# Package 'bigleaf'

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```
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      Covariance Data
Maintainer Juergen Knauer < J. Knauer@westernsydney.edu.au>
Description Calculation of physical (e.g. aerodynamic conductance, surface temperature),
      and physiological (e.g. canopy conductance, water-use efficiency) ecosystem properties
              from eddy covariance data and accompanying meteorological measurements. Calculations
               assume the land surface to behave like a 'big-
      leaf' and return bulk ecosystem/canopy variables.
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```

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aerodynamic.conductance

Aerodynamic Conductance

# **Description**

Bulk aerodynamic conductance, including options for the boundary layer conductance formulation and stability correction functions.

## Usage

```
aerodynamic.conductance(
  data,
 Tair = "Tair",
 pressure = "pressure",
 wind = "wind",
 ustar = "ustar",
 H = "H"
  zr,
  zh,
  d,
  z0m = NULL,
 D1,
 N = 2,
  fc = NULL,
 LAI,
  Cd = 0.2,
 hs = 0.01,
 wind_profile = FALSE,
  stab_correction = TRUE,
  stab_formulation = c("Dyer_1970", "Businger_1971"),
  Rb_model = c("Thom_1972", "Choudhury_1988", "Su_2001", "constant_kB-1"),
  kB_h = NULL,
  Sc = NULL,
  Sc_name = NULL,
```

```
constants = bigleaf.constants()
)
```

#### **Arguments**

data Data.frame or matrix containing all required variables

Tair Air temperature (deg C)
pressure Atmospheric pressure (kPa)

wind Wind speed (m s-1)

ustar Friction velocity (m s-1)

H Sensible heat flux (W m-2)

zr Instrument (reference) height (m)

zh Canopy height (m)

d Zero-plane displacement height (m)

z0m Roughness length for momentum (m), optional; if not provided, it is estimated

from roughness.parameters (method="wind\_profile"). Only used if wind\_profile

= TRUE and/or Rb\_model = "Su\_2001" or "Choudhury\_1988".

D1 Characteristic leaf dimension (m) (if Rb\_model = "Su\_2001") or leaf width (if

Rb\_model = "Choudhury\_1988"); ignored otherwise.

N Number of leaf sides participating in heat exchange (1 or 2); only used if Rb\_model

= "Su\_2001". Defaults to 2.

fc Fractional vegetation cover (-); only used if Rb\_model = "Su\_2001". See De-

tails.

LAI One-sided leaf area index (m2 m-2); only used if Rb\_model = "Choudhury\_1988"

or "Su\_2001".

Cd Foliage drag coefficient (-); only used if Rb\_model = "Su\_2001".

hs Roughness length of bare soil (m); only used if Rb\_model = "Su\_2001".

wind\_profile Should Ga for momentum be calculated based on the logarithmic wind profile

equation? Defaults to FALSE.

stab\_correction

Should stability correction be applied? Defaults to TRUE. Ignored if wind\_profile

= FALSE.

stab\_formulation

Stability correction function. Either "Dyer\_1970" (default) or "Businger\_1971".

Ignored if wind\_profile = FALSE or if stab\_correction = FALSE.

Rb\_model Boundary layer resistance formulation. One of "Thom\_1972", "Choudhury\_1988", "Su\_2001", "constant

kB\_h kB-1 value for heat transfer; only used if Rb\_model = "constant\_kB-1"

Sc Optional: Schmidt number of additional quantities to be calculated

Sc\_name Optional: Name of the additional quantities, has to be of same length than

Sc\_name

constants k - von Karman constant

cp - specific heat of air for constant pressure (J K-1 kg-1)

Kelvin - conversion degree Celsius to Kelvin

g - gravitational acceleration (m s-2)

pressure0 - reference atmospheric pressure at sea level (Pa)

Tair0 - reference air temperature (K) Sc\_CO2 - Schmidt number for CO2 Pr - Prandtl number (if Sc is provided)

#### **Details**

Aerodynamic conductance for heat (Ga\_h) is calculated as:

$$Ga_h = 1/(Ra_m + Rb_h)$$

where Ra\_m is the aerodynamic resistance for momentum and Rb the (quasi-laminar) canopy boundary layer resistance ('excess resistance').

The aerodynamic resistance for momentum Ra\_m is given by:

$$Ra_m = u/ustar^2$$

Note that this formulation accounts for changes in atmospheric stability, and does not require an additional stability correction function.

An alternative method to calculate Ra\_m is provided (calculated if wind\_profile = TRUE):

$$Ra_m = (ln((zr-d)/z0m) - psi_h)/(kustar)$$

If the roughness parameters z0m and d are unknown, they can be estimated using roughness.parameters. The argument stab\_formulation determines the stability correction function used to account for the effect of atmospheric stability on Ra\_m (Ra\_m is lower for unstable and higher for stable stratification). Stratification is based on a stability parameter zeta (z-d/L), where z = reference height, d the zero-plane displacement height, and L the Monin-Obukhov length, calculated with Monin.Obukhov.length The stability correction function is chosen by the argument stab\_formulation. Options are "Dyer\_1970" and "Businger\_1971".

The model used to determine the canopy boundary layer resistance for heat (Rb\_h) is specified by the argument Rb\_model. The following options are implemented: "Thom\_1972" is an empirical formulation based on the friction velocity (ustar) (Thom 1972):

$$Rb_h = 6.2ustar^-0.667$$

The model by Choudhury & Monteith 1988 (Rb\_model = "Choudhury\_1988"), calculates Rb\_h based on leaf width, LAI and ustar (Note that function argument Dl represents leaf width (w) and not characteristic leaf dimension (Dl) if Rb\_model = "Choudhury\_1988"):

$$Gb_h = LAI((0.02/\alpha) * sqrt(u(zh)/w) * (1 - exp(-\alpha/2)))$$

where  $\alpha$  is a canopy attenuation coefficient modeled in dependence on LAI, u(zh) is wind speed at canopy height (calculated from wind.profile), and w is leaf width (m). See Gb.Choudhury for further details.

The option Rb\_model = "Su\_2001" calculates Rb\_h based on the physically-based Rb model by Su et al. 2001, a simplification of the model developed by Massman 1999:

$$kB_h = (kCdfc^2)/(4Ctustar/u(zh)) + kBs - 1(1 - fc)^2$$

where Cd is a foliage drag coefficient (defaults to 0.2), fc is fractional vegetation cover, Bs-1 is the inverse Stanton number for bare soil surface, and Ct is a heat transfer coefficient. See Gb. Su for details on the model.

The models calculate the parameter  $kB^{(-1)}$  (in the code referred to as  $kB_h$ ), which is related to  $Rb_h$ :

$$kB_h = Rb_h * (k * ustar)$$

From version 0.7.6 onwards, the roughness length for heat (z0h) is added to the output if z0m is available (i.e. provided as input or calculated within this function). z0h is calculated from roughness.length.heat:

$$z0h = z0m/exp(kB_h)$$

Rb (and Gb) for water vapor and heat are assumed to be equal in this package. Gb for other quantities x is calculated as (Hicks et al. 1987):

$$Gb_x = Gb/(Sc_x/Pr)^0.67$$

where Sc\_x is the Schmidt number of quantity x, and Pr is the Prandtl number (0.71).

#### Value

a data.frame with the following columns:

Ga_m	Aerodynamic conductance for momentum transfer (m s-1)
Ra_m	Aerodynamic resistance for momentum transfer (s m-1)
Ga_h	Aerodynamic conductance for heat transfer (m s-1)
Ra_h	Aerodynamic resistance for heat transfer (s m-1)
Gb_h	Canopy boundary layer conductance for heat transfer (m s-1)
Rb_h	Canopy boundary layer resistance for heat transfer (s m-1)
kB_h	kB^(-1) parameter for heat transfer
z0h	Roughness length for heat (m) (NA if not input $z0m$ not provided as input or not estimated in this function)
zeta	Stability parameter 'zeta' (NA if wind_profile = FALSE)
psi_h	Integrated stability correction function (NA if wind_profile = FALSE)

Ra_CO2	Aerodynamic resistance for CO2 transfer (s m-1)
Ga_CO2	Aerodynamic conductance for CO2 transfer (m s-1)
Gb_C02	Canopy boundary layer conductance for CO2 transfer (m s-1)
Ga_Sc_name	Aerodynamic conductance for $Sc\_name\ (m\ s-1)$ . Only added if $Sc\_name\ and$ the respective $Sc$ are provided
Gb_Sc_name	Boundary layer conductance for Sc_name (m s-1). Only added if Sc_name and the respective Sc are provided

#### Note

Input variables such as LAI, Dl, or zh can be either constants, or vary with time (i.e. vectors of the same length as data).

Note that boundary layer conductance to water vapor transfer (Gb\_w) is often assumed to equal Gb\_h. This assumption is also made in this R package, for example in the function surface.conductance.

If the roughness length for momentum (z0m) is not provided as input, it is estimated from the function roughness.parameters within wind.profile if wind\_profile = TRUE and/or Rb\_model = "Su\_2001" or "Choudhury\_1988" The roughness.parameters function estimates a single z0m value for the entire time period! If a varying z0m value (e.g. across seasons or years) is required, z0m should be provided as input argument.

#### References

Verma, S., 1989: Aerodynamic resistances to transfers of heat, mass and momentum. In: Estimation of areal evapotranspiration, IAHS Pub, 177, 13-20.

Verhoef, A., De Bruin, H., Van Den Hurk, B., 1997: Some practical notes on the parameter kB-1 for sparse vegetation. Journal of Applied Meteorology, 36, 560-572.

Hicks, B.B., Baldocchi, D.D., Meyers, T.P., Hosker, J.R., Matt, D.R., 1987: A preliminary multiple resistance routine for deriving dry deposition velocities from measured quantities. Water, Air, and Soil Pollution 36, 311-330.

Monteith, J.L., Unsworth, M.H., 2008: Principles of environmental physics. Third Edition. Elsevier Academic Press, Burlington, USA.

## See Also

Gb. Thom, Gb. Choudhury, Gb. Su for calculations of Rb / Gb only

```
df <- data.frame(Tair=25,pressure=100,wind=c(3,4,5),ustar=c(0.5,0.6,0.65),H=c(200,230,250))
# simple calculation of Ga
aerodynamic.conductance(df,Rb_model="Thom_1972")
# calculation of Ga using a model derived from the logarithmic wind profile
aerodynamic.conductance(df,Rb_model="Thom_1972",zr=40,zh=25,d=17.5,z0m=2,wind_profile=TRUE)
# simple calculation of Ga_m, but a physically based canopy boundary layer model</pre>
```

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```
aerodynamic.conductance (df, Rb\_model="Su\_2001", zr=40, zh=25, d=17.5, Dl=0.05, N=2, fc=0.8) \\
```

air.density

Air Density

# Description

Air density of moist air from air temperature and pressure.

## Usage

```
air.density(Tair, pressure, constants = bigleaf.constants())
```

# **Arguments**

Tair Air temperature (deg C)
pressure Atmospheric pressure (kPa)

constants Kelvin - conversion degC to Kelvin

Rd - gas constant of dry air (J kg-1 K-1)

kPa2Pa - conversion kilopascal (kPa) to pascal (Pa)

#### **Details**

Air density  $(\rho)$  is calculated as:

```
\rho = pressure/(Rd * Tair)
```

## Value

```
\rho air density (kg m-3)
```

## References

Foken, T, 2008: Micrometeorology. Springer, Berlin, Germany.

```
# air density at 25degC and standard pressure (101.325kPa)
air.density(25,101.325)
```

Arrhenius.temp.response

(Modified) Arrhenius Temperature Response Function

#### **Description**

(Modified) Arrhenius function describing the temperature response of biochemical parameters.

#### Usage

```
Arrhenius.temp.response(
  param,
  Temp,
  Ha,
  Hd,
  dS,
  constants = bigleaf.constants()
```

## **Arguments**

param	Parameter measured at measurement temperature (umol m-2 s-1)
Temp	Measurement temperature (degC)
На	Activation energy for param (kJ mol-1)
Hd	Deactivation energy for param (kJ mol-1)
dS	Entropy term for param (kJ mol-1 K-1)
constants  Kelvin - conversion degree Celsius to Kelvin  Rgas - universal gas constant (J mol-1 K-1)  kJ2J - conversion kilojoule (kJ) to joule (J)	

## **Details**

The function returns the biochemical rate at a reference temperature of 25degC given a predefined temperature response function. This temperature response is given by a modified form of the Arrhenius function:

```
param25 = param/(exp(Ha*(Temp-Tref)/(Tref*Rgas*Temp))*(1 + exp((Tref*dS-Hd)/(Tref*Rgas)))/(1 + exp((Tref*dS-Hd)/(Tref*Rgas))/(1 + exp((Tref*dS-Hd)/(Tref*Rg
```

where param is the value/rate of the parameter at measurement temperature, Temp is temperature in K, Tref is reference temperature (298.15K), and Rgas is the universal gas constant (8.314 J K-1 mol-1). Ha is the activation energy (kJ mol-1), Hd is the deactivation energy (kJ mol-1), and dS the entropy term (kJ mol-1 K-1) of the respective parameter.

If either Hd or dS or both are not provided, the equation above reduces to the first term (i.e. the common Arrhenius equation without the deactivation term.)

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#### Value

param25 - value of the input parameter at the reference temperature of 25degC (umol m-2 s-1)

#### References

Johnson F.H., Eyring H., Williams R.W. 1942: The nature of enzyme inhibitions in bacterial luminescence: sulfanilamide, urethane, temperature and pressure. Journal of cellular and comparative physiology 20, 247-268.

Kattge J., Knorr W., 2007: Temperature acclimation in a biochemical model of photosynthesis: a reanalysis of data from 36 species. Plant, Cell and Environment 30, 1176-1190.

AT\_Neu\_Jul\_2010

Eddy Covariance Data of AT-Neu (Neustift)

#### **Description**

Halfhourly eddy covariance Data of the site AT-Neu, a mountain meadow in Austria. (https://sites.fluxdata.org/AT-Neu/). Data are from July 2010.

## Usage

```
AT_Neu_Jul_2010
```

## **Format**

```
A data frame with 1488 observations and 31 columns:
```

wind horizontal wind velocity (m s-1) [WS\_F]

```
year year of measurement
month month of measurement
doy day of year
hour hour (0 - 23.5)
Tair Air temperature (degC) [TA_F]
Tair_qc Quality control of Tair [TA_F_QC]
PPFD Photosynthetic photon flux density (umol m-2 s-1) [PPFD_IN]
PPFD_qc Quality control of PPFD [PPFD_IN_QC]
VPD Vapor pressure deficit (kPa) [VPD_F]
VPD_qc Quality control of VPD [VPD_F_QC]
pressure Atmospheric pressure (kPa) [PA_F]
precip_precipitation (mm) [P_F]
precip_qc Quality control of precip [P_F_QC]
ustar friction velocity (m s-1) [USTAR]
```

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```
wind_qc Quality control of wind [WS_F_QC]
Ca CO2 concentration (ppm) [CO2_F_MDS]
Ca_qc Quality control of Ca [CO2_F_MDS_QC]
LW_up upward longwave radiation (W m-2) [LW_OUT]
Rn Net radiation (W m-2) [NETRAD]
LE Latent heat flux (W m-2) [LE_F_MDS]
LE_qc Quality control of LE [LE_F_MDS_QC]
H Sensible heat flux (W m-2) [H_F_MDS]
H_qc Quality control of H [H_F_MDS_QC]
G Ground heat flux (W m-2) [G_F_MDS]
G_qc Quality control of G [G_F_MDS_QC]
NEE Net ecosystem exchange (umol m-2 s-1) [NEE_VUT_USTAR50]
NEE_qc Quality control of NEE [NEE_VUT_USTAR50_QC]
GPP Gross primary productivity from nighttime partitioning (umol m-2 s-1) [GPP_NT_VUT_USTAR50]
GPP_qc Quality control of GPP [NEE_VUT_USTAR50_QC]
Reco Ecosystem respiration from nighttime partitioning (umol m-2 s-1) [RECO_NT_VUT_USTAR50]
```

#### Note

The original variable names as provided by the FLUXNET2015 dataset are given in squared brackets. Note that variable units have been converted in some cases (e.g. VPD from hPa to kPa).

