Package 'LeafGasExchange'

April 14, 2020

Title Modeling photosynthesis at the leaf level

Version 0.0.0.9000

Description Model gas exchanges at the leaf level using a coupled stomatal conductance model (USO) and photosynthesis model (Farquhar) using an analytical solution of the different equations. This package also gathers functions to import data from LICORS 6400 and 6800, fit and display the main types of curves obtained with a gas exchange device: AQ, Aci, Mcurves and simulate data.

License What license it uses

Encoding UTF-8

LazyData true

RoxygenNote 7.1.0

Depends stats4, bbmle, readxl, stringr, tidyverse, readr, tkrplot

Imports stats4, bbmle, readxl, stringr, tidyverse, readr, tkrplot

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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R topics documented:

`f.A` *Coupled conductance photosynthesis model*

Description

Coupled conductance photosynthesis model

Usage

```
f.A(
  PFD,
  cs,
  Tleaf,
  Tair,
  RH,
 param = list(R = 8.314, O2 = 210, TRef = 298.16, Patm = 101, JmaxRef = 160, JmaxHa =
   50300, JmaxHd = 152044, JmaxS = 495, VcmaxRef = 120, VcmaxHa = 73637, VcmaxHd =
  149252, VcmaxS = 486, RdRef = 1, RdHa = 46390, KcRef = 404.9, KcHa = 79430, KoRef =
   278.4, KoHa = 36380, GstarRef = 42.75, GstarHa = 37830, abso = 0.85, f = 0.15,
    LogitTheta = f.logit(0.85), g0 = 0.01, g1 = 2)
)
```

Arguments

`PFD`	Photo Flux Density in micromol.m-2,s-1
`cs`	CO2 at the surface of the leaf in ppm
`Tleaf`	Temperature of the leaf in Kelvin
`Tair`	Temperature of the air in Kelvin
`RH`	Relative Humidity of the air, from 0 to 100
`param`	List of parameters, see f.make.param for details

Value

List of different variables: - A: Raw assimilation of the leaf in micromol.m-2.s-1 - gs: Conductance of the leaf for water vapour - ci: Intracellular CO2 concentration in micromol.mol-1 - ds: Leaf surface to air vapour pressure deficit in Pa

Examples

```
f.A(PFD=2000,cs=400,Tleaf=273.16+29,Tair=273.16+28,RH=70)
```

f.Aci *Photosynthesis model*

Description

Calculate the assimilation according to Farquhar equations. Contrary to f.A, this function uses intracellular CO2 and not ambiant air CO2

Usage

```
f.Aci(
  PFD,
  ci,
  Tleaf,
 param = list(R = 8.314, O2 = 210, TRef = 298.16, Patm = 101, JmaxRef = 160, JmaxHa =
   50300, JmaxHd = 152044, JmaxS = 495, VcmaxRef = 120, VcmaxHa = 73637, VcmaxHd =
  149252, VcmaxS = 486, RdRef = 1, RdHa = 46390, KcRef = 404.9, KcHa = 79430, KoRef =
   278.4, KoHa = 36380, GstarRef = 42.75, GstarHa = 37830, abso = 0.85, f = 0.15,
    LogitTheta = f.logit(0.85))
)
```

Arguments

PFD	Photo Flux Density in micromol.m-2,s-1
ci	Leaf intracellular CO2 in ppm
Tleaf	Temperature of the leaf in Kelvin
param	List of parameters, see f.make.param for details

Value

Assimilation in micromol.m-2.s-1

Examples

```
ci=seq(1,1500,10)
plot(x=ci,y=f.Aci(PFD=2000,ci=ci,Tleaf=300))
```

f.arrhenius *Temperature dependence of Gamma star, Ko, Kc and Rd*

Description

Temperature dependence of Gamma star, Ko, Kc and Rd

Usage

```
f.arrhenius(PRef, Ha, Tleaf, TRef = 298.16, R = 8.314)
```

Arguments

PRef	Value of the parameter at the reference temperature
Ha	Enthalpie of activation in J.mol-1
Tleaf	Temperature of the leaf in Kelvin
TRef	Reference temperature
R	Ideal gas constant

Value

Value of the parameter at the temperature of the leaf

References

VON CAEMMERER, S. (2013), Steady-state models of photosynthesis. Plant Cell Environ, 36: 1617-1630. doi:10.1111/pce.12098 Bernacchi, C.J., Singsaas, E.L., Pimentel, C., Portis Jr, A.R. and Long, S.P. (2001), Improved temperature response functions for models of Rubisco-limited photosynthesis. Plant, Cell & Environment, 24: 253-259. doi:10.1111/j.1365-3040.2001.00668.x

