Package 'LeafGasExchange'

July 6, 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 analytical solutions of the different equations. It is also possible to include leaf energy balance and mesophyll conductance. 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, tealeaves

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

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

Author Julien Lamour [aut, cre]

Maintainer Julien Lamour <jlamour@bnl.gov>

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RemoteUsername TESTgroup-BNL

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GithubRef master

GithubSHA1 77b2bf83bd8a3b74747380b668ae2d9e503a258e

R topics documented:

`f.A` *Coupled conductance photosynthesis model*

Description

Photosynthesis model at the leaf level using the farquhar equations. The parameters can be defined by the function f.make param and corresponds to the parameters inplemented in different Terrestrial Biosphere Modesl such as ORCHIDEE, JULES, CLM4.5 or FATES

Usage

```
f.A(PFD, cs, Tleaf, Tair, RH, param = list())
```

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 - cc: Mesophyll CO2 concentration in micromol.mol-1 (for the models using mesophyll conductance) - 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,param=f.make.param())
```

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())
```

Arguments

param	List of parameters, see f.make.param for details

Value

Assimilation in micromol.m-2.s-1

Examples

```
ci=seq(40,1500,10)
plot(x=ci,y=f.Aci(PFD=2000,ci=ci,Tleaf=300,param=f.make.param())$A)
```

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

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f.AT *Coupled conductance photosynthesis model with energy balance model*

Description

Coupled conductance photosynthesis model with energy balance model

Usage

```
f.AT(PFD, cs, Tair, RH, wind, precision = 0.1, max_it = 10, param = list())
```

Arguments

precision	Precision of the leaf temperature prediction. The resolution of the energy balance coupled with the photosynthesis and stomatal conductance is numerical. The smaller the precision, the longer will be the resolution.
max_it	Maximum number of iterations to find the solution
param	List of parameters given by f.make.param()

Details

This function allo to calculate the photosynthesis from environmental variables PFD, RH, wind, cs, Tair. (There is no boundary layer). The energy balance model comes from the package Tealeaves (see reference). The energy balance calculation involves the stomatal conductance and the cuticular conductance. Here the cuticular conductance is considered to be equal to g0 even if it is wrong for the USO models. Most of the times, no precaution is taken on gs_min when fitting the conductance models so gs_min is often negative. This choice was made to prevent unrealistic energy budgets.

References

tealeaves: an R package for modelling leaf temperature using energy budgets. Christopher. D. Muir. bioRxiv 529487; doi: https://doi.org/10.1101/529487

Examples

```
f.AT(PFD=1500,cs=400,Tair=299,wind=2,RH=70,param=f.make.param())
```

---

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)
```

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.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)
```

f.fitting *Fitting function for photosynthesis datadata (light curve or Aci curve)*

Description

Function to fit 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.fitting(
  measures,
  id.name = NULL,
  Start = list(JmaxRef = 90, VcmaxRef = 70, RdRef = 1),
  param = f.make.param(),
  modify.init = TRUE,
  do.plot = TRUE,
  type = "Aci"
)
```

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
do.plot	TRUE or FALSE, plot data and fitted curves ?

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(TBM='FATES'))$A+rnorm(n = 20,mean = 0,sd = 0.5))

f.fitting(measures=data,id.name=NULL,Start=list(JmaxRef=90,VcmaxRef=70,RdRef=1),param=f.make.param(TBM='FA
```

---

f.gs *Conductance 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, power = 0.5, model = "USO")
```

Arguments

A	Net 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)
power	Power of the VPDl in USO model. By default is is 0.5 as in Medlin publication
model	Stomatal model ("USO" or "USO_simpl")

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,power=0.5)
```

`f.gsmin` *Calculation of the minimal conductance given by a particular coupled conductance and photosynthesis model*

Description

The minimal conductance of a model depends on the parameters of the model (ie g0 and g1) but also on the minimum A value, which corresponds to the dark respiration. Knowing the minimal conductance is important because the conductance can become negative and lead to unrealistic values in photosynthesis models

Usage

```
f.gsmin(
  RdRef = 0.825,
  RdHa = 46390,
  RdHd = 150650,
  RdS = 490,
  Tleaf = 300,
  cs = 400,
  ds = 1000,
  g0 = 0.02,
  g1 = 4.1,
  power = 0.5,
  model = "USO"
)
```

Arguments

`RdRef`	Respiration value at the reference temperature
`RdHa`	Energie of activation for Rd in J.mol-1
`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)
`power`	Power of VPDl in USO model. By default power=0.5 as in Medlyn article

Value

Minimal conductance

Examples

```
gs_min=f.gsmin(RdRef= 0.825,RdHa= 46390,RdHd=150650,RdS=490,Tleaf=300,cs=400,ds=1000,g0=0.02,g1=4.1,power=0
```

`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.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 most of the functions of this package. Depending on the function, all the parameters are not used. For example go and g1 are not used in f.Aci. The parameters from different TBM are implemented and can be chosen by selecting a TBM