#### **Source**

original data were downloaded from https://fluxnet.org/ (accessed 09 November 2016)

bigleaf.constants

Constants Used in the bigleaf Package

#### **Description**

This function defines the following constants:

## Usage

```
bigleaf.constants(

cp = 1004.834,

Rgas = 8.31451,

Rv = 461.5,

Rd = 287.0586,

Md = 0.0289645,

Mw = 0.0180153,

eps = 0.622,
```

bigleaf.constants

```
g = 9.81,
  solar_constant = 1366.1,
 pressure0 = 101325,
 Tair0 = 273.15,
 k = 0.41,
 Cmol = 0.012011,
 Omol = 0.0159994,
 H2Omol = 0.01801528,
  sigma = 5.670367e-08,
 Pr = 0.71,
  Sc_C02 = 1.07,
 Le067 = 0.93,
 Kelvin = 273.15,
 DwDc = 1.6,
  days2seconds = 86400,
  kPa2Pa = 1000,
 Pa2kPa = 0.001,
  umol2mol = 1e-06,
 mol2umol = 1e+06,
 kg2g = 1000,
 g2kg = 0.001,
 kJ2J = 1000,
 J2kJ = 0.001,
  se_median = 1.253,
  frac2percent = 100
)
```

# Arguments

H2Omol

ср	Specific heat of air for constant pressure (J K-1 kg-1)
Rgas	Universal gas constant (J mol-1 K-1)
Rv	Gas constant of water vapor (J kg-1 K-1) (Stull 1988 p.641)
Rd	Gas constant of dry air (J kg-1 K-1) (Foken p. 245)
Md	Molar mass of dry air (kg mol-1)
Mw	Molar mass of water vapor (kg mol-1)
eps	Ratio of the molecular weight of water vapor to dry air (=Mw/Md)
g	Gravitational acceleration (m s-2)
solar_constant	Solar constant (W m-2)
pressure0	Reference atmospheric pressure at sea level (Pa)
Tair0	Reference air temperature (K)
k	von Karman constant
Cmol	Molar mass of carbon (kg mol-1)
Omol	Molar mass of oxygen (kg mol-1)

Molar mass of water (kg mol-1)

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sigma Stefan-Boltzmann constant (W m-2 K-4)

Pr Prandtl number

Sc\_C02 Schmidt number for CO2

Lewis number for water vapor to the power of 0.67

Kelvin Conversion degree Celsius to Kelvin

DwDc Ratio of the molecular diffusivities for water vapor and CO2

days2seconds Seconds per day

kPa2Pa Conversion kilopascal (kPa) to pascal (Pa)
Pa2kPa Conversion pascal (Pa) to kilopascal (kPa)
umo12mo1 Conversion micromole (umol) to mole (mol)
mol2umo1 Conversion mole (mol) to micromole (umol)

kg2g Conversion kilogram (kg) to gram (g)
g2kg Conversion gram (g) to kilogram (kg)
kJ2J Conversion kilojoule (kJ) to joule (J)
J2kJ Conversion joule (J) to kilojoule (kJ)

se\_median Conversion standard error (SE) of the mean to SE of the median

frac2percent Conversion between fraction and percent

#### **Details**

This function is passed as an argument to every function that uses one or more constants. Individual constants passed to a function can be easily altered. E.g. the following command will change the value of the von Karman constant from 0.41 to 0.4:

bigleaf.constants(k=0.4)

the value of a constant can be returned by calling:

bigleaf.constants()\$\*name\_of\_constant\*

To permanently change the constants contained within this function (which makes sense for some of them, e.g. for the von Karman constant), the command fixInNamespace can be used. E.g.

fixInNamespace(bigleaf.constants,ns="bigleaf")

Note that this has to be repeated every time the package is newly installed/loaded.

biochemical.energy Biochemical Energy

## **Description**

Radiant energy absorbed in photosynthesis or heat release by respiration calculated from net ecosystem exchange of CO2 (NEE).

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## Usage

```
biochemical.energy(NEE, alpha = 0.422)
```

## **Arguments**

NEE Net ecosystem exchange (umol CO2 m-2 s-1)

alpha Energy taken up/released by photosynthesis/respiration per mol CO2 fixed/respired

(J umol-1)

#### **Details**

The following sign convention is employed: NEE is negative when carbon is taken up by the ecosystem. Positive values of the resulting biochemical energy mean that energy (heat) is taken up by the ecosystem, negative ones that heat is released. The value of alpha is taken from Nobel 1974 (see Meyers & Hollinger 2004), but other values have been used (e.g. Blanken et al., 1997)

#### Value

Sp - biochemical energy (W m-2)

## References

Meyers, T.P., Hollinger, S.E. 2004: An assessment of storage terms in the surface energy balance of maize and soybean. Agricultural and Forest Meteorology 125, 105-115.

Nobel, P.S., 1974: Introduction to Biophysical Plant Physiology. Freeman, New York.

Blanken, P.D. et al., 1997: Energy balance and canopy conductance of a boreal aspen forest: Partitioning overstory and understory components. Journal of Geophysical Research 102, 28915-28927.

## **Examples**

```
# Calculate biochemical energy taken up by the ecosystem with # a measured NEE of -30umol CO2 m-2 s-1 biochemical.energy(NEE=-30)
```

decoupling

Canopy-Atmosphere Decoupling Coefficient

#### **Description**

The canopy-atmosphere decoupling coefficient 'Omega'.

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## Usage

```
decoupling(
  data,
  Tair = "Tair",
  pressure = "pressure",
  Ga = "Ga_h",
  Gs = "Gs_ms",
  approach = c("Jarvis&McNaughton_1986", "Martin_1989"),
  LAI,
  Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
```

#### **Arguments**

data Data.frame or matrix containing all required input variables

Tair Air temperature (deg C)
pressure Atmospheric pressure (kPa)

Ga Aerodynamic conductance to heat/water vapor (m s-1)

Gs Surface conductance (m s-1)

approach Approach used to calculate omega. Either "Jarvis&McNaughton\_1986" (de-

fault) or "Martin\_1989".

LAI Leaf area index (m2 m-2), only used if approach = "Martin\_1989".

Esat. formula Optional: formula to be used for the calculation of esat and the slope of esat.

One of "Sonntag\_1990" (Default), "Alduchov\_1996", or "Allen\_1998". See

Esat.slope.

constants Kelvin - conversion degree Celsius to Kelvin

cp - specific heat of air for constant pressure (J K-1 kg-1) eps - ratio of the molecular weight of water vapor to dry air (-)

sigma - Stefan-Boltzmann constant (W m-2 K-4) Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)

#### **Details**

The decoupling coefficient Omega ranges from 0 to 1 and quantifies the linkage of the conditions (foremost humidity and temperature) at the canopy surface to the ambient air. Values close to 0 indicate well coupled conditions characterized by high physiological (i.e. stomatal) control on transpiration and similar conditions at the canopy surface compared to the atmosphere above the canopy. Values close to 1 indicate the opposite, i.e. decoupled conditions and a low stomatal control on transpiration (Jarvis & McNaughton 1986).

The "Jarvis&McNaughton\_1986" approach (default option) is the original formulation for the decoupling coefficient, given by (for an amphistomatous canopy):

$$\Omega = \frac{\epsilon + 1}{\epsilon + 1 + \frac{Ga}{Gc}}$$

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where  $\epsilon = \frac{s}{\gamma}$  is a dimensionless coefficient with s being the slope of the saturation vapor pressure curve (Pa K-1), and  $\gamma$  the psychrometric constant (Pa K-1).

The approach "Martin\_1989" by Martin 1989 additionally takes radiative coupling into account:

$$\Omega = \frac{\epsilon + 1 + \frac{Gr}{Ga}}{\epsilon + (1 + \frac{Ga}{Gs})(1 + \frac{Gr}{Ga})}$$

#### Value

 $\Omega$  - the decoupling coefficient Omega (-)

#### References

Jarvis P.G., McNaughton K.G., 1986: Stomatal control of transpiration: scaling up from leaf to region. Advances in Ecological Research 15, 1-49.

Martin P., 1989: The significance of radiative coupling between vegetation and the atmosphere. Agricultural and Forest Meteorology 49, 45-53.

#### See Also

aerodynamic.conductance, surface.conductance, equilibrium.imposed.ET

## **Examples**

dew.point

Dew Point

#### **Description**

calculates the dew point, the temperature to which air must be cooled to become saturated (i.e. e = Esat(Td))

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## Usage

```
dew.point(
   Tair,
   VPD,
   accuracy = 0.001,
   Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
   constants = bigleaf.constants()
)
```

## **Arguments**

Tair Air temperature (degC)

VPD Vapor pressure deficit (kPa)

accuracy Accuracy of the result (deg C)

Esat.formula Optional: formula to be used for the calculation of esat and the slope of esat. One of "Sonntag\_1990" (Default), "Alduchov\_1996", or "Allen\_1998". See Esat.slope.

constants Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)

#### **Details**

Dew point temperature (Td) is defined by:

$$e = Esat(Td)$$

where e is vapor pressure of the air and Esat is the vapor pressure deficit. This equation is solved for Td using optimize.

## Value

```
Td - dew point temperature (degC)
```

#### References

Monteith J.L., Unsworth M.H., 2008: Principles of Environmental Physics. 3rd edition. Academic Press, London.

```
dew.point(c(25,30),1.5)
```

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DE\_Tha\_Jun\_2014

Eddy Covariance Data of DE-Tha (Tharandt)

#### **Description**

Halfhourly eddy covariance Data of the site DE-Tha, a spruce forest in Eastern Germany (https://sites.fluxdata.org/DE-Tha/). Data are from June 2014.

#### Usage

```
DE_Tha_Jun_2014
```

#### **Format**

```
A data frame with 1440 observations and 32 columns:
```

year year of measurement

month month of measurement

doy day of year

hour hour (0 - 23.5)

**Tair** Air temperature (degC) [TA\_F]

**Tair\_qc** Quality control of Tair [TA\_F\_QC]

**PPFD** Photosynthetic photon flux density (umol m-2 s-1) [PPFD\_IN]

PPFD\_qc Quality control of PPFD [PPFD\_IN\_QC]

**VPD** Vapor pressure deficit (kPa) [VPD\_F]

**VPD\_qc** Quality control of VPD [VPD\_F\_QC]

**pressure** Atmospheric pressure (kPa) [PA\_F]

**precip** precipitation (mm) [P\_F]

precip\_qc Quality control of precip [P\_F\_QC]

ustar friction velocity (m s-1) [USTAR]

wind horizontal wind velocity (m s-1) [WS\_F]

wind\_qc Quality control of wind [WS\_F\_QC]

Ca CO2 concentration (ppm) [CO2\_F\_MDS]

Ca\_qc Quality control of Ca [CO2\_F\_MDS\_QC]

**LW\_up** upward longwave radiation (W m-2) [LW\_OUT]

LW\_down downward longwave radiation (W m-2) [LW\_IN\_F]

**Rn** Net radiation (W m-2) [NETRAD]

LE Latent heat flux (W m-2) [LE\_F\_MDS]

LE\_qc Quality control of LE [LE\_F\_MDS\_QC]

**H** Sensible heat flux (W m-2) [H\_F\_MDS]

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```
H_qc Quality control of H [H_F_MDS_QC]

G Ground heat flux (W m-2) [G_F_MDS]

G_qc Quality control of G [G_F_MDS_QC]

NEE Net ecosystem exchange (umol m-2 s-1) [NEE_VUT_USTAR50]

NEE_qc Quality control of NEE [NEE_VUT_USTAR50_QC]

GPP Gross primary productivity from nighttime partitioning (umol m-2 s-1) [GPP_NT_VUT_USTAR50]

GPP_qc Quality control of GPP [NEE_VUT_USTAR50_QC]

Reco Ecosystem respiration from nighttime partitioning (umol m-2 s-1) [RECO_NT_VUT_USTAR50]
```

#### Note

The original variable names as provided by the FLUXNET2015 dataset are given in squared brackets. Note that variable units have been converted in some cases (e.g. VPD from hPa to kPa).

#### Source

original data were downloaded from https://fluxnet.org/ (accessed 09 November 2016)

energy.closure

Energy Balance Closure

## **Description**

Calculates the degree of the energy balance non-closure for the entire time span based on the ratio of two sums (energy balance ratio), and ordinary least squares (OLS).

## Usage

```
energy.closure(
  data,
  Rn = "Rn",
  G = NULL,
  S = NULL,
  LE = "LE",
  H = "H",
  instantaneous = FALSE,
  missing.G.as.NA = FALSE,
  missing.S.as.NA = FALSE)
```

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#### **Arguments**

data	Data.frame or matrix containing all required variables.
Rn	Net radiation (W m-2)
G	Ground heat flux (W m-2); optional
S	Sum of all storage fluxes (W m-2); optional
LE	Latent heat flux (W m-2)
Н	Sensible heat flux (W m-2)
instantaneous	should the energy balance be calculated at the time step of the observations (TRUE), or over the entire time period provided as input (FALSE)
missing.G.as.NA	
	if TRUE, missing G are treated as NAs ,otherwise set to 0.
missing.S.as.NA	

if TRUE, missing S are treated as NAs, otherwise set to 0.

#### **Details**

The energy balance ratio (EBR) is calculated as:

$$EBR = sum(LE + H)/sum(Rn - G - S)$$

the sum is taken for all time steps with complete observations (i.e. where all energy balance terms are available).

#### Value

a named vector containing:

n number of complete (all energy balance terms available) observations

 $\begin{array}{ll} \text{intercept} & \text{intercept of the OLS regression} \\ \text{slope} & \text{slope of the OLS regression} \\ \text{r\_squared} & \text{r^2 of the OLS regression} \\ \text{EBR} & \text{energy balance ratio} \end{array}$ 

if instantaneous = TRUE, only EBR is returned.

#### References

Wilson K., et al. 2002: Energy balance closure at FLUXNET sites. Agricultural and Forest Meteorology 113, 223-243.

```
## characterize energy balance closure for DE-Tha in June 2014
energy.closure(DE_Tha_Jun_2014,instantaneous=FALSE)

## look at half-hourly closure
EBR_inst <- energy.closure(DE_Tha_Jun_2014,instantaneous=TRUE)
summary(EBR_inst)</pre>
```

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```
energy.use.efficiency Energy-Use Efficiency (EUE)
```

# Description

Fraction of net radiation fixed by primary productivity.

## Usage

```
energy.use.efficiency(GPP, alpha = 0.422, Rn)
```

## **Arguments**

GPP Gross primary productivity exchange (umol CO2 m-2 s-1)

alpha Energy taken up/released by photosynthesis/respiration (J umol-1)

Rn Net radiation (W m-2)

## **Details**

Energy use efficiency is calculated as:

$$EUE = sum(GPP)/sum(Rn)$$

where the sums are calculated for complete cases of GPP and Rn over the entire time period.

## Value

```
EUE - Energy use efficiency (-)
```

## See Also

```
light.use.efficiency
```

```
energy.use.efficiency(GPP=20,Rn=500)
```

```
equilibrium.imposed.ET
```

Equilibrium and Imposed Evapotranspiration

# **Description**

Evapotranspiration (ET) split up into imposed ET and equilibrium ET.

## Usage

```
equilibrium.imposed.ET(
   data,
   Tair = "Tair",
   pressure = "pressure",
   VPD = "VPD",
   Gs = "Gs_ms",
   Rn = "Rn",
   G = NULL,
   S = NULL,
   missing.G.as.NA = FALSE,
   missing.S.as.NA = FALSE,
   Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
   constants = bigleaf.constants()
)
```

# **Arguments**

data Data.frame or matrix containing all required input variables Air temperature (deg C) Tair Atmospheric pressure (kPa) pressure **VPD** Air vapor pressure deficit (kPa) surface conductance to water vapor (m s-1) Gs Net radiation (W m-2) Rn G Ground heat flux (W m-2); optional Sum of all storage fluxes (W m-2); optional missing.G.as.NA if TRUE, missing G are treated as NAs, otherwise set to 0. missing.S.as.NA if TRUE, missing S are treated as NAs, otherwise set to 0. Esat.formula Optional: formula to be used for the calculation of esat and the slope of esat. One of "Sonntag\_1990" (Default), "Alduchov\_1996", or "Allen\_1998". See Esat.slope. constants cp - specific heat of air for constant pressure (J K-1 kg-1) eps - ratio of the molecular weight of water vapor to dry air (-) Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)

#### **Details**

Total evapotranspiration can be written in the form (Jarvis & McNaughton 1986):

$$ET = \Omega ET_e q + (1 - \Omega)ET_i mp$$

where  $\Omega$  is the decoupling coefficient as calculated from decoupling. ET\_eq is the equilibrium evapotranspiration rate, the ET rate that would occur under uncoupled conditions, where the heat budget is dominated by radiation (when Ga -> 0):

$$ET_eq = (\Delta * (Rn - G - S) * \lambda)/(\Delta + \gamma)$$

where  $\Delta$  is the slope of the saturation vapor pressure curve (kPa K-1),  $\lambda$  is the latent heat of vaporization (J kg-1), and  $\gamma$  is the psychrometric constant (kPa K-1). ET\_imp is the imposed evapotranspiration rate, the ET rate that would occur under fully coupled conditions (when Ga -> inf):

$$ET_imp = (\rho * cp * VPD * Gs * \lambda)/\gamma$$

where  $\rho$  is the air density (kg m-3).

#### Value

A data.frame with the following columns:

ET_eq	Equilibrium ET (kg m-2 s-1)
ET_imp	Imposed ET (kg m-2 s-1)
LE_eq	Equilibrium LE (W m-2)
LE_imp	Imposed LE (W m-2)

#### Note

Surface conductance (Gs) can be calculated with surface.conductance. Aerodynamic conductance (Ga) can be calculated using aerodynamic.conductance.

# References

Jarvis, P.G., McNaughton, K.G., 1986: Stomatal control of transpiration: scaling up from leaf to region. Advances in Ecological Research 15, 1-49.

Monteith, J.L., Unsworth, M.H., 2008: Principles of Environmental Physics. 3rd edition. Academic Press, London.

#### See Also

decoupling

```
\label{eq:continuous} \begin{split} &\text{df <- data.frame(Tair=20,pressure=100,VPD=seq(0.5,4,0.5),} \\ &\text{Gs\_ms=seq(0.01,0.002,length.out=8),Rn=seq(50,400,50))} \\ &\text{equilibrium.imposed.ET(df)} \end{split}
```

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Esat.slope

Saturation Vapor Pressure (Esat) and Slope of the Esat Curve

#### **Description**

Calculates saturation vapor pressure (Esat) over water and the corresponding slope of the saturation vapor pressure curve.

## Usage

```
Esat.slope(
   Tair,
   formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
   constants = bigleaf.constants()
)
```

## **Arguments**

Tair Air temperature (deg C)

formula Formula to be used. Either "Sonntag\_1990" (Default), "Alduchov\_1996", or

"Allen\_1998".

constants Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)

## **Details**

Esat (kPa) is calculated using the Magnus equation:

$$Esat = a * exp((b * Tair)/(c + Tair))/1000$$

where the coefficients a, b, c take different values depending on the formula used. The default values are from Sonntag 1990 (a=611.2, b=17.62, c=243.12). This version of the Magnus equation is recommended by the WMO (WMO 2008; p1.4-29). Alternatively, parameter values determined by Alduchov & Eskridge 1996 or Allen et al. 1998 can be used (see references). The slope of the Esat curve  $(\Delta)$  is calculated as the first derivative of the function:

$$\Delta = dEsat/dTair$$

which is solved using D.

