coruna, Spain, 183-206 (2005).

Examples

```
## Polycarbonate dataset
data(PC)
x=PC
## TTS function applied to polycarbonate.
derive=TTS(x,reference.temperature=150, method=c("derived","WLF","Arrhenius"))
names(derive)
##[1] "data"      "aT"        "bT"        "TTS.data"  "ref.temp"  "TTS.gam"
##[7] "I.lower"   "I.upper"   "residuals"
## Horizontal shifts vector of modulus versus frequency curves.
derive$aT
## Reference temperature
derive$ref.temp
```

`TTS_10` *Time-Temperature Superposition (TTS) analysis*

Description

This function provides an estimate of the Master Curve in a similar way to the TTS function, with the difference that, in this case, a thin plate spline fit is performed (instead the B-splines smoothing), within the framework of the application of generalized additive models (GAM), as implemented in the mgcv package.

Usage

```
TTS_10(
  x,
  reference.temperature = 40,
  n = 100,
  nB = 100,
  method = c("derived", "WLF", "Arrhenius")
)
```

Arguments

`x` Matrix or data frame composed of three columns: a numeric column vector with the experimental frequencies (in logarithmic scale, base-ten), the response variable (E' or G' modulus, compliance, etc.) base-ten logarithm vector and, finally the corresponding temperatures vector.

`reference.temperature` Value of the selected reference temperature at which the Master Curve of the response variable (E' or G' modulus, compliance, etc.) will be obtained, the default value of temperature is 40.

`n` Number of partitions in the frequency domain in order to fit the B-spline basis. The default value is 100.

`nB` Number of bootstrap replicates to estimate confidence intervals of Master Curve fitting. The default is 100.

`method` A string vector composed of one of the following options: "derived" (by default), "WLF" and "Arrhenius".

Value

The function returns a list composed of the following outputs:

`data` Input experimental data.

`aT` Numerical vector of horizontal shifts between the modulus curves.

`bT` Numerical vector of vertical shifts between the modulus curves.

`TTS.data` Master Curve Data frame defined by three columns: Log10_time, Log10_Compliance and Temperature.

`ref.temp` Reference temperature value.

`TTS.gam` Data frame of the Generalized Additive Model with B-splines (GAM) estimate of the Master Curve. It contains two columns: time and Prediction.

`I.lower` Lower limit of bootstrap confidence interval corresponding to the estimated B-splines Master Curve.

`I.upper` Upper limit of bootstrap confidence interval corresponding to the estimated B-splines Master Curve.

`residuals` Residuals corresponding to the GAM with B-splines Master Curve fitting.

Author(s)

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References

Naya, S., Meneses A., Tarrio-Saavedra, J., Artiaga R., Lopez-Beceiro, J. and Gracia-Fernandez C. (2013) New method for estimating shift factors in time-temperatura superposition models. Journal of Thermal Analysis and Calorimetry. ISSN 1388-6150. DOI 10.1007/s10973-013-3193-1.

Williams, M. L. (1964) Structural analysis of Viscoelastic materials. AIAA Journal, 785-808.

Artiaga R., Garcia A. Fundamentals of DMA. In: 'Thermal analysis. Fundamentals and applications to material characterization' (ed.: Artiaga R.) Publicaciones de la Universidade da Coruna, A Coruna, Spain, 183-206 (2005).

Wood, S.N. (2017) Generalized Additive Models: An Introduction with R (2nd edition). Chapman and Hall/CRC.

Examples

```
## Epoxy
data(Epoxy)
x=Epoxy
## TTS_10 function applied to Epoxy.
Q=TTS_10(x,reference.temperature=40, method=c("derived","WLF","Arrhenius"))
names(Q)
## Horizontal shifts vector of compliance versus time curves.
Q$aT
## Reference temperature
Q$ref.temp
PLOT <- PLOT.TTS(Q)
## Generic plots of: data, aT, bT, TTS.data and TTS.gam
PLOT$PLOT.data(main="PLOT: Data",xlab="Log_time",
ylab="Log_Compliance")
PLOT$PLOT.aT(main="PLOT: horizontal shift factors",
xlab="Temperature", ylab="aT")
PLOT$PLOT.bT(main="PLOT: vertical shift factors",
xlab="Temperature",ylab="bT")
PLOT$PLOT.TTS.data(xlab="Log_time",
ylab="Log_Compliance")
PLOT$PLOT.TTS.gam( xlab="Log_time",
ylab="Log_Compliance",
main = "Fitted gam, Bootstrap confidence intervals",
sub = "Reference temperature = 40 Celsius degrees")
```

Index