Examples

```
plot(x=seq(25,35,0.1),y=f.arrhenius(PRef=1,Ha=46390,Tleaf=seq(273.15+25,273.15+35,0.1),R=8.314),xlab='Tempe
```

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f.arrhenius.inv *Temperature dependence of Gamma star, Ko, Kc and Rd*

Description

Temperature dependence of Gamma star, Ko, Kc and Rd

Usage

```
f.arrhenius.inv(P, Ha, Tleaf, TRef = 298.16, R = 8.314)
```

Arguments

P	Value of the parameter at Tleaf
Ha	Enthalpie of activation in J.mol-1
Tleaf	Temperature of the leaf in Kelvin
TRef	Reference temperature
R	Ideal gas constant

Details

Retrieve the value of the parameter at Tref knowing its value at Tleaf

f.AWc *Carbon assimilation under rubisco carboxylation limitation*

Description

Carbon assimilation under rubisco carboxylation limitation

Usage

```
f.AWc(
  ci,
  Tleaf,
 param = list(ci, Tleaf, RdHa, GstarRef, GstarHa, RdRef, VcmaxRef, VcmaxHa, VcmaxHd,
    VcmaxS, KoRef, KoHa, KcRef, KcHa)
)
```

Arguments

Tleaf	Temperature of the leaf in Kelvin
param	List of parameters, see f.make.param for details

Examples

```
plot(x=seq(1,1500,10),y=f.AWc(ci=seq(1,1500,10),Tleaf=300,param=f.make.param()),xlab='Intracellular CO2 in p
```

f.AWj *Carbon assimilation under electron transport limitation*

Description

Carbon assimilation under electron transport limitation

Usage

```
f.AWj(
  PFD,
  ci,
  Tleaf,
 param = list(RdHa, GstarRef, GstarHa, JmaxHa, JmaxHd, JmaxS, JmaxRef, RdRef, abso, f,
    LogitTheta)
)
```

Arguments

PFD	Photo Flux Density in micromol.m-2,s-1
Tleaf	Temperature of the leaf in Kelvin
param	List of parameters, see f.make.param for details

Value

Assimilation under Jmax limitation

Examples

```
plot(x=seq(0,1500,10),y=f.AWj(PFD=seq(0,1500,10),ci=270,Tleaf=300,param=f.make.param()),xlab='PFD',ylab='Aw
```

`f.ci.treshold` *Intracellular CO2 threshold between electron transport and carboxylation limitations*

Description

Intracellular CO2 threshold between electron transport and carboxylation limitations

Usage

```
f.ci.treshold(
  PFD,
  Tleaf,
 param = list(GstarRef, GstarHa, KoRef, KoHa, KcRef, KcHa, VcmaxHa, VcmaxHd, VcmaxS,
    JmaxHa, JmaxHd, JmaxS, VcmaxRef, JmaxRef, abso, f, LogitTheta)
)
```

Arguments

`PFD`	Photo Flux Density in micromol.m-2,s-1
`Tleaf`	Temperature of the leaf in Kelvin
`param`	List of parameters, see f.make.param for details

Value

Intracellular CO2 such as Wc==Wj

Examples

```
f.ci.treshold(PFD=2000,Tleaf=300,param=f.make.param(VcmaxRef=60,JmaxRef=85))
f.ci.treshold(PFD=2000,Tleaf=300,param=f.make.param(VcmaxRef=70,JmaxRef=85))
```

f.CO2.fitting *Fitting function for Aci data*

Description

Function to fit f.Aci model to data. The parameters to fit have to be described in the list Start. All the other parameters of the f.Aci functions have to be in param. If the parameters from Start are repeated in param, the later one will be ignored. This function uses two methods to fit the data. First by minimizing the residual sum-of-squares of the residuals and then by maximizing the likelihood function. The first method is more robust but the second one allows to calculate the confident interval of the parameters.