## Value

A dataframe with the following columns:

Esat Saturation vapor pressure (kPa)

Delta Slope of the saturation vapor pressure curve (kPa K-1)

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#### References

Sonntag D. 1990: Important new values of the physical constants of 1986, vapor pressure formulations based on the ITS-90 and psychrometric formulae. Zeitschrift fuer Meteorologie 70, 340-344.

World Meteorological Organization 2008: Guide to Meteorological Instruments and Methods of Observation (WMO-No.8). World Meteorological Organization, Geneva. 7th Edition.

Alduchov, O. A. & Eskridge, R. E., 1996: Improved Magnus form approximation of saturation vapor pressure. Journal of Applied Meteorology, 35, 601-609

Allen, R.G., Pereira, L.S., Raes, D., Smith, M., 1998: Crop evapotranspiration - Guidelines for computing crop water requirements - FAO irrigation and drainage paper 56, FAO, Rome.

#### **Examples**

```
Esat.slope(seq(0,45,5))[,"Esat"] # Esat in kPa
Esat.slope(seq(0,45,5))[,"Delta"] # the corresponding slope of the Esat curve (Delta) in kPa K-1
```

extraterrestrial.radiation

Extraterrestrial solar radiation

## **Description**

Compute the extraterrestrial solar radiation with the

## Usage

```
extraterrestrial.radiation(doy, constants = bigleaf.constants())
```

## **Arguments**

```
doy integer vector with day of year (DoY)
constants solar constant - solar constant (W m-2)
```

#### **Details**

Computation follows Lanini, 2010 (Master thesis, Bern University)

#### Value

```
numeric vector of extraterrestrial radiation (W_m-2)
```

```
plot(1:365, extraterrestrial.radiation(1:365), type = "l"
   , ylab = "radiation (W m-2)", xlab = "day of year")
```

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filter.data

Basic Eddy Covariance Data Filtering

# **Description**

Filters time series of EC data for high-quality values and specified meteorological conditions.

# Usage

```
filter.data(
  data,
  quality.control = TRUE,
  filter.growseas = FALSE,
  filter.precip = FALSE,
  filter.vars = NULL,
  filter.vals.min,
  filter.vals.max,
 NA.as.invalid = TRUE,
  vars.qc = NULL,
  quality.ext = "_qc",
  good.quality = c(0, 1),
 missing.qc.as.bad = TRUE,
  GPP = "GPP",
  doy = "doy",
  year = "year",
  tGPP = 0.5,
 ws = 15,
 min.int = 5,
  precip = "precip",
  tprecip = 0.01,
  precip.hours = 24,
  records.per.hour = 2,
  filtered.data.to.NA = TRUE,
  constants = bigleaf.constants()
)
```

# Arguments

,	
data	Data.frame or matrix containing all required input variables in half-hourly or hourly resolution. Including year, month, day information
quality.control	
	Should quality control be applied? Defaults to TRUE.
filter.growseas	
	Should data be filtered for growing season? Defaults to FALSE.
filter.precip	Should precipitation filtering be applied? Defaults to FALSE.
filter.vars	Additional variables to be filtered. Vector of type character.

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filter.vals.min

Minimum values of the variables to be filtered. Numeric vector of the same length than filter.vars. Set to NA to be ignored.

filter.vals.max

Maximum values of the variables to be filtered. Numeric vector of the same length than filter.vars. Set to NA to be ignored.

NA. as. invalid If TRUE (the default) missing data are filtered out (applies to all variables).

vars.qc Character vector indicating the variables for which quality filter should be applied. Ignored if quality.control = FALSE.

quality.ext The extension to the variables' names that marks them as quality control variables. Ignored if quality.control = FALSE.

good.quality Which values indicate good quality (i.e. not to be filtered) in the quality control (qc) variables? Ignored if quality.control = FALSE.

missing.qc.as.bad

If quality control variable is NA, should the corresponding data point be treated as bad quality? Defaults to TRUE. Ignored if quality.control = FALSE.

GPP Gross primary productivity (umol m-2 s-1); Ignored if filter.growseas = FALSE.

doy Day of year; Ignored if filter.growseas = FALSE.

year Year; Ignored if filter.growseas = FALSE.

tGPP GPP threshold (fraction of 95th percentile of the GPP time series). Must be

between 0 and 1. Ignored if filter.growseas is FALSE.

ws Window size used for GPP time series smoothing. Ignored if filter.growseas

= FALSE.

min.int Minimum time interval in days for a given state of growing season. Ignored if

filter.growseas = FALSE.

precip Precipitation (mm time-1)

tprecip Precipitation threshold used to identify a precipitation event (mm). Ignored if

filter.precip = FALSE.

precip. hours Number of hours removed following a precipitation event (h). Ignored if filter.precip

= FALSE.

records.per.hour

Number of observations per hour. I.e. 2 for half-hourly data.

filtered.data.to.NA

Logical. If TRUE (the default), all variables in the input data.frame/matrix are set to NA for the time step where ANY of the filter.vars were beyond their acceptable range (as determined by filter.vals.min and filter.vals.max). If FALSE, values are not filtered, and an additional column 'valid' is added to the data.frame/matrix, indicating if any value of a row did (1) or did not fulfill the

filter criteria (0).

constants frac2percent - conversion between fraction and percent

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#### **Details**

This routine consists of two parts:

1) Quality control: All variables included in vars.qc are filtered for good quality data. For these variables a corresponding quality variable with the same name as the variable plus the extension as specified in quality.ext must be provided. For time steps where the value of the quality indicator is not included in the argument good.quality, i.e. the quality is not considered as 'good', its value is set to NA.

2) Meteorological filtering. Under certain conditions (e.g. low ustar), the assumptions of the EC method are not fulfilled. Further, some data analysis require certain meteorological conditions, such as periods without rainfall, or active vegetation (growing season, daytime). The filter applied in this second step serves to exclude time periods that do not fulfill the criteria specified in the arguments. More specifically, time periods where one of the variables is higher or lower than the specified thresholds (filter.vals.min and filter.vals.max) are set to NA for all variables. If a threshold is set to NA, it will be ignored.

#### Value

If filtered.data.to.NA = TRUE (default), the input data.frame/matrix with observations which did not fulfill the filter criteria set to NA. If filtered.data.to.NA = FALSE, the input data.frame/matrix with an additional column "valid", which indicates whether all the data of a time step fulfill the filtering criteria (1) or not (0).

#### Note

The thresholds set with filter.vals.min and filter.vals.max filter all data that are smaller than ("<"), or greater than (">") the specified thresholds. That means if a variable has exactly the same value as the threshold, it will not be filtered. Likewise, tprecip filters all data that are greater than tprecip.

Variables considered of bad quality (as specified by the corresponding quality control variables) will be set to NA by this routine. Data that do not fulfill the filtering criteria are set to NA if filtered.data.to.NA = TRUE. Note that with this option \*all\* variables of the same time step are set to NA. Alternatively, if filtered.data.to.NA = FALSE data are not set to NA, and a new column "valid" is added to the data.frame/matrix, indicating if any value of a row did (1) or did not fulfill the filter criteria (0).

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```
year="year",tGPP=0.5,ws=15,min.int=5,precip="precip",
                                tprecip=0.1,precip.hours=24,records.per.hour=2,
                                filtered.data.to.NA=TRUE)
## same, but with filtered.data.to.NA=FALSE
DE_Tha_Jun_2014_3 <- filter.data(DE_Tha_Jun_2014,quality.control=FALSE,</pre>
                                vars.qc=c("Tair","precip","H","LE"),
                                filter.growseas=FALSE,filter.precip=TRUE,
                                filter.vars=c("Tair","PPFD","ustar"),
                                filter.vals.min=c(5,200,0.2),
                                filter.vals.max=c(NA,NA,NA),NA.as.invalid=TRUE,
                                quality.ext="_qc",good.quality=c(0,1),
                                missing.qc.as.bad=TRUE,GPP="GPP",doy="doy",
                                year="year",tGPP=0.5,ws=15,min.int=5,precip="precip",
                                tprecip=0.1,precip.hours=24,records.per.hour=2,
                                filtered.data.to.NA=FALSE)
# note the additional column 'valid' in DE_Tha_Jun_2014_3.
# To remove time steps marked as filtered out (i.e. 0 values in column 'valid'):
DE_Tha_Jun_2014_3[DE_Tha_Jun_2014_3["valid"] == 0,] <- NA
```

filter.growing.season GPP-based Growing Season Filter

#### **Description**

Filters annual time series for growing season based on smoothed daily GPP data.

# Usage

```
filter.growing.season(GPPd, tGPP, ws = 15, min.int = 5)
```

#### **Arguments**

GPPd	daily GPP (any unit)
tGPP	GPP threshold (fraction of 95th percentile of the GPP time series). Takes values between $0$ and $1$ .
WS	window size used for GPP time series smoothing
min.int	minimum time interval in days for a given state of growing season

## **Details**

The basic idea behind the growing season filter is that vegetation is considered to be active when its carbon uptake (GPP) is above a specified threshold, which is defined relative to the peak GPP (95th percentile) observed in the year. The GPP-threshold is calculated as:

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$$GPP_threshold = quantile(GPPd, 0.95) * tGPP$$

GPPd time series are smoothed with a moving average to avoid fluctuations in the delineation of the growing season. The window size defaults to 15 days, but depending on the ecosystem, other values can be appropriate.

The argument min.int serves to avoid short fluctuations in the status growing season vs. no growing season by defining a minimum length of the status. If a time interval shorter than min.int is labeled as growing season or non-growing season, it is changed to the status of the neighboring values.

#### Value

a vector of type integer of the same length as the input GPPd in which 0 indicate no growing season (dormant season) and 1 indicate growing season.

FR\_Pue\_May\_2012

Eddy Covariance Data of FR-Pue (Puechabon)

# **Description**

Halfhourly eddy covariance Data of the site FR-Pue, a Mediterranean evergreen oak forest in Southern France (https://sites.fluxdata.org/FR-Pue/). Data are from May 2012.

#### Usage

```
FR_Pue_May_2012
```

#### **Format**

A data frame with 1488 observations and 29 columns:

year year of measurement

month month of measurement

doy day of year

**hour** hour (0 - 23.5)

**Tair** Air temperature (degC) [TA\_F]

Tair\_qc Quality control of Tair [TA\_F\_QC]

**PPFD** Photosynthetic photon flux density (umol m-2 s-1) [PPFD\_IN]

PPFD\_qc Quality control of PPFD [PPFD\_IN\_QC]

**VPD** Vapor pressure deficit (kPa) [VPD\_F]

**VPD\_qc** Quality control of VPD [VPD\_F\_QC]

pressure Atmospheric pressure (kPa) [PA\_F]

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```
precip precipitation (mm) [P_F]
precip_qc Quality control of precip [P_F_QC]
ustar friction velocity (m s-1) [USTAR]
wind horizontal wind velocity (m s-1) [WS_F]
wind_qc Quality control of wind [WS_F_QC]
Ca CO2 concentration (ppm) [CO2 F MDS]
Ca_qc Quality control of Ca [CO2_F_MDS_QC]
LW_up upward longwave radiation (W m-2) [LW_OUT]
Rn Net radiation (W m-2) [NETRAD]
LE Latent heat flux (W m-2) [LE_F_MDS]
LE_qc Quality control of LE [LE_F_MDS_QC]
H Sensible heat flux (W m-2) [H_F_MDS]
H_qc Quality control of H [H_F_MDS_QC]
NEE Net ecosystem exchange (umol m-2 s-1) [NEE_VUT_USTAR50]
NEE qc Quality control of NEE [NEE VUT USTAR50 QC]
GPP Gross primary productivity from nighttime partitioning (umol m-2 s-1) [GPP_NT_VUT_USTAR50]
GPP_qc Quality control of GPP [NEE_VUT_USTAR50_QC]
Reco Ecosystem respiration from nighttime partitioning (umol m-2 s-1) [RECO_NT_VUT_USTAR50]
```

#### Note

The original variable names as provided by the FLUXNET2015 dataset are given in squared brackets. Note that variable units have been converted in some cases (e.g. VPD from hPa to kPa).

#### Source

original data were downloaded from https://fluxnet.org/ (accessed 09 November 2016)

Gb.Choudhury Boundary Layer Conductance according to Choudhury & M. 1988	lonteith
--	----------

#### **Description**

A formulation for the canopy boundary layer conductance for heat transfer according to Choudhury & Monteith 1988.

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#### Usage

```
Gb.Choudhury(
  data,
  Tair = "Tair",
 pressure = "pressure",
 wind = "wind",
  ustar = "ustar",
 H = "H",
  leafwidth,
 LAI,
  zh,
  zr,
  d,
  z0m = NULL,
  stab_formulation = c("Dyer_1970", "Businger_1971"),
  Sc = NULL,
  Sc_name = NULL,
  constants = bigleaf.constants()
)
```

# **Arguments**

data Data.frame or matrix containing all required variables

Tair Air temperature (degC)
pressure Atmospheric pressure (kPa)

wind Wind speed at sensor height (m s-1)

ustar Friction velocity (m s-1)

H Sensible heat flux (W m-2)

leafwidth Leaf width (m)

LAI One-sided leaf area index

zh Canopy height (m)

zr Instrument (reference) height (m)

d Zero-plane displacement height (-), can be calculated using roughness.parameters

z0m Roughness length for momentum (m). If not provided, calculated from roughness.parameters

within wind.profile

stab\_formulation

Stability correction function used (If stab\_correction = TRUE). Either "Dyer\_1970"

or "Businger\_1971".

Sc Optional: Schmidt number of additional quantities to be calculated

Sc\_name Optional: Name of the additional quantities, has to be of same length than

Sc\_name

constants k - von-Karman constant

Sc\_CO2 - Schmidt number for CO2 Pr - Prandtl number (if Sc is provided) Gb.Choudhury 33

#### **Details**

Boundary layer conductance according to Choudhury & Monteith 1988 is given by:

$$Gb_h = LAI((2a/\alpha) * sqrt(u(h)/w) * (1 - exp(-\alpha/2)))$$

where u(zh) is the wind speed at the canopy surface, approximated from measured wind speed at sensor height zr and a wind extinction coefficient  $\alpha$ :

$$u(zh) = u(zr)/(exp(\alpha(zr/zh - 1)))$$

.

 $\alpha$  is modeled as an empirical relation to LAI (McNaughton & van den Hurk 1995):

$$\alpha = 4.39 - 3.97 * exp(-0.258 * LAI)$$

Gb (=1/Rb) for water vapor and heat are assumed to be equal in this package. Gb for other quantities x is calculated as (Hicks et al. 1987):

$$Gb_x = Gb/(Sc_x/Pr)^0.67$$

where  $Sc_x$  is the Schmidt number of quantity x, and Pr is the Prandtl number (0.71).

#### Value

A data frame with the following columns:

Gb\_h Boundary layer conductance for heat transfer (m s-1)
Rb\_h Boundary layer resistance for heat transfer (s m-1)

kB\_h kB-1 parameter for heat transfer

Gb\_Sc\_name Boundary layer conductance for Sc\_name (m s-1). Only added if Sc\_name and

Sc\_name are provided

#### Note

If the roughness length for momentum (z0m) is not provided as input, it is estimated from the function roughness.parameters within wind.profile. This function estimates a single z0m value for the entire time period! If a varying z0m value (e.g. across seasons or years) is required, z0m should be provided as input argument.

## References

Choudhury, B. J., Monteith J.L., 1988: A four-layer model for the heat budget of homogeneous land surfaces. Q. J. R. Meteorol. Soc. 114, 373-398.

McNaughton, K. G., Van den Hurk, B.J.J.M., 1995: A 'Lagrangian' revision of the resistors in the two-layer model for calculating the energy budget of a plant canopy. Boundary-Layer Meteorology 74, 261-288.

Hicks, B.B., Baldocchi, D.D., Meyers, T.P., Hosker, J.R., Matt, D.R., 1987: A preliminary multiple resistance routine for deriving dry deposition velocities from measured quantities. Water, Air, and Soil Pollution 36, 311-330.

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#### See Also

```
Gb. Thom, Gb. Su, aerodynamic.conductance
```

# Examples

```
## bulk canopy boundary layer resistance for a closed canopy (LAI=5)
## with large leaves (leafwdith=0.1)
df <- data.frame(Tair=25,pressure=100,wind=c(3,4,5),ustar=c(0.5,0.6,0.65),H=c(200,230,250))
Gb.Choudhury(data=df,leafwidth=0.1,LAI=5,zh=25,d=17.5,zr=40)
## same conditions, but smaller leaves (leafwidth=0.01)
Gb.Choudhury(data=df,leafwidth=0.01,LAI=5,zh=25,d=17.5,zr=40)</pre>
```

Gb.Su

Boundary Layer Conductance according to Su et al. 2001

# Description

A physically based formulation for the canopy boundary layer conductance to heat transfer according to Su et al. 2001.

# Usage

```
Gb.Su(
  data,
  Tair = "Tair",
  pressure = "pressure",
  ustar = "ustar",
 wind = "wind",
 H = "H"
  zh,
  zr,
  d,
  z0m = NULL
 Dl,
  fc = NULL,
  LAI = NULL,
 N = 2,
  Cd = 0.2,
  hs = 0.01,
  stab_formulation = c("Dyer_1970", "Businger_1971"),
  Sc = NULL,
  Sc_name = NULL,
  constants = bigleaf.constants()
)
```

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#### **Arguments**

data Data.frame or matrix containing all required variables

Tair Air temperature (degC)

pressure Atmospheric pressure (kPa)

ustar Friction velocity (m s-1)

wind Wind speed (m s-1)

H Sensible heat flux (W m-2)

zh Canopy height (m) zr Reference height (m)

d Zero-plane displacement height (-), can be calculated using roughness.parameters

z0m Roughness length for momentum (m). If not provided, calculated from roughness.parameters

within wind.profile

D1 Leaf characteristic dimension (m)

fc Fractional vegetation cover [0-1] (if not provided, calculated from LAI)

LAI One-sided leaf area index (-)

N Number of leaf sides participating in heat exchange (defaults to 2)

Cd Foliage drag coefficient (-)
hs Roughness height of the soil (m)

stab\_formulation

Stability correction function used (If stab\_correction = TRUE). Either "Dyer\_1970"

or "Businger\_1971".