Usage

```
f.make.param(
  TBM = "FATES",
  R = NA,
  O2 = NA,
  TRef = NA,
  Patm = NA,
  JmaxRef = NA,
  JmaxHa = NA,
  JmaxHd = NA,
  JmaxS = NA,
  VcmaxRef = NA,
  VcmaxHa = NA,
  VcmaxHd = NA,
  VcmaxS = NA,
  VcmaxQ10 = NA,
  Tlow = NA,
  Tup = NA,
  TpRef = NA,
  TpHa = NA,
  TpHd = NA,
  TpS = NA,
  thetacj = NA,
  thetaip = NA,
  RdRef = NA,
  RdHa = NA,
  RdHd = NA,
  RdS = NA,
  KcRef = NA,
  KcHa = NA,
  KcQ10 = NA,
  KoRef = NA,
  KoHa = NA,
  KoQ10 = NA,
  GstarRef = NA,
  GstarHa = NA,
  TauRef = NA,
  TauQ10 = NA,
  abso = NA,
  aQY = NA,
  Theta = NA,
```

```
  model.gs = NA,
  g0 = NA,
  g1 = NA,
  power = NA,
  gmRef = NA,
  gmS = NA,
  gmHa = NA,
  gmHd = NA
)
```

Arguments

TBM	Type of model (FATES, ORCHIDEE, CLM4.5 or JULES). Default is FATES
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
aQY	Apparent quantum yield
Theta	Theta is the empirical curvacture factor for the response of J to PFD. It takes its values between 0 and 1.
model.gs	Type of conductance model (USO, USO_simpl)
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)
power	Power of VPDl in USO model. By default power=0.5 as in Medlyn article

gmRef	Mesophyll conductance at Tref (25 deg C) mol m-2 s-1
gmS	Entropy term for gm J K-1 mol-1
gmHa	Energy of activation for gm in J.mol-1
gmHd	Energy of deactivation for gm in J.mol-1

Details

The call of this function is made using f.make.param(). If a parameter is modified for example writting f.make.param(VcmaxRef=10), this function will return all the default parameters from FATES TBM with VcmaxRef = 10 instead of its default value

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 CLM4.5: http://www.cesm.ucar.edu/models/cesm2/land/CL
ORCHIDEE: https://forge.ipsl.jussieu.fr/orchidee/wiki/Documentation/OrchideeParameters AND https://agupubs.online
JULES: https://www.geosci-model-dev.net/4/701/2011/gmd-4-701-2011.pdf FATES: https://fates-docs.readthedocs.io/en/latest/fates_tech_note.html#

Examples

```
param1=f.make.param(TBM='FATES',JmaxRef=100,VcmaxRef=60,RdRef=1,TpRef=10)
 param2=f.make.param(TBM='CLM4.5',JmaxRef=100,VcmaxRef=60,RdRef=1,TpRef=10)
 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 *Plot data and model*

Description

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

Usage

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

Arguments

measures	Data frame obtained from CO2 or light curve with at least columns Photo, Ci, PARi and Tleaf Data frame obtained from CO2 or light curve with at least columns Photo, Ci, PARi and Tleaf
list_legend	Named list where the name and values will appear in the legend
name	Name of the curve to be displayed
type	Type of the curve to plot (light curve: Aq or CO2 curve Aci)

Value

Plot a figure

Examples

```
param=f.make.param()
Photo=f.Aci(PFD=2000,Tleaf=300,ci=seq(40,1500,50),param=param)$A+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(measures=data,param=param,list_legend=param['VcmaxRef'],name='Example 01',type='Aci')
```

f.Q10 *Temperature dependence of photosynthetic parameters*

Description

Temperature dependence of photosynthetic parameters

Usage

```
f.Q10(Pref, Q10, Tleaf, TRef)
```

Arguments

TRef	Reference temperature for Kc, Ko, Rd,GammaStar Vcmax, Jmax

Details

This equation is used in JULES TBM model

Value

Value of the photosynthetic parameter at the specified leaf temperature

References

Clark, D. B., Mercado, L. M., Sitch, S., Jones, C. D., Gedney, N., Best, M. J., . Cox, P. M. (2011). The Joint UK Land Environment Simulator (JULES), model description - Part 2: Carbon fluxes and vegetation dynamics. Geoscientific Model Development, 4(3), 701-722. doi:10.5194/gmd-4-701-2011

`f.Q10.modified` *Temperature dependence of photosynthetic parameters*

Description

Temperature dependence of photosynthetic parameters

Usage

```
f.Q10.modified(Pref, Q10, Tleaf, TRef, Tlow, Tup)
```

Arguments

`TRef`	Reference temperature for Kc, Ko, Rd,GammaStar Vcmax, Jmax

Details

This equation is used in JULES TBM model

Value

Value of the photosynthetic parameter at the specified leaf temperature

References

Clark, D. B., Mercado, L. M., Sitch, S., Jones, C. D., Gedney, N., Best, M. J., . Cox, P. M. (2011). The Joint UK Land Environment Simulator (JULES), model description - Part 2: Carbon fluxes and vegetation dynamics. Geoscientific Model Development, 4(3), 701-722. doi:10.5194/gmd-4-701-2011

`f.smooth` *Smoothing functions between photosynthesis limitations (for example between rubisco carboxylation and light limitation)*

Description

Smoothing functions between photosynthesis limitations (for example between rubisco carboxylation and light limitation)

Usage

```
f.smooth(A1, A2, theta)
```

Arguments

`theta`	Smoothing factor

Value

Smoothed value

Examples

```
A1= seq(0,20,1)
A2= seq(9,11,2/20)
Asmooth=f.smooth(A1=A1,A2=A2,theta=0.99)
plot(A1,type='l')
lines(A2)
lines(Asmooth,col='blue')
```

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