Usage

```
f.CO2.fitting(
  measures,
  id.name = NULL,
  Start = list(JmaxRef = 90, VcmaxRef = 70, RdRef = 1),
  param = f.make.param(),
  modify.init = TRUE
)
```

Arguments

measures	Data frame of measures obtained from gas exchange analyser with at least the columns Photo, Ci, PARi and Tleaf (in K)
id.name	Name of the colums in measures with the identifier for the curve.
Start	List of parameters to fit with their initial values.
param	See f.make.param() for details.
modify.init	TRUE or FALSE, allows to modify the Start values before fitting the data

Examples

```
##Simulation of a CO2 curve
data=data.frame(Tleaf=rep(300,20),
Ci=seq(40,1500,75),PARi=rep(2000,20),Photo=f.Aci(PFD=2000,Tleaf=300,ci=seq(40,1500,75),
param=f.make.param(RdRef=1.25,VcmaxRef=57,JmaxRef=92))+rnorm(n = 20,mean = 0,sd = 0.5))

f.CO2.fitting(measures=data,id.name=NULL,Start=list(JmaxRef=90,VcmaxRef=70,RdRef=1))
```

f.ds *Leaf water vapour pressure deficit calculation*

Description

This function calculates the leaf water pressure deficit (VPDl or Ds) using the temperature of the leaf, the temperature of the air and its relative humidity

Usage

```
f.ds(Tleaf, Tair, RH)
```

Arguments

Tleaf	Temperature of the leaf in Kelvin
Tair	Temperature of the air in Kelvin
RH	Humidity of the air (0 to 100)

Value

Ds in Pascal

Examples

```
f.ds(Tleaf=273.16 + 30, Tair=273.16+28, RH=70)
```

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f.gs *USO model for stomatal conductance to water vapour*

Description

Semi-empirical model of the leaf conductance to water vapour

Usage

```
f.gs(A, cs, ds, g0, g1, Rd)
```

Arguments

A	Raw assimilation in micromol.m-2.s-1, i-e, the assimilation in presence of respiration
cs	CO2 at the surface of the leaf in ppm
ds	Leaf surface to air vapour pressure deficit in Pa
g0	Constant of the USO model, representing the conductance when A is 0, in mol.m-2.s-1
g1	Slope parameter, between 1.14 and 3.58 KPa^0.5 (Wu et al., 2019)
Rd	Respiration rate in micromol.m-2.s-1

Value

This function returns the optimal stomatal conductance to water vapour in mol.m-2.s-1

References

Medlyn, B.E., Duursma, R.A., Eamus, D., Ellsworth, D.S., Colin Prentice, I., Barton, C.V.M., Crous, K.Y., de Angelis, P., Freeman, M. and Wingate, L. (2012), Reconciling the optimal and empirical approaches to modelling stomatal conductance. Glob Change Biol, 18: 3476-3476. doi:10.1111/j.1365-2486.2012.02790.x Wu, J, Serbin, SP, Ely, KS, et al. The response of stomatal conductance to seasonal drought in tropical forests. Glob Change Biol. 2020; 26: 823– 839. https://doi.org/10.1111/gcb.14820

Examples

```
gs=f.gs(A=30,cs=400,ds=1500,g0=0.01,g1=2,Rd=1)
```

`f.import_licor6400` *Import Licor 6400 file*

Description

This functions allows to import the text file produced by LICOR as a data.frame

Usage

```
f.import_licor6400(
  file,
  column_display = c("Photo", "Cond", "PARi", "Ci", "Leaf_Barcode", "Species",
    "Tree Canopy", "Age", "file")
)
```

Arguments

`file`	File to import by the function
`column_display`	The first lines of the file which are part of this list are displayed by this function after being imported.

Value

dataframe

References

Adapted from http://www.ericrscott.com/2018/01/17/li-cor-wrangling/

`f.import_licor6800` *Import Licor 6800 excel file*

Description

This functions allows to import the excel file produced by LICOR as a data.frame. The files have to be open in Excel and saved before using his function so the result of the formula are calculated. The formula are sotred into the Excel file but not computed until the file is open.

Usage

```
f.import_licor6800(
  file,
  column_display = c("A", "gsw", "Qin", "Ci", "Species", "Canopy", "Pheno_Age",
    "Barcode", "file")
)
```

Arguments

file	File to import by the function
column_display	The first lines of the file which are part of this list are displayed by this function after being imported.