Sc Optional: Schmidt number of additional quantities to be calculated

Sc\_name Optional: Name of the additional quantities, has to be of same length than

Sc\_name

constants Kelvin - conversion degree Celsius to Kelvin

pressure0 - reference atmospheric pressure at sea level (Pa)

Tair0 - reference air temperature (K) Sc\_CO2 - Schmidt number for CO2 Pr - Prandtl number (if Sc is provided)

#### **Details**

The formulation is based on the kB-1 model developed by Massman 1999. Su et al. 2001 derived the following approximation:

$$kB - 1 = (kCdfc^2)/(4Ctustar/u(zh)) + kBs - 1(1 - fc)^2$$

If fc (fractional vegetation cover) is missing, it is estimated from LAI:

$$fc = 1 - exp(-LAI/2)$$

The wind speed at the top of the canopy is calculated using function wind.profile.

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Ct is the heat transfer coefficient of the leaf (Massman 1999):

$$Ct = Pr^-2/3Reh^-1/2N$$

where Pr is the Prandtl number (set to 0.71), and Reh is the Reynolds number for leaves:

$$Reh = Dlwind(zh)/v$$

kBs-1, the kB-1 value for bare soil surface, is calculated according to Su et al. 2001:

$$kBs^{-}1 = 2.46(Re)^{0}.25 - ln(7.4)$$

Gb (=1/Rb) for water vapor and heat are assumed to be equal in this package. Gb for other quantities x is calculated as (Hicks et al. 1987):

$$Gb_x = Gb/(Sc_x/Pr)^0.67$$

where  $Sc_x$  is the Schmidt number of quantity x, and Pr is the Prandtl number (0.71).

#### Value

A data frame with the following columns:

Gb\_h Boundary layer conductance for heat transfer (m s-1)

Rb\_h Boundary layer resistance for heat transfer (s m-1)

kB\_h kB-1 parameter for heat transfer

Gb\_Sc\_name Boundary layer conductance for Sc\_name (m s-1). Only added if Sc\_name and

Sc\_name are provided

# Note

If the roughness length for momentum (z0m) is not provided as input, it is estimated from the function roughness parameters within wind profile. This function estimates a single z0m value for the entire time period! If a varying z0m value (e.g. across seasons or years) is required, z0m should be provided as input argument.

#### References

Su, Z., Schmugge, T., Kustas, W. & Massman, W., 2001: An evaluation of two models for estimation of the roughness height for heat transfer between the land surface and the atmosphere. Journal of Applied Meteorology 40, 1933-1951.

Massman, W., 1999: A model study of kB H- 1 for vegetated surfaces using 'localized near-field' Lagrangian theory. Journal of Hydrology 223, 27-43.

Hicks, B.B., Baldocchi, D.D., Meyers, T.P., Hosker, J.R., Matt, D.R., 1987: A preliminary multiple resistance routine for deriving dry deposition velocities from measured quantities. Water, Air, and Soil Pollution 36, 311-330.

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### See Also

Gb. Thom, Gb. Choudhury, aerodynamic. conductance

#### **Examples**

```
# Canopy boundary layer resistance (and kB-1 parameter) for a set of meteorological conditions, # a leaf characteristic dimension of 1cm, and an LAI of 5 df <- data.frame(Tair=25,pressure=100,wind=c(3,4,5),ustar=c(0.5,0.6,0.65),H=c(200,230,250)) Gb.Su(data=df,zh=25,zr=40,d=17.5,Dl=0.01,LAI=5) # the same meteorological conditions, but larger leaves Gb.Su(data=df,zh=25,zr=40,d=17.5,Dl=0.1,LAI=5) # same conditions, large leaves, and sparse canopy cover (LAI = 1.5) Gb.Su(data=df,zh=25,zr=40,d=17.5,Dl=0.1,LAI=1.5)
```

Gb.Thom

Boundary Layer Conductance according to Thom 1972

### **Description**

An empirical formulation for the canopy boundary layer conductance for heat transfer based on a simple ustar dependency.

### Usage

```
Gb.Thom(ustar, Sc = NULL, Sc_name = NULL, constants = bigleaf.constants())
```

## **Arguments**

ustar Friction velocity (m s-1)

Sc Optional: Schmidt number of additional quantities to be calculated

Sc\_name Optional: Name of the additional quantities, has to be of same length than

Sc\_name

constants k - von-Karman constant

Sc\_CO2 - Schmidt number for CO2 Pr - Prandtl number (if Sc is provided)

#### **Details**

The empirical equation for Rb suggested by Thom 1972 is:

$$Rb = 6.2ustar^-0.67$$

Gb (=1/Rb) for water vapor and heat are assumed to be equal in this package. Gb for other quantities x is calculated as (Hicks et al. 1987):

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$$Gb_x = Gb/(Sc_x/Pr)^0.67$$

where Sc\_x is the Schmidt number of quantity x, and Pr is the Prandtl number (0.71).

#### Value

a data.frame with the following columns:

Gb\_h Boundary layer conductance for heat transfer (m s-1)

Rb\_h Boundary layer resistance for heat transfer (s m-1)

kB\_h kB-1 parameter for heat transfer

Gb\_Sc\_name Boundary layer conductance for Sc\_name (m s-1). Only added if Sc\_name and

Sc\_name are provided

#### References

Thom, A., 1972: Momentum, mass and heat exchange of vegetation. Quarterly Journal of the Royal Meteorological Society 98, 124-134.

Hicks, B.B., Baldocchi, D.D., Meyers, T.P., Hosker, J.R., Matt, D.R., 1987: A preliminary multiple resistance routine for deriving dry deposition velocities from measured quantities. Water, Air, and Soil Pollution 36, 311-330.

#### See Also

Gb.Choudhury, Gb.Su, aerodynamic.conductance

### **Examples**

```
Gb.Thom(seq(0.1,1.4,0.1))
## calculate Gb for SO2 as well
Gb.Thom(seq(0.1,1.4,0.1),Sc=1.25,Sc_name="SO2")
```

intercellular.CO2

Bulk Intercellular CO2 Concentration

## Description

Bulk canopy intercellular CO2 concentration (Ci) calculated based on Fick's law given surface conductance (Gs), gross primary productivity (GPP) and atmospheric CO2 concentration (Ca).

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### Usage

```
intercellular.CO2(
  data,
  Ca = "Ca",
  GPP = "GPP",
  Gs = "Gs_mol",
  Rleaf = NULL,
  missing.Rleaf.as.NA = FALSE,
  constants = bigleaf.constants()
)
```

#### **Arguments**

data	Data.Frame or matrix with all required columns		
Ca	Atmospheric or surface CO2 concentration (umol mol-1)		
GPP	Gross primary productivity (umol CO2 m-2 s-1)		
Gs	Surface conductance to water vapor (mol m-2 s-1)		
Rleaf	Ecosystem respiration stemming from leaves (umol CO2 m-2 s-1); defaults to 0		
missing.Rleaf.as.NA			
	if Rleaf is provided, should missing values be treated as NA (TRUE) or set to 0		
	(FALSE, the default)?		
constants	DwDc - Ratio of the molecular diffusivities for water vapor and CO2 (-)		

### **Details**

Bulk intercellular CO2 concentration (Ci) is given by:

$$Ci = Ca - (GPP - Rleaf)/(Gs/1.6)$$

where Gs/1.6 (mol m-2 s-1) represents the surface conductance to CO2. Note that Gs is required in mol m-2 s-1 for water vapor. Gs is converted to its value for CO2 internally. Ca can either be atmospheric CO2 concentration (as measured), or surface CO2 concentration as calculated from surface.CO2.

#### Value

Ci - Bulk canopy intercellular CO2 concentration (umol mol-1)

# Note

The equation is based on Fick's law of diffusion and is equivalent to the often used equation at leaf level (ci = ca - An/gs). Note that GPP and Gs have a different interpretation than An and gs. Gs comprises non-physiological contributions (i.e. physical evaporation) and is confounded by physical factors (e.g. energy balance non-closure). GPP does not account for dark respiration and is further subject to uncertainties in the NEE partitioning algorithm used. Leaf respiration can be provided, but it is usually not known at ecosystem level (as a consequence, Ci is likely to be slightly underestimated) This function should be used with care and the resulting Ci might not be readily comparable to its leaf-level analogue and/or physiological meaningful.

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### References

Kosugi Y. et al., 2013: Determination of the gas exchange phenology in an evergreen coniferous forest from 7 years of eddy covariance flux data using an extended big-leaf analysis. Ecol Res 28, 373-385.

Keenan T., Sabate S., Gracia C., 2010: The importance of mesophyll conductance in regulating forest ecosystem productivity during drought periods. Global Change Biology 16, 1019-1034.

# Examples

```
# calculate bulk canopy Ci of a productive ecosystem
intercellular.CO2(Ca=400,GPP=40,Gs=0.7)
# note the sign convention for NEE
```

isothermal.Rn

Isothermal Net Radiation

# **Description**

Calculates the isothermal net radiation, i.e. the net radiation that the surface would receive if it had the same temperature than the air.

# Usage

```
isothermal.Rn(
  data,
  Rn = "Rn",
  Tair = "Tair",
  Tsurf = "Tsurf",
  emissivity,
  constants = bigleaf.constants()
)
```

# **Arguments**

data Data.frame or matrix containing all required variables

Rn Net radiation (W m-2)

Tair Air temperature (degC)

Tsurf Surface temperature (degC)

emissivity Emissivity of the surface (-)

constants sigma - Stefan-Boltzmann constant (W m-2 K-4)

Kelvin - conversion degree Celsius to Kelvin

kg.to.mol 41

### **Details**

The isothermal net radiation (Rni) is given by:

$$Rni = Rn + \epsilon * \sigma * (Tsur f^4 - Tair^4)$$

where  $\epsilon$  is the emissivity of the surface. Tsurf and Tair are in Kelvin.

### Value

Rni - isothermal net radiation (W m-2)

### References

Jones, H. 2014: Plants and Microclimate. 3rd edition, Cambridge University Press.

# **Examples**

# calculate isothermal net radiation of a surface that is 2degC warmer than the air. isothermal.Rn(Rn=400,Tair=25,Tsurf=27,emissivity=0.98)

kg.to.mol

Conversion between Mass and Molar Units

# **Description**

Converts mass units of a substance to the corresponding molar units and vice versa.

### Usage

```
kg.to.mol(mass, molarMass = bigleaf.constants()$H2Omol)
```

# **Arguments**

mass Numeric vector of mass in kg

molarMass Numeric vector of molar mass of the substance (kg mol-1) e.g. as provided by

bigleaf.constants()\$H2Omol Default is molar mass of Water.

### Value

Numeric vector of amount of substance in mol.

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kinematic.viscosity Kiner

Kinematic Viscosity of Air

# **Description**

calculates the kinematic viscosity of air.

# Usage

```
kinematic.viscosity(Tair, pressure, constants = bigleaf.constants())
```

# Arguments

Tair Air temperature (deg C)

pressure Atmospheric pressure (kPa)

constants Kelvin - conversion degree Celsius to Kelvin

pressure0 - reference atmospheric pressure at sea level (Pa)

Tair0 - reference air temperature (K)

kPa2Pa - conversion kilopascal (kPa) to pascal (Pa)

#### **Details**

where v is the kinematic viscosity of the air (m2 s-1), given by (Massman 1999b):

$$v = 1.327 * 10^{-5} (pressure0/pressure) (Tair/Tair0)^{1}.81$$

# Value

v - kinematic viscosity of air (m2 s-1)

# References

Massman, W.J., 1999b: Molecular diffusivities of Hg vapor in air, O2 and N2 near STP and the kinematic viscosity and thermal diffusivity of air near STP. Atmospheric Environment 33, 453-457.

# **Examples**

kinematic.viscosity(25,100)

latent.heat.vaporization 43

latent.heat.vaporization

Latent Heat of Vaporization

# Description

Latent heat of vaporization as a function of air temperature.

# Usage

latent.heat.vaporization(Tair)

# Arguments

Tair

Air temperature (deg C)

# **Details**

The following formula is used:

$$\lambda = (2.501 - 0.00237 * Tair)10^6$$

#### Value

 $\lambda$  - Latent heat of vaporization (J kg-1)

# References

Stull, B., 1988: An Introduction to Boundary Layer Meteorology (p.641) Kluwer Academic Publishers, Dordrecht, Netherlands

Foken, T, 2008: Micrometeorology. Springer, Berlin, Germany.

# **Examples**

latent.heat.vaporization(seq(5,45,5))

LE.to.ET

LE.to.ET

Conversion between Latent Heat Flux and Evapotranspiration

# Description

converts evaporative water flux from mass (ET=evapotranspiration) to energy (LE=latent heat flux) units, or vice versa.

# Usage

```
LE.to.ET(LE, Tair)
ET.to.LE(ET, Tair)
```

# **Arguments**

LE Latent heat flux (W m-2)

Tair Air temperature (deg C)

ET Evapotranspiration (kg m-2 s-1)

### **Details**

The conversions are given by:

$$ET = LE/\lambda$$

$$LE = \lambda ET$$

where  $\lambda$  is the latent heat of vaporization (J kg-1) as calculated by latent.heat.vaporization.

# **Examples**

```
\# LE of 200 Wm-2 and air temperature of 25degC LE.to.ET(200,25)
```

light.response 45

light	response	
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Ecosystem Light Response

### **Description**

calculates GPP\_ref at a reference (usually saturating) PPFD and ecosystem quantum yield (alpha) using a rectangular light response curve.

### Usage

```
light.response(
  data,
  NEE = "NEE",
  Reco = "Reco",
  PPFD = "PPFD",
  PPFD_ref = 2000,
  ...
)
```

# Arguments

data	Data.frame or matrix containing all required columns
NEE	Net ecosystem exchange (umol CO2 m-2 s-1)
Reco	Ecosystem respiration (umol CO2 m-2 s-1)
PPFD	Photosynthetic photon flux density (umol m-2 s-1)
PPFD_ref	Reference PPFD (umol m-2 s-1) for which GPP_ref is estimated. Default is $2000 \ \text{umol} \ \text{m-2 s-1}.$
	Additional arguments to nls

#### **Details**

A rectangular light response curve is fitted to NEE data. The curve takes the form as described in Falge et al. 2001:

```
-NEE = \alpha PPFD/(1 - (PPFD/PPFD_ref) + \alpha PPFD/GPP_ref) - Reco
```

where  $\alpha$  is the ecosystem quantum yield (umol CO2 m-2 s-1) (umol quanta m-2 s-1)-1, and GPP\_ref is the GPP at the reference PPFD (usually at saturating light).  $\alpha$  represents the slope of the light response curve, and is a measure for the light use efficiency of the canopy.

The advantage of this equation over the standard rectangular light response curve is that GPP\_ref at PPFD\_ref is more readily interpretable as it constitutes a value observed in the ecosystem, in contrast to GPP\_ref (mostly named 'beta') in the standard model that occurs at infinite light. PPFD\_ref defaults to 2000 umol m-2 s-1, but other values can be used. For further details refer to Falge et al. 2001.

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#### Value

A nls model object containing estimates (+/- SE) for alpha and GPP\_ref.

#### Note

Note the sign convention. Negative NEE indicates that carbon is taken up by the ecosystem. Reco has to be 0 or larger.

#### References

Falge E., et al. 2001: Gap filling strategies for defensible annual sums of net ecosystem exchange. Agricultural and Forest Meteorology 107, 43-69.

Gilmanov T.G., et al. 2003: Gross primary production and light response parameters of four Southern Plains ecosystems estimated using long-term CO2-flux tower measurements. Global Biogeochemical Cycles 17, 1071.

Reichstein M., Stoy P.C., Desai A.R., Lasslop G., Richardson A. 2012: Partitioning of net fluxes. In: Eddy Covariance. A practical guide to measurement and data analysis. Aubinet M., Vesala T., Papale D. (Eds.). Springer.

light.use.efficiency Light-Use Efficiency (LUE)

# Description

Amount of carbon fixed (GPP) per incoming light.

### Usage

```
light.use.efficiency(GPP, PPFD)
```

## Arguments

GPP Gross ecosystem productivity (umol CO2 m-2 s-1)

PPFD Photosynthetic photon flux density (umol quanta m-2 s-1)

### **Details**

Light use efficiency is calculated as

$$LUE = sum(GPP)/sum(PPFD)$$

where both GPP and PPFD are in umol m-2 s-1. A more meaningful (as directly comparable across ecosystems) approach is to take absorbed PPFD rather than incoming PPFD as used here.

### Value

LUE - Light use efficiency (-)

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### See Also

```
energy.use.efficiency
```

### **Examples**

light.use.efficiency(GPP=20,PPFD=1500)

longwave.conductance Longwave Radiative Transfer Conductance of the Canopy

# Description

Longwave Radiative Transfer Conductance of the Canopy

# Usage

longwave.conductance(Tair, LAI, constants = bigleaf.constants())

# **Arguments**

Tair Air temperature (deg C)
LAI Leaf area index (m2 m-2)

constants Kelvin - conversion degree Celsius to Kelvin

sigma - Stefan-Boltzmann constant (W m-2 K-4)

cp - specific heat of air for constant pressure (J K-1 kg-1)

#### **Details**

the following formula is used (Martin, 1989):

$$Gr = 4\sigma Tair^3 LAI/cp$$

# Value

Gr - longwave radiative transfer conductance of the canopy (m s-1)

# References

Martin P., 1989: The significance of radiative coupling between vegetation and the atmosphere. Agricultural and Forest Meteorology 49, 45-53.

# **Examples**

longwave.conductance(25, seq(1,8,1))

Monin.Obukhov.length Monin-Obukhov Length

### **Description**

calculates the Monin-Obukhov length.

# Usage

```
Monin.Obukhov.length(
  data,
  Tair = "Tair",
  pressure = "pressure",
  ustar = "ustar",
  H = "H",
  constants = bigleaf.constants()
)
```

# **Arguments**

data Data.frame or matrix containing all required variables

Tair Air temperature (deg C)
pressure Atmospheric pressure (kPa)
ustar Friction velocity (m s-1)
H Sensible heat flux (W m-2)

constants Kelvin - conversion degree Celsius to Kelvin

cp - specific heat of air for constant pressure (J K-1 kg-1)

k - von Karman constant (-)

g - gravitational acceleration (m s-2)  $\,$ 

#### **Details**

The Monin-Obukhov length (L) is given by:

$$L = -(\rho * cp * ustar^3 * Tair)/(k * g * H)$$

where rho is air density (kg m-3).

### Value

L - Monin-Obukhov length (m)

#### Note

Note that L gets very small for very low ustar values with implications for subsequent functions using L as input. It is recommended to filter data and exclude low ustar values (ustar  $< \sim 0.2$ ) beforehand.

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### References

Foken, T, 2008: Micrometeorology. Springer, Berlin, Germany.

#### See Also

```
stability.parameter
```

# **Examples**

```
Monin.0bukhov.length(Tair=25,pressure=100,ustar=seq(0.2,1,0.1),H=seq(40,200,20))
```

ms.to.mol

Conversion between Conductance Units

# **Description**

Converts conductances from mass (m s-1) to molar units (mol m-2 s-1), or vice versa.

### Usage

```
ms.to.mol(G_ms, Tair, pressure, constants = bigleaf.constants())
mol.to.ms(G_mol, Tair, pressure, constants = bigleaf.constants())
```

# **Arguments**

G_ms	Conductance (m s-1)
Tair	Air temperature (deg C)
pressure	Atmospheric pressure (kPa)
	** 4 1

constants Kelvin - conversion degree Celsius to Kelvin Rgas - universal gas constant (J mol-1 K-1)

kPa2Pa - conversion kilopascal (kPa) to pascal (Pa)

G\_mol Conductance (mol m-2 s-1)

### **Details**

The conversions are given by:

$$G_mol = G_ms * pressure/(Rgas * Tair)$$

$$G_m s = G_m ol * (Rgas * Tair)/pressure$$

where Tair is in Kelvin and pressure in Pa (converted from kPa internally)

optimum.temperature

### References

Jones, H.G. 1992. Plants and microclimate: a quantitative approach to environmental plant physiology. 2nd Edition., Cambridge University Press, Cambridge. 428 p

# **Examples**

```
ms.to.mol(0.005, 25, 100)
```

optimum.temperature

Optimum temperature of Gross Primary Productivity

# Description

Calculates the relationship between Gross Primary Productivity (GPP) and Air Temperature (Tair) using boundary line analysis and derives the thermal optima. This function can also be used to find the boundary line relationship and optima of other variables such as NPP and NEP.

# Usage

```
optimum.temperature(
  data,
  GPP = "GPP",
  Tair = "Tair",
  BLine = 0.9,
  Obs_filter = 30
)
```

# Arguments

data	Dataframe containing the Gross Primary Productivity and Air Temperature observations
GPP	Name of column (in quotations, eg. "GPP") containing the Gross Primary Productivity observations (umol CO2 m-2 s-1).
Tair	Name of column (in quotations, eg. "Tair") containing the air temperature (degrees celcius) observations.
BLine	Quantile at which to place the boundary line in format "0.XX". Defaults to 0.90.
Obs_filter	Filter to remove air temperature bins with an insufficient number of observations. Defaults to 30.

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#### **Details**

This function works by first binning GPP and air temperature observations to 1 degree temperature bins and then deriving the relationship between GPP and air temperature at a defined quantile using boundary line analysis. Observations are binned using a rounding function, so that each bin is centered on the degree integer value (eg. bin 18 contains values between 17.5 and 18.49). The boundary line is usually placed at the upper boundary of the distribution (see Webb 1972) however this functional allows the user to select any quantile, with the default of 0.9 selected for use with eddy covariance flux observations due to the high level of noise in these data (see Bennett et al, 2021). After binning observations, the function removes temperature bins with fewer observations than the default of 30 (this value can also be user defined). It then calculates the smoothed curve between GPP and air temperature using the loess function and derives the thermal optima of GPP (Topt). Topt is defined as the temperature bin at which GPP reaches its maximum along the smoothed boundary line.

#### Value

A list containing the following objects:

- 1. df.bl: A four column dataframe:
  - Tair\_bin: air temperature bins in 1 degree increments
  - GPP Bline: Value of GPP at the BLine
  - n\_obs: number of observations in the air temperature bin
  - GPP Bline smooth: Value of GPP at the smoothed Bline
- 2. opt.temp: A named vector with two elements:
  - Topt: Thermal optima of GPP the air temperature bin with maximum GPP along the smoothed Bline
  - GPP\_bl: The boundary line GPP observation at Topt

### References

Bennett A. et al., 2021: Thermal optima of gross primary productivity are closely aligned with mean air temperatures across Australian wooded ecosystems. Global Change Biology 32(3), 280-293

Webb, R. A. 1972. Use of the Boundary Line in the analysis of biological data. Journal of Horticultural Science 47, 309-319

#### **Examples**

```
photosynthetic.capacity
```

Bulk Canopy Photosynthetic Capacity (Vcmax and Jmax)

# **Description**

Bulk canopy maximum carboxylation rate (Vcmax25), and maximum electron transport rate (Jmax25) at 25 degrees Celsius from bulk intercellular CO2 concentration using the Farquhar et al. 1980 model for C3 photosynthesis.

# Usage

```
photosynthetic.capacity(
  data,
 C3 = TRUE,
 Temp,
 GPP = "GPP",
 Ci,
 PPFD = "PPFD",
 PPFD_j = c(200, 500),
 PPFD_c = 1000,
 Rleaf = NULL,
 0i = 0.21,
 Kc25 = 404.9,
 Ko25 = 278.4
 Gam25 = 42.75,
 Kc_{Ha} = 79.43,
 Ko_{Ha} = 36.38,
 Gam_{Ha} = 37.83,
  Vcmax_Ha = 65.33,
  Vcmax_Hd = 200,
  Vcmax_dS = 0.635,
  Jmax_Ha = 43.9,
  Jmax_Hd = 200,
  Jmax_dS = 0.64,
  Theta = 0.7,
  alpha_canopy = 0.8,
 missing.Rleaf.as.NA = FALSE,
 Ci_C4 = 100,
  constants = bigleaf.constants()
)
```

### **Arguments**

Data.Frame or matrix with all required columns
C3 C3 vegetation (TRUE, the default) or C4 vegetation (FALSE)?

	Temp	Surface (or air) temperature (degC)
	GPP	Gross primary productivity (umol m-2 s-1)
	Ci	Bulk canopy intercellular CO2 concentration (umol mol-1)
	PPFD	Photosynthetic photon flux density (umol m-2 s-1)
	PPFD_j	PPFD threshold, below which the canopy is considered to be RuBP regeneration limited. Defaults to $500$ umol m-2 s-1.
	PPFD_c	PPFD threshold, above which the canopy is considered to be Rubisco limited. Defaults to $1000 \text{ umol } \text{m-}2 \text{ s-}1.$
	Rleaf	Ecosystem respiration stemming from leaves (umol CO2 m-2 s-1); defaults to $0$
	Oi	Intercellular O2 concentration (mol mol-1)
	Kc25	Michaelis-Menten constant for CO2 at 25 degC (umol mol-1)
	Ko25	Michaelis-Menten constant for O2 at 25 degC (mmol mol-1)
	Gam25	Photorespiratory CO2 compensation point ('Gamma star') at 25 degC (umol $$ mol-1)
	Kc_Ha	Activation energy for Kc (kJ mol-1)
	Ko_Ha	Activation energy for Ko (kJ mol-1)
	Gam_Ha	Activation energy for Gam (kJ mol-1)
	Vcmax_Ha	Activation energy for Vcmax (kJ mol-1)
	Vcmax_Hd	Deactivation energy for Vcmax (kJ mol-1)
	Vcmax_dS	Entropy term for Vcmax (kJ mol-1 K-1)
	Jmax_Ha	Activation energy for Jmax (kJ mol-1)
	Jmax_Hd	Deactivation energy for Jmax (kJ mol-1)
	Jmax_dS	Entropy term for Jmax (kJ mol-1 K-1)
	Theta	Curvature term in the light response function of J (-)
alpha_canopy Canopy absorptance (-)		Canopy absorptance (-)
	missing.Rleaf.a	
		if Rleaf is provided, should missing values be treated as NA (TRUE) or set to 0 (FALSE, the default)?
	Ci_C4	intercellular CO2 concentration below which photosynthesis is considered to be CO2-limited (umol mol-1), ignored if C3 = TRUE.
	constants	Kelvin - conversion degree Celsius to Kelvin Rgas - universal gas constant (J mol-1 K-1) kJ2J - conversion kilojoule (kJ) to joule (J) J2kJ - conversion joule (J) to kilojoule (kJ) se_median - conversion standard error (SE) of the mean to SE of the median

# **Details**

The maximum carboxylation rate at 25 degC (Vcmax25) and the maximum electron transport rate at 25 degC (Jmax25), which characterize photosynthetic capacity, are calculated as at leaf level. The required variables Gs and Ci can be calculated from surface.conductance and intercellular.CO2, respectively.

Gas exchange parameters are taken from Bernacchi et al. 2001 (apparent values, which assume an infinite mesophyll conductance). Negative and very low Ci values (the threshold is set to Ci < 80umol mol-1 at the moment) are filtered out.

Vcmax is calculated from the photosynthesis model by Farquhar et al. 1980. If net photosynthesis is Rubisco-limited (RuBP-saturated carboxylation rate, i.e. light has to be (near-)saturating):

$$Vcmax = (GPP * (Ci + Kc * (1.0 + Oi/Ko)))/(Ci - Gam)$$

where Kc and Ko are the Michaelis-Menten constants for CO2 and O2 (mmol mol-1), respectively, Oi is the O2 concentration, and Gam is the photorespiratory CO2 compensation point (umol mol-1). Under low-light conditions, the electron transport rate J is calculated from the RuBP regeneration-limited photosynthesis rate:

$$J = (GPP * (4.0 * Ci + 8.0 * Gam)/(Ci - Gam))$$

In this function, bulk canopy photosynthesis is assumed to be Rubisco/RuBP-regeneration limited, if incoming PPFD is above/below a specified threshold or range. These ranges are determined by the parameters PPFD\_j and PPFD\_c. If, for example, PPFD\_j = c(100,400), all conditions with a PPFD between 100 and 400 are assumed to be in the RuBP-regeneration (i.e. light-limited) photosynthesis domain. The electron transport rate J is then only calculated for periods that meet this criterion.

Jmax is calculated from J and absorbed irradiance:

$$J = (APPFD_PSII + Jmax - sqrt((APPFD_PSII + Jmax)^2 - 4.0*Theta*APPFD_PSII*Jmax))/(2.0*Theta)$$

where APPFD\_PSII is the absorbed PPFD by photosystem II (PS II), and Theta is a curvature parameter. APPFD\_PSII is calculated as

$$PPFD * alpha_canopy * 0.85 * beta$$

where alpha\_canopy is canopy-scale absorptance, 0.85 is a correction factor, and beta is the fraction of photons absorbed by PS II (assumed 0.5). alpha\_canopy accounts for non-absorbing components of the ecosystem such as stems or soil, and is very likely ecosystem-specific. This parameter is relatively sensitive for the determination of Jmax25 at some sites.

Vcmax and Jmax at canopy level are assumed to follow the same temperature response as at leaf level. Hence, the respective parameter k at 25degC (k25) is calculated as (see e.g. Kattge & Knorr 2007):

$$k25 = k/(exp(Ha*(Temp-Tref)/(Tref*Rgas*Temp))*(1 + exp((Tref*dS-Hd)/(Tref*Rgas)))/(1 + exp((Temp-Tref)/(Tref*Rgas*Temp)))$$

where Ha is the activation energy (kJ mol-1), Hd is the deactivation energy (kJ mol-1), and dS is the entropy term (kJ mol-1 K-1) of the respective parameter. Tref is set to 298.15 K.

For C4 photosynthesis, the simplified model by von Caemmerer 2000 is used. For light-saturated photosynthesis, Vcmax is given by:

$$Vcmax = GPP$$

Note that in addition to the range PPFD\_c, the range Ci\_C4 discards all periods with low Ci, in which photosynthesis is likely to be CO2-limited (see von Caemmerer 2000 for details).

In the light-limited case, J is calculated as:

$$J = 3 * GPPj/(1 - 0.5)$$

The calculation of Jmax25 and Vcmax25 is identical to C3 photosynthesis as described above.

#### Value

a data.frame with the following columns:

Vcmax25 maximum bulk canopy carboxylation rate at 25degC (umol m-2 (ground) s-1)

Jmax25 maximum bulk canopy electron transport rate at 25degC (umol m-2 (ground) s-1)

#### Note

The critical assumption is that bulk canopy photosynthesis is limited by one of the two limitation states. Incoming PPFD is assumed to determine the limitation states. Note however that the ranges (PPFD\_j and PPFD\_c) are likely ecosystem-specific. E.g. dense canopies presumably require higher PPFD\_c thresholds than open canopies. A threshold of 500 umol m-2 s-1 PPFD for Rubisco-limited photosynthesis was assumed a reasonable working assumption (see Kosugi et al. 2013). Here, PPFD\_c defaults to 1000 umol m-2 s-1. Note that even under very high/low irradiances, not all photosynthetically active plant material of an ecosystem will be in the same limitation state. Note that parameters describing bulk canopy photosynthetic capacity are not directly comparable to their leaf-level counterparts, as the former integrate over the entire canopy depth (i.e. are given per ground area, and not per leaf area). In general, the function should be used with care!

#### References

Lloyd J. et al., 1995: A simple calibrated model of Amazon rainforest productivity based on leaf biochemical properties. Plant, Cell and Environment 18, 1129-1145.

Rayment M.B., Loustau D., Jarvis P.G., 2002: Photosynthesis and respiration of black spruce at three organizational scales: shoot, branch and canopy. Tree Physiology 22, 219-229.

Kosugi Y. et al., 2013: Determination of the gas exchange phenology in an evergreen coniferous forest from 7 years of eddy covariance flux data using an extended big-leaf analysis. Ecol Res 28, 373-385.

Ueyama M. et al, 2016: Optimization of a biochemical model with eddy covariance measurements in black spruce forests of Alaska for estimating CO2 fertilization effects. Agricultural and Forest Meteorology 222, 98-111.

Bernacchi C.J., Singsaas E.L., Pimentel C., Portis JR A.R., Long S.P., 2001: Improved temperature response functions for models of Rubisco-limited photosynthesis. Plant, Cell and Environment 24, 253-259.

Bernacchi C.J., Pimentel C., Long S.P., 2003: In vivo temperature response functions of parameters required to model RuBP-limited photosynthesis. Plant, Cell and Environment 26, 1419-1430.

von Caemmerer, 2000: Biochemical models of leaf photosynthesis. Techniques in plant sciences No. 2. CSIRO Publishing, Collingwood VIC, Australia.

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### See Also

```
intercellular.CO2, Arrhenius.temp.response
```

### **Examples**

```
DE_Tha_Jun_2014_2 <- filter.data(DE_Tha_Jun_2014, quality.control=FALSE,
                                 vars.qc=c("Tair","precip","VPD","H","LE"),
                                 filter.growseas=FALSE,filter.precip=TRUE,
                                 filter.vars=c("Tair","PPFD","ustar","LE"),
                                 filter.vals.min=c(5,200,0.2,0),
                                 filter.vals.max=c(NA,NA,NA,NA),NA.as.invalid=TRUE,
                                 quality.ext="_qc",good.quality=c(0,1),
                                 missing.qc.as.bad=TRUE,GPP="GPP",doy="doy",
                                 year="year",tGPP=0.5,ws=15,min.int=5,precip="precip",
                                 tprecip=0.1,precip.hours=24,records.per.hour=2)
# calculate Ga
Ga <- aerodynamic.conductance(DE_Tha_Jun_2014_2,Rb_model="Thom_1972")[,"Ga_h"]
# calculate Gs from the the inverted PM equation
Gs_PM <- surface.conductance(DE_Tha_Jun_2014_2,Tair="Tair",pressure="pressure",
                             Rn="Rn", G="G", S=NULL, VPD="VPD", Ga=Ga,
                             formulation="Penman-Monteith")[,"Gs_mol"]
# calculate Ci
Ci <- intercellular.CO2(DE_Tha_Jun_2014_2, Ca="Ca", GPP="GPP", Gs=Gs_PM)
# calculate Vcmax25 and Jmax25
photosynthetic.capacity(DE_Tha_Jun_2014_2,Temp="Tair",Ci=Ci,PPFD_j=c(200,500),PPFD_c=1000)
```

potential.ET

Potential Evapotranspiration

### Description

Potential evapotranspiration according to Priestley & Taylor 1972 or the Penman-Monteith equation with a prescribed surface conductance.