Value

dataframe

References

Adapted from http://www.ericrscott.com/2018/01/17/li-cor-wrangling/

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f.light.fitting *Fitting function for AQ data*

Description

Fitting function for AQ data

Usage

```
f.light.fitting(
  measures,
  id.name = NULL,
  Start = list(JmaxRef = 90, LogitTheta = 0.6, RdRef = 1),
  param = f.make.param(),
  modify.init = TRUE
)
```

Arguments

measures	Data frame of measures obtained from gas exchange analyser with at least the columns Photo, Ci, PARi and Tleaf (in K)
id.name	Name of the colums in measures with the identifier for the curve.
Start	List of parameters to fit with their initial values.
param	See f.make.param() for details.
modify.init	TRUE or FALSE, allows to modify the Start values before fitting the data

Examples

```
data=data.frame(Tleaf=300,Ci=280,PARi=seq(0,2000,67),Photo=f.AWj(PFD=seq(0,2000,67),Tleaf=300,ci=280,param=
Start=list(JmaxRef=50,LogitTheta=f.logit(0.8),RdRef=0.5)
f.light.fitting(measures=data,Start=Start)
```

f.logistic *Logistic function*

Description

This function takes it values in -Inf;+Inf and returns values in 0;1. It is the inverse function of f.logit, ie f.logistic(logit(x))=x

Usage

```
f.logistic(x)
```

Details

f.logistic(x)=1/(1+exp(-x)) if x<0, = exp(x)/(1+exp(x)) if x<=0

Examples

```
plot(x=seq(-10,10,0.1),y=f.logistic(x=seq(-10,10,0.1)))
```

f.logit *Function logit*

Description

This function takes it values in 0;1- and returns values in Inf;+Inf. It is the inverse function of f.logistic

Usage

```
f.logit(x)
```

Examples

```
plot(x=seq(0,1,0.01),y=f.logit(x=seq(0,1,0.01)))
```

f.make.param *Photosynthesis and stomata model parameters*

Description

Function to create a list of parameters to be used in f.A, f.Aci, f.AWc and f.AWj function. Depending on the function, all the parameters are not used. For example go and g1 are not used in f.Aci

Usage

```
f.make.param(
  R = 8.314,
  O2 = 210,
  TRef = 298.16,
  Patm = 101,
  JmaxRef = 85,
  JmaxHa = 50300,
  JmaxHd = 152044,
  JmaxS = 495,
  VcmaxRef = 55,
  VcmaxHa = 73637,
  VcmaxHd = 149252,
  VcmaxS = 486,
  RdRef = 1,
  RdHa = 46390,
  KcRef = 404.9,
  KcHa = 79430,
  KoRef = 278.4,
  KoHa = 36380,
  GstarRef = 42.75,
  GstarHa = 37830,
  abso = 0.85,
  f = 0.15,
  LogitTheta = f.logit(0.85),
  g0 = 0.01,
  g1 = 2
)
```

Arguments

R	Ideal gas constant
O2	O2 concentration in ppm
TRef	Reference temperature for Kc, Ko, Rd,GammaStar Vcmax, Jmax
Patm	Atmospheric pressure in Pa
JmaxRef	Maximum electron transport rate in micromol.m-2.s-1
JmaxHa	Energy of activation for Jmax in J.mol-1
JmaxHd	Energy of desactivation for Jmax in J.mol-1
JmaxS	Entropy term for Jmax in J.mol-1.K-1

VcmaxRef	Maximum rate of Rubisco for carboxylation micromol.m-2.s-1
VcmaxHa	Energy of activation for Vcmax in J.mol-1
VcmaxHd	Energy of desactivation for Vcmax in J.mol-1
VcmaxS	Entropy term for Vcmax in J.mol-1.K-1
RdRef	Respiration value at the reference temperature
RdHa	Energie of activation for Rd in J.mol-1
KcRef	Michaelis-Menten constant of Rubisco for CO2 at the reference temperature in micromol.mol-1
KcHa	Energy of activation for Kc in J.mol-1
KoRef	ichaelis-Menten constant of Rubisco for CO2 at the reference temperature in milimol.mol-1
KoHa	Energy of activation for Ko in J.mol-1
GstarRef	CO2 compensation point in absence of respiration in micromol.mol-1
GstarHa	Enthalpie of activation for Gstar in J.mol-1
abso	Absorptance of the leaf in the photosynthetic active radiation wavelenghts
f	Correcting factor for the spectral quality of the light
LogitTheta	Theta is the empirical curvacture factor for the response of J to PFD. It takes its values between 0 and 1. To avoid numerical issues when fitting data, this parameters is transformed in this model and called LogitTheta. The transformation between Theta and LogitTheta is: Theta=f.logistic(LogitTheta) and LogitTheta=f.logit(Theta)
g0	Constant of the USO model, representing the conductance when A is 0, in mol.m-2.s-1
g1	Slope parameter, between 1.14 and 3.58 KPa^0.5 (Wu et al., 2019)