# Usage

```
potential.ET(
  data,
  Tair = "Tair",
  pressure = "pressure",
  Rn = "Rn",
  G = NULL,
  S = NULL,
  VPD = "VPD",
```

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```
Ga = "Ga_h",
approach = c("Priestley-Taylor", "Penman-Monteith"),
alpha = 1.26,
Gs_pot = 0.6,
missing.G.as.NA = FALSE,
missing.S.as.NA = FALSE,
Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
constants = bigleaf.constants()
```

# Arguments

data	Data.frame or matrix containing all required variables; optional			
Tair	Air temperature (degC)			
pressure	Atmospheric pressure (kPa)			
Rn	Net radiation (W m-2)			
G	Ground heat flux (W m-2); optional			
S	Sum of all storage fluxes (W m-2); optional			
VPD	Vapor pressure deficit (kPa); only used if approach = "Penman-Monteith".			
Ga	Aerodynamic conductance to heat/water vapor (m s-1); only used if approach = "Penman-Monteith".			
approach	Approach used. Either "Priestley-Taylor" (default), or "Penman-Monteith".			
alpha	Priestley-Taylor coefficient; only used if approach = "Priestley-Taylor".			
Gs_pot	Potential/maximum surface conductance (mol m-2 s-1); defaults to 0.6 mol m-2 s-1; only used if approach = "Penman-Monteith".			
missing.G.as.NA				
	if TRUE, missing G are treated as NAs, otherwise set to 0.			
missing.S.as.NA				
	if TRUE, missing S are treated as NAs, otherwise set to 0.			
Esat.formula	Optional: formula to be used for the calculation of esat and the slope of esat. One of "Sonntag_1990" (Default), "Alduchov_1996", or "Allen_1998". See Esat.slope.			
constants	cp - specific heat of air for constant pressure (J K-1 kg-1) eps - ratio of the molecular weight of water vapor to dry air Pa2kPa - conversion pascal (Pa) to kilopascal (kPa) Rd - gas constant of dry air (J kg-1 K-1) (only used if approach = "Penman-Monteith") Rgas - universal gas constant (J mol-1 K-1) (only used if approach = "Penman-Monteith") Kelvin - conversion degree Celsius to Kelvin (only used if approach = "Penman-Monteith")			

# **Details**

Potential evapotranspiration is calculated according to Priestley & Taylor, 1972 if approach = "Priestley-Taylor" (the default):

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$$LE_pot, PT = (\alpha * \Delta * (Rn - G - S))/(\Delta + \gamma)$$

 $\alpha$  is the Priestley-Taylor coefficient,  $\Delta$  is the slope of the saturation vapor pressure curve (kPa K-1), and  $\gamma$  is the psychrometric constant (kPa K-1). if approach = "Penman-Monteith", potential evapotranspiration is calculated according to the Penman-Monteith equation:

$$LE_not, PM = (\Delta * (Rn - G - S) + \rho * cp * VPD * Ga)/(\Delta + \gamma * (1 + Ga/Gs_not))$$

where  $\Delta$  is the slope of the saturation vapor pressure curve (kPa K-1),  $\rho$  is the air density (kg m-3), and  $\gamma$  is the psychrometric constant (kPa K-1). The value of Gs\_pot is typically a maximum value of Gs observed at the site, e.g. the 90th percentile of Gs within the growing season.

#### Value

a data.frame with the following columns:

ET\_pot Potential evapotranspiration (kg m-2 s-1)

LE\_pot Potential latent heat flux (W m-2)

#### Note

If the first argument data is provided (either a matrix or a data.frame), the following variables can be provided as character (in which case they are interpreted as the column name of data) or as numeric vectors, in which case they are taken directly for the calculations. If data is not provided, all input variables have to be numeric vectors.

# References

Priestley, C.H.B., Taylor, R.J., 1972: On the assessment of surface heat flux and evaporation using large-scale parameters. Monthly Weather Review 100, 81-92.

Allen, R.G., Pereira L.S., Raes D., Smith M., 1998: Crop evapotranspiration - Guidelines for computing crop water requirements - FAO Irrigation and drainage paper 56.

Novick, K.A., et al. 2016: The increasing importance of atmospheric demand for ecosystem water and carbon fluxes. Nature Climate Change 6, 1023 - 1027.

### See Also

```
surface.conductance
```

### **Examples**

```
# Calculate potential ET of a surface that receives a net radiation of 500 Wm-2
# using Priestley-Taylor:
potential.ET(Tair=30,pressure=100,Rn=500,alpha=1.26,approach="Priestley-Taylor")
# Calculate potential ET for a surface with known Gs (0.5 mol m-2 s-1) and Ga (0.1 m s-1)
# using Penman-Monteith:
```

potential.radiation 59

potential.radiation Potential radiation

# **Description**

Compute potential radiation for given geolocation and day of year.

### Usage

```
potential.radiation(doy, hour, latDeg, longDeg, timezone, useSolartime = TRUE)
```

### Arguments

doy Integer vector with day of year (start at 1), same length as hour or length 1.

hour Numeric vector with daytime as decimal hour of local time zone

latDeg Latitude (decimal degrees)
longDeg Longitude (decimal degrees)

timezone Time zone (hours)

useSolartime by default corrects hour (given in local winter time) for latitude to solar time

(where noon is exactly at 12:00). Set this to FALSE to directly use local winter

time.

### Value

vector of potential radiation (W m-2)

# **Examples**

```
hour <- seq(5, 18, by = 0.1)
potRadApparentLocal <- potential.radiation(
  160, hour, 39.94, -5.77, timezone = +1)
potRadTimezone <- potential.radiation(
  160, hour, 39.94, -5.77, timezone = +1, useSolartime = FALSE)
plot(potRadApparentLocal ~ hour, type = 'l'
  , ylab = 'potential radiation (W m-2)')
lines(potRadTimezone ~ hour, col = "blue")
abline(v = 12, col = "blue", lty = "dotted")
legend("bottomright", legend = c("solar time", "local winter time")
, col = c("black", "blue"), inset = 0.05, lty = 1)</pre>
```

```
pressure.from.elevation
```

Atmospheric Pressure from Hypsometric Equation

#### **Description**

An estimate of mean pressure at a given elevation as predicted by the hypsometric equation.

### Usage

```
pressure.from.elevation(
  elev,
  Tair,
  VPD = NULL,
  constants = bigleaf.constants()
)
```

### **Arguments**

elev Elevation a.s.l. (m)
Tair Air temperature (deg C)

VPD Vapor pressure deficit (kPa); optional constants Kelvin-conversion degC to Kelvin

pressure0 - reference atmospheric pressure at sea level (Pa)

Rd - gas constant of dry air (J kg-1 K-1) g - gravitational acceleration (m s-2)

Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)

#### **Details**

Atmospheric pressure is approximated by the hypsometric equation:

```
pressure = pressure_0/(exp(g * elevation/(RdTemp)))
```

#### Value

```
pressure - Atmospheric pressure (kPa)
```

# Note

The hypsometric equation gives an estimate of the standard pressure at a given altitude. If VPD is provided, humidity correction is applied and the virtual temperature instead of air temperature is used. VPD is internally converted to specific humidity.

# References

Stull B., 1988: An Introduction to Boundary Layer Meteorology. Kluwer Academic Publishers, Dordrecht, Netherlands.

psychrometric.constant 61

### **Examples**

```
# mean pressure at 500m altitude at 25 deg C and VPD of 1 kPa
pressure.from.elevation(500,Tair=25,VPD=1)
```

psychrometric.constant

Psychrometric Constant

# **Description**

Calculates the psychrometric 'constant'.

# Usage

```
psychrometric.constant(Tair, pressure, constants = bigleaf.constants())
```

### **Arguments**

Tair Air temperature (deg C)
pressure Atmospheric pressure (kPa)

constants cp - specific heat of air for constant pressure (J K-1 kg-1)

eps - ratio of the molecular weight of water vapor to dry air (-)

# **Details**

The psychrometric constant  $(\gamma)$  is given as:

```
\gamma = cp * pressure/(eps * \lambda)
```

where  $\lambda$  is the latent heat of vaporization (J kg-1), as calculated from latent.heat.vaporization.

### Value

 $\gamma$  - the psychrometric constant (kPa K-1)

### References

Monteith J.L., Unsworth M.H., 2008: Principles of Environmental Physics. 3rd Edition. Academic Press, London.

# **Examples**

```
psychrometric.constant(seq(5,45,5),100)
```

```
radiometric.surface.temp
```

Radiometric Surface Temperature

### **Description**

Radiometric surface temperature from longwave radiation measurements.

## Usage

```
radiometric.surface.temp(
  data,
  LW_up = "LW_up",
  LW_down = "LW_down",
  emissivity,
  constants = bigleaf.constants()
)
```

# **Arguments**

data Data.frame or matrix containing all required input variables

LW\_up Longwave upward radiation (W m-2)
LW\_down Longwave downward radiation (W m-2)

emissivity Emissivity of the surface (-)

constants sigma - Stefan-Boltzmann constant (W m-2 K-4) Kelvin - conversion degree Celsius to Kelvin

#### **Details**

Radiometric surface temperature (Trad) is calculated as:

$$Trad = ((LW_u p - (1 - \epsilon) * LW_d own)/(\sigma \epsilon))^{(1/4)}$$

# Value

a data.frame with the following columns:

Trad\_K Radiometric surface temperature (K)

Trad\_degC Radiometric surface temperature (degC)

## References

Wang, W., Liang, S., Meyers, T. 2008: Validating MODIS land surface temperature products using long-term nighttime ground measurements. Remote Sensing of Environment 112, 623-635.

reference.ET 63

### **Examples**

```
# determine radiometric surface temperature for the site DE-Tha in June 2014
# assuming an emissivity of 0.98.
# (Note that variable 'LW_down' was only included for the DE-Tha example dataset
# and not for the others due restrictions on file size)
Trad <- radiometric.surface.temp(DE_Tha_Jun_2014,emissivity=0.98)
summary(Trad)</pre>
```

reference.ET

Reference Evapotranspiration

# **Description**

Reference evapotranspiration calculated from the Penman-Monteith equation with a prescribed surface conductance. This function is deprecated. Use potential.ET(...,approach="Penman-Monteith") instead.

# Usage

```
reference.ET(
  data,
  Gs_ref = 0.0143,
  Tair = "Tair",
  pressure = "pressure",
  VPD = "VPD",
  Rn = "Rn",
  Ga = "Ga_h",
  G = NULL,
  S = NULL,
  missing.G.as.NA = FALSE,
  missing.S.as.NA = FALSE,
  Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
```

# **Arguments**

data	Data.frame or matrix containing all required variables; optional
Gs_ref	Reference surface conductance (m s-1); defaults to 0.0143 m s-1.
Tair	Air temperature (degC)
pressure	Atmospheric pressure (kPa)
VPD	Vapor pressure deficit (kPa)
Rn	Net radiation (W m-2)
Ga	Aerodynamic conductance to heat/water vapor (m s-1)

Reynolds.Number

G Ground heat flux (W m-2); optional

S Sum of all storage fluxes (W m-2); optional

missing.G.as.NA

if TRUE, missing G are treated as NAs, otherwise set to 0.

missing.S.as.NA

if TRUE, missing S are treated as NAs, otherwise set to 0.

Esat. formula Optional: formula to be used for the calculation of esat and the slope of esat.

One of "Sonntag\_1990" (Default), "Alduchov\_1996", or "Allen\_1998". See

Esat.slope.

constants cp - specific heat of air for constant pressure (J K-1 kg-1)

eps - ratio of the molecular weight of water vapor to dry air

Rd - gas constant of dry air (J kg-1 K-1) (only if approach = "Penman-Monteith") Rgas - universal gas constant (J mol-1 K-1) (only if approach = "Penman-Monteith") Kelvin - conversion degree Celsius to Kelvin (only if approach = "Penman-Monteith")

Reynolds.Number

Roughness Reynolds Number

# Description

calculates the Roughness Reynolds Number.

## Usage

Reynolds.Number(Tair, pressure, ustar, z0m, constants = bigleaf.constants())

### **Arguments**

Tair Air temperature (deg C)

pressure Atmospheric pressure (kPa)

ustar Friction velocity (m s-1)

zom Roughness length (m)

constants Kelvin - conversion degree Celsius to Kelvin

pressure0 - reference atmospheric pressure at sea level (Pa)

Tair0 - reference air temperature (K)

#### **Details**

The Roughness Reynolds Number is calculated as in Massman 1999a:

$$Re = z0m * ustar/v$$

where v is the kinematic viscosity (m2 s-1).

Rg.to.PPFD 65

# Value

Re - Roughness Reynolds Number (-)

# References

Massman, W.J., 1999a: A model study of kB H- 1 for vegetated surfaces using 'localized near-field' Lagrangian theory. Journal of Hydrology 223, 27-43.

# Examples

Reynolds.Number(25,100,0.5,z0m=0.5)

Rg.to.PPFD	Conversions	between	Global	Radiation	and	Photosynthetic	Photon
	Flux Density						

# Description

Converts radiation from W m-2 to umol m-2 s-1 and vice versa.

# Usage

```
Rg.to.PPFD(Rg, J_to_mol = 4.6, frac_PAR = 0.5)
PPFD.to.Rg(PPFD, J_to_mol = 4.6, frac_PAR = 0.5)
```

# **Arguments**

Rg	Global radiation = incoming short-wave radiation at the surface (W m-2)
J_to_mol	Conversion factor from J m-2 s-1 (= W m-2) to umol (quanta) m-2 s-1
frac_PAR	Fraction of incoming solar irradiance that is photosynthetically active radiation (PAR); defaults to $0.5$
PPFD	Photosynthetic photon flux density (umol m-2 s-1)

# **Details**

The conversion is given by:

$$PPFD = Rg * frac_PAR * J_to_mol$$

by default, the combined conversion factor (frac\_PAR \* J\_to\_mol) is 2.3

### **Examples**

```
\# convert a measured incoming short-wave radiation of 500 Wm-2 to \# PPFD in umol m-2 s-1 and backwards Rg.to.PPFD(500) PPFD.to.Rg(1150)
```

roughness.length.heat Roughness length for heat

# **Description**

Roughness length for heat (thermal roughness length, z0h) from the kB-1 parameter and roughness length for momentum (z0m).

## Usage

```
roughness.length.heat(z0m, kB_h)
```

# **Arguments**

z0m Roughness length for momentum (m) kB\_h kB-1 parameter for heat transfer

## **Details**

The roughness length for heat (z0h) can be calculated from the following relationship (e.g. Verma 1989):

$$kB_h = ln(z0m/z0h)$$

it follows:

$$z0h = z0m/exp(kB_h)$$

# Value

Roughness length for heat, z0h (m)

## Note

If unknown, z0m can be calculated from roughness.parameters. kB\_h can be calculated from Gb.Thom, Gb.Choudhury, Gb.Su or aerodynamic.conductance.

roughness.parameters 67

### References

Verma, S., 1989: Aerodynamic resistances to transfers of heat, mass and momentum. In: Estimation of areal evapotranspiration, IAHS Pub, 177, 13-20.

Rigden, A., Li, D., Salvucci, G., 2018: Dependence of thermal roughness length on friction velocity across land cover types: A synthesis analysis using AmeriFlux data. Agricultural and Forest Meteorology 249, 512-519.

### **Examples**

```
roughness.length.heat(2,2.5)
```

roughness.parameters Roughness Parameters

### **Description**

A simple approximation of the two roughness parameters displacement height (d) and roughness length for momentum (z0m).

# Usage

```
roughness.parameters(
 method = c("canopy_height", "canopy_height&LAI", "wind_profile"),
  frac_d = 0.7,
  frac_z0m = 0.1,
 LAI,
 zr,
  cd = 0.2,
 hs = 0.01,
 data,
  Tair = "Tair",
  pressure = "pressure",
 wind = "wind",
 ustar = "ustar",
 H = "H",
 d = NULL
 z0m = NULL
  stab_roughness = TRUE,
 stab_formulation = c("Dyer_1970", "Businger_1971"),
  constants = bigleaf.constants()
)
```

#### **Arguments**

method Method to use, one of "canopy\_height", "canopy\_height&LAI", "wind\_profile"

NOTE: if method = "canopy\_height", only the following three arguments are used. If method = "canopy\_height&LAI", only zh, LAI, cd, and hs are re-

quired.

zh Vegetation height (m)

frac\_d Fraction of displacement height on canopy height (-)
frac\_z0m Fraction of roughness length on canopy height (-)

LAI Leaf area index (-)

zr Instrument (reference) height (m)

cd Mean drag coefficient for individual leaves. Defaults to 0.2. Only needed if

method = "canopy\_height&LAI".

hs roughness length of the soil surface (m). Only needed if method = "canopy\_height&LAI"

The following arguments are only needed if method = "wind\_profile"!

data Data.frame or matrix containing all required variables

Tair Air temperature (deg C)

pressure Atmospheric pressure (kPa)

wind Wind speed at height zr (m s-1)

ustar Friction velocity (m s-1)
H Sensible heat flux (W m-2)

d Zero-plane displacement height (m); optional z0m Roughness length for momentum (m); optional

stab\_roughness Should stability correction be considered? Default is TRUE.

stab\_formulation

Stability correction function used (If stab\_correction = TRUE). Either "Dyer\_1970"

or "Businger\_1971".

constants k - von-Karman constant (-)

Kelvin - conversion degree Celsius to Kelvin

cp - specific heat of air for constant pressure (J K-1 kg-1)

g - gravitational acceleration (m s-2)

se median - conversion standard error (SE) of the mean to SE of the median

#### Details

The two main roughness parameters, the displacement height (d) and the roughness length for momentum (z0m) can be estimated from simple empirical relationships with canopy height (zh). If method = "canopy\_height", the following formulas are used:

$$d = frac_d * zh$$

$$z0m = frac_z 0m * zh$$

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where frac\_d defaults to 0.7 and frac\_z0m to 0.1.

Alternatively, d and z0m can be estimated from both canopy height and LAI (If method = "canopy\_height&LAI"). Based on data from Shaw & Pereira 1982, Choudhury & Monteith 1988 proposed the following semi-empirical relations:

$$X = cd * LAI$$

$$d = 1.1 * zh * ln(1 + X^{(1/4)})$$

$$z0m = hs + 0.3 * zh * X^{(1/2)} for 0 \le X \le 0.2$$

$$z0m = hs * zh * (1 - d/zh) for 0.2 < X$$

If method = "wind\_profile", z0m is estimated by solving the wind speed profile for z0m:

$$z0m = median((zr - d) * exp(-k * wind/ustar - psi_m))$$

By default, d in this equation is fixed to 0.7\*zh, but can be set to any other value. psi\_m is 0 if stab\_roughness = FALSE.

## Value

a data.frame with the following columns:

d Zero-plane displacement height (m)

z0m Roughness length for momentum (m)

z0m\_se Only if method = wind\_profile: Standard Error of the median for z0m (m)

### References

Choudhury, B. J., Monteith J.L., 1988: A four-layer model for the heat budget of homogeneous land surfaces. Q. J. R. Meteorol. Soc. 114, 373-398.

Shaw, R. H., Pereira, A., 1982: Aerodynamic roughness of a plant canopy: a numerical experiment. Agricultural Meteorology, 26, 51-65.

#### See Also

wind.profile

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### **Examples**