Value

List of parameters that can be used in f.A

References

Bernacchi, C.J., Singsaas, E.L., Pimentel, C., Portis Jr, A.R. and Long, S.P. (2001), Improved temperature response functions for models of Rubisco-limited photosynthesis. Plant, Cell & Environment, 24: 253-259. doi:10.1111/j.1365-3040.2001.00668.x

Examples

```
param1=f.make.param(JmaxRef=100,VcmaxRef=60,RdRef=1)
 param2=f.make.param(JmaxRef=100,VcmaxRef=80,RdRef=1)
 f.A(PFD=1500,cs=400,Tleaf=300,Tair=299,RH=70,param=param1)
 f.A(PFD=1500,cs=400,Tleaf=300,Tair=299,RH=70,param=param2)
```

`f.modified.arrhenius` *Temperature dependence of Jmax and Vcmax*

Description

The temperature dependence of the photosynthetic parameters Vcmax, the maximum catalytic rate of the enzyme Rubisco, and Jmax, the maximum electron transport rate is modelled by a modified Arrehenius equation. It is modified to account for decreases in each parameter at high temperatures.

Usage

```
f.modified.arrhenius(PRef, Ha, Hd, s, Tleaf, TRef = 298.16, R = 8.314)
```

Arguments

`PRef`	Value of the parameter, here Vcmax or Jmax, at the reference temperature in micromol.m-2.s-1
`Ha`	Energy of activation in J.mol-1
`Hd`	Energy of desactivation in J.mol-1
`s`	Entropy term in J.mol-1.K-1
`Tleaf`	Temperature of the leaf in Kelvin
`TRef`	Reference temperature
`R`	Ideal gas constant

Value

Value of the parameter Jmax or Vcmax at a given temperature

References

Leuning, R. (2002), Temperature dependence of two parameters in a photosynthesis model. Plant, Cell & Environment, 25: 1205-1210. doi:10.1046/j.1365-3040.2002.00898.x

Examples

```
plot(x=seq(25,35,0.1),y=f.modified.arrhenius(PRef=50,Ha=73637,Hd=149252,s=486,Tleaf=seq(273.15+25,273.15+35
```

`f.modified.arrhenius.inv` *Temperature dependence of Jmax and Vcmax*

Description

Retrieve the reference temperature value of a parameter knowing its value at Tleaf

Usage

```
f.modified.arrhenius.inv(P, Ha, Hd, s, Tleaf, TRef = 298.16, R = 8.314)
```

Arguments

P	Value of the parameter, here Vcmax or Jmax, at the leaf temperature in micromol.m-2.s-1
Ha	Energy of activation in J.mol-1
Hd	Energy of desactivation in J.mol-1
s	Entropy term in J.mol-1.K-1
Tleaf	Temperature of the leaf in Kelvin
TRef	Reference temperature
R	Ideal gas constant

---

f.plot.Aci *Plot Aci data and model*

Description

Plot a generic graphic with observed data and predictions. Be careful to sort the data.frame beforehand.

Usage

```
f.plot.Aci(measures = NULL, list_legend, param, name = "")
```

Arguments

measures	Data frame obtained from CO2 curve with at least columns Photo, Ci, PARi and Tleaf
param	List of parameters, see f.make.param for details
name	Name of the curve to be displayed

Value

Plot a figure

Examples

```
param=f.make.param()
Photo=f.Aci(PFD=2000,Tleaf=300,ci=seq(40,1500,50),param=param)+rnorm(n = 30,mean = 0,sd = 0.5)
data=data.frame(Tleaf=rep(300,30),Ci=seq(40,1500,50),PARi=rep(2000,30),Photo=Photo)
f.plot.Aci(measures=data,param=param,list_legend=param['VcmaxRef'],name='Example 01')
```

f.plot.AQ *Plot AQ data and model*

Description

Plot a generic graphic with observed data and predictions. Be careful to sort the data.frame beforehand.

Usage

```
f.plot.AQ(measures = NULL, param, list_legend = NULL, name = "")
```

Arguments

measures	Data frame obtained from CO2 curve with at least columns Photo, Ci, PARi and Tleaf
param	List of parameters, see f.make.param for details
name	Name of the curve to be displayed

Value

Plot a figure

Examples

```
param=f.make.param()
data=data.frame(Tleaf=seq(298,305,0.24),Ci=seq(300,271),PARi=seq(0,2000,67),Photo=f.AWj(PFD=seq(0,2000,67)
f.plot.AQ(measures=data,param=param,list_legend=param[c('VcmaxRef','RdRef','JmaxRef')],name='Example 01')
```

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