```
# estimate d and z0m from canopy height for a dense (LAI=5) and open (LAI=2) canopy
roughness.parameters(method="canopy_height&LAI",zh=25,LAI=5)
roughness.parameters(method="canopy_height&LAI",zh=25,LAI=2)

# fix d to 0.7*zh and estimate z0m from the wind profile
df <- data.frame(Tair=c(25,25,25),pressure=100,wind=c(3,4,5),ustar=c(0.5,0.6,0.65),H=200)
roughness.parameters(method="wind_profile",zh=25,zr=40,frac_d=0.7,data=df)

# assume d = 0.8*zh
roughness.parameters(method="wind_profile",zh=25,zr=40,frac_d=0.8,data=df)</pre>
```

stability.correction Integrated Stability Correction Functions for Heat and Momentum

### **Description**

dimensionless stability functions needed to correct deviations from the exponential wind profile under non-neutral conditions.

# Usage

```
stability.correction(zeta, formulation = c("Dyer_1970", "Businger_1971"))
```

### **Arguments**

zeta Stability parameter zeta (-)

formulation Formulation for the stability function. Either "Dyer\_1970", or "Businger\_1971"

### **Details**

The functions give the integrated form of the universal functions. They depend on the value of the stability parameter  $\zeta$ , which can be calculated from the function stability parameter. The integration of the universal functions is:

$$\psi = -x * zeta$$

for stable atmospheric conditions ( $\zeta >= 0$ ), and

$$\psi = 2 * log((1+y)/2)$$

for unstable atmospheric conditions ( $\zeta < 0$ ).

The different formulations differ in their value of x and y.

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### Value

a data.frame with the following columns:

```
psi_h the value of the stability function for heat and water vapor (-)
psi_m the value of the stability function for momentum (-)
```

#### References

Dyer, A.J., 1974: A review of flux-profile relationships. Boundary-Layer Meteorology 7, 363-372.

Dyer, A. J., Hicks, B.B., 1970: Flux-Gradient relationships in the constant flux layer. Quart. J. R. Meteorol. Soc. 96, 715-721.

Businger, J.A., Wyngaard, J. C., Izumi, I., Bradley, E. F., 1971: Flux-Profile relationships in the atmospheric surface layer. J. Atmospheric Sci. 28, 181-189.

Paulson, C.A., 1970: The mathematical representation of wind speed and temperature profiles in the unstable atmospheric surface layer. Journal of Applied Meteorology 9, 857-861.

Foken, T, 2008: Micrometeorology. Springer, Berlin, Germany.

# Examples

```
zeta <- seq(-2,0.5,0.05)
stability.correction(zeta)
stability.correction(zeta,formulation="Businger_1971")</pre>
```

stability.parameter

Stability Parameter "zeta"

# **Description**

calculates "zeta", a parameter characterizing stratification in the lower atmosphere.

# Usage

```
stability.parameter(
  data,
  Tair = "Tair",
  pressure = "pressure",
  ustar = "ustar",
  H = "H",
  zr,
  d,
  constants = bigleaf.constants()
```

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### **Arguments**

data Data.frame or matrix containing all required variables

Tair Air temperature (degC)

pressure Atmospheric pressure (kPa)
ustar Friction velocity (m s-1)
H Sensible heat flux (W m-2)

zr Instrument (reference) height (m)
d Zero-plane displacement height (m)

constants Kelvin - conversion degree Celsius to Kelvin

cp - specific heat of air for constant pressure (J K-1 kg-1)

k - von Karman constant (-)

g - gravitational acceleration (m s-2)

### **Details**

The stability parameter  $\zeta$  is given by:

$$\zeta = (zr - d)/L$$

where L is the Monin-Obukhov length (m), calculated from the function Monin.Obukhov.length. The displacement height d can be estimated from the function roughness.parameters.

#### Value

$$\zeta$$
 - stability parameter (-)

# **Examples**

```
df <- data.frame(Tair=25,pressure=100,ustar=seq(0.2,1,0.1),H=seq(40,200,20)) stability.parameter(df,zr=40,d=15)
```

stomatal.sensitivity Stomatal Sensitivity to VPD

# **Description**

Sensitivity of surface conductance to vapor pressure deficit.

# Usage

```
stomatal.sensitivity(data, Gs = "Gs_mol", VPD = "VPD", ...)
```

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## Arguments

data	Data.frame or matrix containing all required columns
Gs	Surface conductance to water vapor (mol m-2 s-1)
VPD	Vapor pressure deficit (kPa)
	Additional arguments to nls

## **Details**

The function fits the following equation (Oren et al. 1999):

$$Gs = -mln(VPD) + b$$

where b is the reference surface conductance (Gs) at VPD=1kPa (in mol m-2 s-1), and m is the sensitivity parameter of Gs to VPD (in mol m-2 s-1 log(kPa)-1). The two parameters b and m are fitted using nls. VPD can be the one directly measured at instrument height, or the one at the surface, as returned by surface.conditions.

#### Value

A nls model object containing (amongst others) estimates for the mean and standard errors of the parameters m and b.

#### References

Oren R., et al. 1999: Survey and synthesis of intra- and interspecific variation in stomatal sensitivity to vapour pressure deficit. Plant, Cell & Environment 22, 1515-1526.

Novick K.A., et al. 2016: The increasing importance of atmospheric demand for ecosystem water and carbon fluxes. Nature Climate Change 6, 1023 - 1027.

#### See Also

```
surface.conductance
```

## **Examples**

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```
stomatal.sensitivity(FR_Pue_May_2012_2,Gs=Gs[,"Gs_mol"],VPD="VPD")
```

stomatal.slope

Stomatal Slope Parameter "g1"

## **Description**

Estimation of the intrinsic WUE metric "g1" (stomatal slope) from nonlinear regression.

# Usage

```
stomatal.slope(
  data,
 Tair = "Tair",
 pressure = "pressure",
 GPP = "GPP",
 Gs = "Gs_mol",
  VPD = "VPD",
 Ca = "Ca",
 Rleaf = NULL,
 model = c("USO", "Ball&Berry", "Leuning"),
  robust.nls = FALSE,
  nmin = 40,
  fitg0 = FALSE,
  g0 = 0,
  fitD0 = FALSE,
 D0 = 1.5
 Gamma = 50,
 missing.Rleaf.as.NA = FALSE,
  constants = bigleaf.constants(),
)
```

# Arguments

data	Data.frame or matrix containing all required columns
Tair	Air (or surface) temperature (deg C)
pressure	Atmospheric pressure (kPa)
GPP	Gross primary productivity (umol CO2 m-2 s-1)
Gs	Surface conductance to water vapor (mol m-2 s-1)
VPD	Vapor pressure deficit (kPa)
Ca	Atmospheric CO2 concentration (air or surface) (umol mol-1)
Rleaf	Ecosystem respiration stemming from leaves (umol CO2 m-2 s-1); defaults to 0
model	Stomatal model used. One of "USO", "Ball&Berry", "Leuning".

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	robust.nls	Use robust nonlinear regression (nlrob)? Default is FALSE.
	nmin	Minimum number of data required to perform the fit; defaults to 40.
	fitg0	Should g0 and g1 be fitted simultaneously?
	g0	Minimum stomatal conductance (mol m-2 s-1); ignored if fitg0 = TRUE.
	fitD0	Should D0 be fitted along with g1 (and g0 if fitg0 = TRUE)?; only used if model = "Leuning".
	D0	Stomatal sensitivity parameter to VPD; only used if $model = "Leuning"$ and $fitD0 = FALSE$ .
	Gamma	Canopy CO2 compensation point (umol mol-1); only used if model = "Leuning". Can be a constant or a variable. Defaults to 50 umol mol-1.
missing.Rleaf.as.NA		
		if Rleaf is provided, should missing values be treated as NA (TRUE) or set to $0$ (FALSE, the default)?
	constants	Kelvin - conversion degree Celsius to Kelvin Rgas - universal gas constant (J mol-1 K-1) DwDc - Ratio of the molecular diffusivities for water vapor and CO2

#### **Details**

All stomatal models were developed at leaf-level, but its parameters can also be estimated at ecosystem level (but be aware of caveats).

Additional arguments to nls or nlrob if robust.nls = TRUE.

The unified stomatal optimization (USO) model is given by (Medlyn et al. 2011):

$$gs = g0 + 1.6 * (1.0 + g1/sqrt(VPD)) * An/ca$$

The semi-empirical model by Ball et al. 1987 is defined as:

$$gs = g0 + g1 * ((An * rH)/ca)$$

Leuning 1995 suggested a revised version of the Ball&Berry model:

$$gs = g0 + g1 * An/((ca - \Gamma) * (1 + VPD/D0))$$

where  $\Gamma$  is by default assumed to be constant, but likely varies with temperature and among plant species. The equations above are valid at leaf-level. At ecosystem level, An is replaced by GPP (or GPP - Rleaf, where Rleaf is leaf respiration), and gs (stomatal conductance) by Gs (surface conductance). The parameters in the models are estimated using nonlinear regression (nls) if robust.nls = FALSE and weighted nonlinear regression if robust.nls = TRUE. The weights are calculated from nlrob, and nls is used for the actual fitting. Alternatively to measured VPD and Ca (i.e. conditions at instrument height), conditions at the big-leaf surface can be provided. Those can be calculated using surface.conditions.

#### Value

A nls model object, containing information on the fitted parameters, their uncertainty range, model fit, etc.

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#### References

Medlyn B.E., et al., 2011: Reconciling the optimal and empirical approaches to modelling stomatal conductance. Global Change Biology 17, 2134-2144.

Ball T.J., Woodrow I.E., Berry J.A. 1987: A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions. In: Progress in Photosynthesis Research, edited by J.Biggins, pp. 221-224, Martinus Nijhoff Publishers, Dordrecht, Netherlands.

Leuning R., 1995: A critical appraisal of a combined stomatal-photosynthesis model for C3 plants. Plant, Cell and Environment 18, 339-355.

Knauer, J. et al., 2018: Towards physiologically meaningful water-use efficiency estimates from eddy covariance data. Global Change Biology 24, 694-710.

#### See Also

surface.conductance

## **Examples**

```
## filter data to ensure that Gs is a meaningful proxy to canopy conductance (Gc)
DE_Tha_Jun_2014_2 <- filter.data(DE_Tha_Jun_2014,quality.control=FALSE,
                                 vars.qc=c("Tair","precip","VPD","H","LE"),
                                 filter.growseas=FALSE,filter.precip=TRUE,
                                 filter.vars=c("Tair","PPFD","ustar","LE"),
                                 filter.vals.min=c(5,200,0.2,0),
                                 filter.vals.max=c(NA,NA,NA,NA),NA.as.invalid=TRUE,
                                 quality.ext="_qc",good.quality=c(0,1),
                                 missing.qc.as.bad=TRUE,GPP="GPP",doy="doy",
                                 year="year",tGPP=0.5,ws=15,min.int=5,precip="precip",
                                 tprecip=0.1,precip.hours=24,records.per.hour=2)
# calculate Gs from the the inverted PM equation
Ga <- aerodynamic.conductance(DE_Tha_Jun_2014_2,Rb_model="Thom_1972")[,"Ga_h"]
# if G and/or S are available, don't forget to indicate (they are ignored by default).
Gs_PM <- surface.conductance(DE_Tha_Jun_2014_2,Tair="Tair",pressure="pressure",
                             Rn="Rn", G="G", S=NULL, VPD="VPD", Ga=Ga,
                             formulation="Penman-Monteith")[,"Gs_mol"]
### Estimate the stomatal slope parameter g1 using the USO model
mod_USO <- stomatal.slope(DE_Tha_Jun_2014_2,model="USO",GPP="GPP",Gs=Gs_PM,</pre>
                          robust.nls=FALSE,nmin=40,fitg0=FALSE)
### Use robust regression to minimize influence of outliers in Gs
mod_USO <- stomatal.slope(DE_Tha_Jun_2014_2,model="USO",GPP="GPP",Gs=Gs_PM,</pre>
                          robust.nls=TRUE,nmin=40,fitg0=FALSE)
### Estimate the same parameter from the Ball&Berry model and prescribe g0
mod_BB <- stomatal.slope(DE_Tha_Jun_2014_2,model="Ball&Berry",GPP="GPP",</pre>
                         robust.nls=FALSE,Gs=Gs_PM,g0=0.01,nmin=40,fitg0=FALSE)
```

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surface.CO2

CO2 Concentration at the Canopy Surface

## **Description**

the CO2 concentration at the canopy surface derived from net ecosystem CO2 exchange and measured atmospheric CO2 concentration.

## Usage

```
surface.CO2(Ca, NEE, Ga_CO2, Tair, pressure)
```

# **Arguments**

Ca	Atmospheric CO2 concentration (umol mol-1)
NEE	Net ecosystem exchange (umol CO2 m-2 s-1)
Ga_CO2	Aerodynamic conductance for CO2 (m s-1)

Tair Air temperature (degC)
pressure Atmospheric pressure (kPa)

## **Details**

CO2 concentration at the canopy surface is calculated as:

$$Ca_surf = Ca + NEE/Ga_CO2$$

Note that this equation can be used for any gas measured (with NEE replaced by the net exchange of the respective gas and Ga\_CO2 by the Ga of that gas).

## Value

Ca\_surf - CO2 concentration at the canopy surface (umol mol-1)

## Note

the following sign convention is employed: negative values of NEE denote net CO2 uptake by the ecosystem.

## **Examples**

```
surface.C02(Ca=400,NEE=-30,Ga_C02=0.05,Tair=25,pressure=100)
```

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surface.conditions

Big-Leaf Surface Conditions

# Description

Calculates meteorological conditions at the big-leaf surface by inverting bulk transfer equations for water, energy, and carbon fluxes.

# Usage

```
surface.conditions(
 data,
 Tair = "Tair",
 pressure = "pressure",
 LE = "LE",
 H = "H",
 VPD = "VPD",
 Ga = "Ga_h",
 calc.surface.CO2 = FALSE,
 Ca = "Ca",
 Ga_CO2 = "Ga_CO2",
 NEE = "NEE",
 Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
 constants = bigleaf.constants()
)
```

# **Arguments**

data	Data.frame or matrix containing all required input variables	
Tair	Air temperature (deg C)	
pressure	Atmospheric pressure (kPa)	
LE	Latent heat flux (W m-2)	
Н	Sensible heat flux (W m-2)	
VPD	Vapor pressure deficit (kPa)	
Ga	Aerodynamic conductance for heat/water vapor (m s-1)	
calc.surface.CO2		
	Calculate surface CO2 concentration? Defaults to FALSE.	
Ca	Atmospheric CO2 concentration (mol mol-1). Required if calc.surface.CO2 = TRUE.	
Ga_CO2	Aerodynamic conductance for CO2 (m s-1). Required if calc.surface.CO2 = TRUE.	
NEE	Net ecosystem exchange (umol m-2 s-1). Required if calc.surface.CO2 = TRUE.	

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Esat. formula Optional: formula to be used for the calculation of esat and the slope of esat.

One of "Sonntag\_1990" (Default), "Alduchov\_1996", or "Allen\_1998". See

Esat.slope.

constants cp - specific heat of air for constant pressure (J K-1 kg-1)

eps - ratio of the molecular weight of water vapor to dry air (-)

Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)

#### **Details**

Canopy surface temperature and humidity are calculated by inverting bulk transfer equations of sensible and latent heat, respectively. 'Canopy surface' in this case refers to the surface of the big-leaf (i.e. at height d + z0h; the apparent sink of sensible heat and water vapor). Aerodynamic canopy surface temperature is given by:

$$Tsurf = Tair + H/(\rho * cp * Ga)$$

where  $\rho$  is air density (kg m-3). Vapor pressure at the canopy surface is:

$$esurf = e + (LE * \gamma)/(Ga * \rho * cp)$$

where  $\gamma$  is the psychrometric constant (kPa K-1). Vapor pressure deficit (VPD) at the canopy surface is calculated as:

$$VPD_surf = Esat_surf - esurf$$

CO2 concentration at the canopy surface is given by:

$$Ca_surf = Ca + NEE/Ga_CO2$$

Note that Ga is assumed to be equal for water vapor and sensible heat. Ga is further assumed to be the inverse of the sum of the turbulent part and the canopy boundary layer conductance (1/Ga = 1/Ga\_m + 1/Gb; see aerodynamic.conductance). Ga\_CO2, the aerodynamic conductance for CO2 is also calculated by aerodynamic.conductance. If Ga is replaced by Ga\_m (i.e. only the turbulent conductance part), the results of the functions represent conditions outside the canopy boundary layer, i.e. in the canopy airspace.

#### Value

a data.frame with the following columns:

Tsurf Surface temperature (deg C)

esat\_surf Saturation vapor pressure at the surface (kPa)

esurf vapor pressure at the surface (kPa)

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VPD_surf	vapor pressure deficit at the surface (kPa)
qsurf	specific humidity at the surface (kg kg-1)
rH_surf	relative humidity at the surface (-)
Ca_surf	CO2 concentration at the surface (umol mol-1)

#### Note

The following sign convention for NEE is employed (relevant if calc.surface.CO2 = TRUE): negative values of NEE denote net CO2 uptake by the ecosystem.

## References

Knauer, J. et al., 2018: Towards physiologically meaningful water-use efficiency estimates from eddy covariance data. Global Change Biology 24, 694-710.

Blanken, P.D. & Black, T.A., 2004: The canopy conductance of a boreal aspen forest, Prince Albert National Park, Canada. Hydrological Processes 18, 1561-1578.

Shuttleworth, W. J., Wallace, J.S., 1985: Evaporation from sparse crops- an energy combination theory. Quart. J. R. Met. Soc. 111, 839-855.

## **Examples**

surface.conductance Surface Conductance to Water Vapor

## **Description**

Calculates surface conductance to water vapor from the inverted Penman-Monteith equation (by default) or from a simple flux-gradient approach.

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## Usage

```
surface.conductance(
 data,
 Tair = "Tair",
 pressure = "pressure",
 Rn = "Rn",
 G = NULL
 S = NULL,
 VPD = "VPD",
 LE = "LE",
 Ga = "Ga_h",
 missing.G.as.NA = FALSE,
 missing.S.as.NA = FALSE,
 formulation = c("Penman-Monteith", "Flux-Gradient"),
 Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
 constants = bigleaf.constants()
)
```

# Arguments

data	Data.frame or matrix containing all required input variables
Tair	Air temperature (deg C)
pressure	Atmospheric pressure (kPa)
Rn	Net radiation (W m-2)
G	Ground heat flux (W m-2); optional
S	Sum of all storage fluxes (W m-2); optional
VPD	Vapor pressure deficit (kPa)
LE	Latent heat flux (W m-2)
Ga	Aerodynamic conductance to heat/water vapor (m s-1)
missing.G.as.N	A
	if TRUE, missing G are treated as NAs, otherwise they are set to 0. Only used if formulation = "Penman-Monteith".
missing.S.as.N	A
	if TRUE, missing $S$ are treated as NAs, otherwise they are set to $O$ . Only used if formulation = "Penman-Monteith".
formulation	Formulation used. Either "Penman-Monteith" (the default) using the inverted Penman-Monteith equation, or "Flux-Gradient", for a simple flux-gradient approach requiring ET, pressure, and VPD only.
Esat.formula	Optional: formula to be used for the calculation of esat and the slope of esat. One of "Sonntag_1990" (Default), "Alduchov_1996", or "Allen_1998". Only used if formulation = "Penman-Monteith". See Esat.slope.
constants	cp - specific heat of air for constant pressure (J K-1 kg-1) eps - ratio of the molecular weight of water vapor to dry air (-) Rd - gas constant of dry air (J kg-1 K-1) Rgas - universal gas constant (J mol-1 K-1)

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Kelvin - conversion degree Celsius to Kelvin Mw - molar mass of water vapor (kg mol-1) Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)

#### **Details**

If formulation = "Penman-Monteith" (the default), surface conductance (Gs) in m s-1 is calculated from the inverted Penman-Monteith equation:

$$Gs = (LE * Ga * \gamma)/(\Delta * A + \rho * cp * Ga * VPD - LE * (\Delta + \gamma))$$

Where  $\gamma$  is the psychrometric constant (kPa K-1),  $\Delta$  is the slope of the saturation vapor pressure curve (kPa K-1), and  $\rho$  is air density (kg m-3). Available energy (A) is defined as A = Rn - G - S. If G and/or S are not provided, A = Rn.

By default, any missing data in G and S are set to 0. If missing. S. as. NA = TRUE or missing. S. as. NA = TRUE, Gs will give NA for these timesteps.

If formulation="Flux-Gradient", Gs (in mol m-2 s-1) is calculated from VPD and ET only:

$$Gs = ET/pressure * VPD$$

where ET is in mol m-2 s-1. Note that this formulation assumes fully coupled conditions (i.e. Ga = inf). This formulation is equivalent to the inverted form of Eq.6 in McNaughton & Black 1973:

$$Gs = LE * \gamma/(\rho * cp * VPD)$$

which gives Gs in m s-1. Note that Gs > Gc (canopy conductance) under conditions when a significant fraction of ET comes from interception or soil evaporation.

If pressure is not available, it can be approximated by elevation using the function pressure.from.elevation

## Value

a dataframe with the following columns:

Gs\_ms Surface conductance in m s-1

Gs\_mol Surface conductance in mol m-2 s-1

#### References

Monteith, J., 1965: Evaporation and environment. In Fogg, G. E. (Ed.), The state and movement of water in living organisms (pp.205-234). 19th Symp. Soc. Exp. Biol., Cambridge University Press, Cambridge

McNaughton, K.G., Black, T.A., 1973: A study of evapotranspiration from a Douglas Fir forest using the energy balance approach. Water Resources Research 9, 1579-1590.

umolCO2.to.gC

## **Examples**

```
## filter data to ensure that Gs is a meaningful proxy to canopy conductance (Gc)
DE_Tha_Jun_2014_2 <- filter.data(DE_Tha_Jun_2014,quality.control=FALSE,
                                 vars.gc=c("Tair","precip","VPD","H","LE"),
                                 filter.growseas=FALSE,filter.precip=TRUE,
                                 filter.vars=c("Tair","PPFD","ustar","LE"),
                                 filter.vals.min=c(5,200,0.2,0),
                                 filter.vals.max=c(NA,NA,NA,NA),NA.as.invalid=TRUE,
                                 quality.ext="_qc",good.quality=c(0,1),
                                 missing.qc.as.bad=TRUE,GPP="GPP",doy="doy",
                                 year="year",tGPP=0.5,ws=15,min.int=5,precip="precip",
                                 tprecip=0.1,precip.hours=24,records.per.hour=2)
# calculate Gs based on a simple gradient approach
Gs_gradient <- surface.conductance(DE_Tha_Jun_2014_2,Tair="Tair",pressure="pressure",
                                   VPD="VPD", formulation="Flux-Gradient")
summary(Gs_gradient)
# calculate Gs from the the inverted PM equation (now Rn, and Ga are needed),
# using a simple estimate of Ga based on Thom 1972
Ga <- aerodynamic.conductance(DE_Tha_Jun_2014_2,Rb_model="Thom_1972")[,"Ga_h"]
# if G and/or S are available, don't forget to indicate (they are ignored by default).
# Note that Ga is not added to the data.frame 'DE_Tha_Jun_2014'
Gs_PM <- surface.conductance(DE_Tha_Jun_2014_2,Tair="Tair",pressure="pressure",</pre>
                             Rn="Rn", G="G", S=NULL, VPD="VPD", Ga=Ga,
                             formulation="Penman-Monteith")
summary(Gs_PM)
# now add Ga to the data.frame 'DE_Tha_Jun_2014' and repeat
DE_Tha_Jun_2014_2$Ga <- Ga
Gs_PM2 <- surface.conductance(DE_Tha_Jun_2014_2, Tair="Tair", pressure="pressure",
                              Rn="Rn", G="G", S=NULL, VPD="VPD", Ga="Ga",
                              formulation="Penman-Monteith")
# note the difference to the previous version (Ga="Ga")
summary(Gs_PM2)
```

umolCO2.to.gC

Conversion between Mass and Molar Units of Carbon and CO2

## Description

Converts CO2 quantities from umol CO2 m-2 s-1 to g C m-2 d-1 and vice versa.

# Usage

```
umolCO2.to.gC(CO2_flux, constants = bigleaf.constants())
gC.to.umolCO2(C_flux, constants = bigleaf.constants())
```

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## **Arguments**

constants Cmol - molar mass of carbon (kg mol-1)

umol2mol - conversion micromole (umol) to mol (mol) mol2umol - conversion mole (mol) to micromole (umol)

kg2g - conversion kilogram (kg) to gram (g) g2kg - conversion gram (g) to kilogram (kg)

days2seconds - seconds per day

C\_flux Carbon (C) flux (gC m-2 d-1)

# Examples

```
umolCO2.to.gC(20) # gC m-2 d-1
```

virtual.temp

Virtual Temperature

## **Description**

Virtual temperature, defined as the temperature at which dry air would have the same density as moist air at its actual temperature.

# Usage

```
virtual.temp(
  Tair,
  pressure,
  VPD,
  Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
```

## **Arguments**

Tair Air temperature (deg C)

pressure Atmospheric pressure (kPa)

VPD Vapor pressure deficit (kPa)

Esat. formula Optional: formula to be used for the calculation of esat and the slope of esat.

One of "Sonntag\_1990" (Default), "Alduchov\_1996", or "Allen\_1998". See

Esat.slope.

constants Kelvin - conversion degree Celsius to Kelvin

eps - ratio of the molecular weight of water vapor to dry air (-)

VPD.to.rH

## **Details**

the virtual temperature is given by:

$$Tv = Tair/(1 - (1 - eps)e/pressure)$$

where Tair is in Kelvin (converted internally). Likewise, VPD is converted to actual vapor pressure (e in kPa) with VPD. to.e internally.

## Value

Tv - virtual temperature (deg C)

## References

Monteith J.L., Unsworth M.H., 2008: Principles of Environmental Physics. 3rd edition. Academic Press, London.

## **Examples**

```
virtual.temp(25,100,1.5)
```

VPD.to.rH

Conversions between Humidity Measures

## **Description**

Conversion between vapor pressure (e), vapor pressure deficit (VPD), specific humidity (q), and relative humidity (rH).

## Usage

```
VPD.to.rH(
    VPD,
    Tair,
    Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
    constants = bigleaf.constants()
)

rH.to.VPD(
    rH,
    Tair,
    Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
    constants = bigleaf.constants()
)
e.to.rH(
```

VPD.to.rH

```
e,
  Tair,
  Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
VPD.to.e(
  VPD,
  Tair,
 Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
e.to.VPD(
  e,
 Tair,
 Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
e.to.q(e, pressure, constants = bigleaf.constants())
q.to.e(q, pressure, constants = bigleaf.constants())
q.to.VPD(
  q,
  Tair,
  pressure,
 Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
VPD.to.q(
  VPD,
  Tair,
  pressure,
  Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
  constants = bigleaf.constants()
)
```

## **Arguments**

VPD Vapor pressure deficit (kPa)

Tair Air temperature (deg C)

Esat.formula Optional: formula to be used for the calculation of esat and the slope of esat. One of "Sonntag\_1990" (Default), "Alduchov\_1996", or "Allen\_1998". See Esat.slope.

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constants	eps - ratio of the molecular weight of water vapor to dry air (-) Pa2kPa - conversion pascal (Pa) to kilopascal (kPa)
rH	Relative humidity (-)
е	Vapor pressure (kPa)
pressure	Atmospheric pressure (kPa)
q	Specific humidity (kg kg-1)

## References

Foken, T, 2008: Micrometeorology. Springer, Berlin, Germany.

wetbulb.temp	Wet-Bulb Temperature	

# Description

calculates the wet bulb temperature, i.e. the temperature that the air would have if it was saturated.

# Usage

```
wetbulb.temp(
   Tair,
   pressure,
   VPD,
   accuracy = 0.001,
   Esat.formula = c("Sonntag_1990", "Alduchov_1996", "Allen_1998"),
   constants = bigleaf.constants()
)
```

# Arguments

Tair	Air temperature (deg C)
pressure	Atmospheric pressure (kPa)
VPD	Vapor pressure deficit (kPa)
accuracy	Accuracy of the result (deg C)
Esat.formula	Optional: formula to be used for the calculation of esat and the slope of esat. One of "Sonntag_1990" (Default), "Alduchov_1996", or "Allen_1998". See Esat.slope.
constants	cp - specific heat of air for constant pressure (J K-1 kg-1) eps - ratio of the molecular weight of water vapor to dry air (-) Pa2kPa - conversion pascal (Pa) to kilopascal (kPa) Le067 - Lewis number for water vapor to the power of 0.67

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## **Details**

Wet-bulb temperature (Tw) is calculated from the following expression:

```
e = Esat(Tw) - Le067 * gamma * (Tair - Tw)
```

The equation is solved for Tw using optimize. Actual vapor pressure e (kPa) is calculated from VPD using the function VPD.to.e. The psychrometric constant gamma (kPa K-1) is calculated from psychrometric.constant. Le067 is the Lewis number for water vapor to the power of 0.67 and represents the ratio of aerodynamic resistance to water vapor and heat. Le067 \* gamma is sometimes referred to as the 'modified psychrometric constant (gamma\*).

#### Value

```
Tw - wet-bulb temperature (degC)
```

## References

Monteith J.L., Unsworth M.H., 2013: Principles of Environmental Physics. Plants, Animals, and the Atmosphere. 4th edition. Academic Press.

#### **Examples**

```
wetbulb.temp(Tair=c(20,25),pressure=100,VPD=c(1,1.6))
```

wind.profile

Wind Speed at a Given Height in the Surface Layer

## **Description**

Wind speed at a given height above the canopy estimated from single-level measurements of wind speed.

## Usage

```
wind.profile(
  data,
  z,
  Tair = "Tair",
  pressure = "pressure",
  ustar = "ustar",
  H = "H",
  wind = "wind",
  zr,
  zh,
  d = NULL,
  frac_d = 0.7,
```

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```
z0m = NULL
  frac_z0m = NULL,
  estimate_z0m = TRUE,
  stab_correction = TRUE,
  stab_formulation = c("Dyer_1970", "Businger_1971"),
  constants = bigleaf.constants()
)
```

## **Arguments**

data

Data.frame or matrix containing all required variables z Height above ground for which wind speed is calculated. Air temperature (deg C) Tair Atmospheric pressure (kPa) pressure Friction velocity (m s-1) ustar Н Sensible heat flux (W m-2) wind Wind speed at height zr (m s-1); only used if stab\_correction = TRUE Instrument (reference) height (m) zr zh Canopy height (m) d Zero-plane displacement height (-) frac d Fraction of displacement height on canopy height (-); only used if d is not availz0m Roughness length (m), optional; only used if stab\_correction = FALSE (default=0.1) Fraction of roughness length on canopy height (-), optional; only used if z0m is frac\_z0m not provided. Default is 0.1. estimate\_z0m Should z0m be estimated from the logarithmic wind profile? If TRUE (the default), arguments z0m and frac\_z0m are ignored. See roughness.parameters for details. stab\_correction Should stability correction be applied? Defaults to TRUE stab\_formulation Stability correction function used (If stab\_correction = TRUE). Either "Dyer\_1970" or "Businger\_1971". constants k - von-Karman constant (-)

## **Details**

The underlying assumption is the existence of a logarithmic wind profile above the height d + z0m(the height at which wind speed mathematically reaches zero according to the Monin-Obukhov similarity theory). In this case, the wind speed at a given height z is given by:

cp - specific heat of air for constant pressure (J K-1 kg-1)

Kelvin - conversion degree Celsius to Kelvin

g - gravitational acceleration (m s-2)

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$$u(z) = (ustar/k) * (ln((z-d)/z0m) - \psi m$$

The roughness parameters zero-plane displacement height (d) and roughness length (z0m) can be approximated from roughness.parameters.  $\psi m$  is omitted if stab\_correction = FALSE (not recommended). If estimate\_z0m = TRUE, z0m is first estimated from the wind profile equation and then used in the equation above for the calculation of u(z) (see e.g. Newman & Klein 2014).

#### Value

A vector of wind speed at heights z.

## Note

Note that this equation is only valid for  $z \ge d + z0m$ , and it is not meaningful to calculate values closely above d + z0m. All values in heights smaller than d + z0m will return 0.

#### References

Monteith, J.L., Unsworth, M.H., 2008: Principles of Environmental Physics. 3rd edition. Academic Press, London.

Newman, J.F., Klein, P.M., 2014: The impacts of atmospheric stability on the accuracy of wind speed extrapolation methods. Resources 3, 81-105.

## See Also

roughness.parameters

## **Examples**

```
heights <- seq(18,40,2) # heights above ground for which to calculate wind speed df <- data.frame(Tair=25,pressure=100,wind=c(3,4,5),ustar=c(0.5,0.6,0.65),H=c(200,230,250)) ws <- sapply(heights,function(x) wind.profile(df,z=x,zr=40,zh=25,d=16)) colnames(ws) <- paste0(heights,"m")
```

WUE.metrics

Water-Use Efficiency Metrics

#### **Description**

Calculation of various water use efficiency (WUE) metrics.

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## Usage

```
WUE.metrics(
  data,
  GPP = "GPP",
  NEE = "NEE",
  LE = "LE",
  VPD = "VPD",
  Tair = "Tair",
  constants = bigleaf.constants()
)
```

## **Arguments**

data	Data.frame or matrix containing all required variables
GPP	Gross primary productivity (umol CO2 m-2 s-1)
NEE	Net ecosystem exchange (umol CO2 m-2 s-1)
LE	Latent heat flux (W m-2)
VPD	Vapor pressure deficit (kPa)
Tair	Air temperature (deg C)
constants	Cmol - molar mass of carbon (kg mol-1) umol2mol - conversion micromole (umol) to mole (mol) kg2g - conversion kilogram (kg) to gram (g)

## **Details**

the following metrics are calculated:

Water-use efficiency (WUE):

$$WUE = GPP/ET$$

Water-use efficiency based on NEE (WUE\_NEE):

$$WUE_NEE = NEE/ET$$

Inherent water-use efficiency (IWUE; Beer et al. 2009):

$$IWUE = (GPP * VPD)/ET$$

Underlying water-use efficiency (uWUE; Zhou et al. 2014):

$$uWUE = (GPP * sqrt(VPD))/ET$$

All metrics are calculated based on the median of all values. E.g. WUE = median(GPP/ET,na.rm=TRUE)

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#### Value

a named vector with the following elements:

WUE Water-use efficiency (gC (kg H20)-1)

WUE\_NEE Water-use efficiency based on NEE (gC (kg H20)-1)

IWUE Inherent water-use efficiency (gC kPa (kg H20)-1)

uWUE Underlying water-use efficiency (gC kPa^0.5 (kg H20)-1)

#### Note

Units for VPD can also be hPa. Units change accordingly. WUE\_NEE is calculated based on the absolute value of NEE (the sign convention does not matter here).

#### References

Beer, C., et al., 2009: Temporal and among-site variability of inherent water use efficiency at the ecosystem level. Global Biogeochemical Cycles 23, GB2018.

Zhou, S., et al., 2014: The effect of vapor pressure deficit on water use efficiency at the sub-daily time scale. Geophysical Research Letters 41.

#### See Also

stomatal.slope for a measure of intrinsic WUE

## **Examples**

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