Package 'ddpart'

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 ${\tt CalculateAerodynamicResistance}$

 ${\it Calculate Aerodynamic Resistance}$

Description

Calculates aerodynamic resistance according to Erisman and Draaijers (1995) page 58. equation 3.4.

Usage

```
CalculateAerodynamicResistance(
  FrictionVelocity_ms,
  ReferenceHeight_m,
  ZeroPlaneDisplacementHeight_m,
  RoughnessLength_m,
  MoninObukhovLength_m
)
```

Arguments

FrictionVelocity_ms

Friction velocity in in m/s.

ReferenceHeight_m

Reference height in m. Aerodynamic resistance will be calculated between ReferenceHeight_m and the sum of ZeroPlaneDisplacementHeight_m + RoughnessLength_m.

```
ZeroPlaneDisplacementHeight_m
```

Displacement height in m.

RoughnessLength_m

Roughness length in m.

MoninObukhovLength_m

Monin-Obkukhiv length in m. Monin-Obkukhiv length for neutral stratification (Pasquill class D) is "infinity". This case is encoded by a value defined in GetConstants()\$InfLength in this package.

Value

Aerodynamic resistance in s/m.

References

Erisman JW, Draaijers GPJ. Atmospheric Deposition In Relation to Acidification and Eutrophication. 1995.

```
# Aerodynamic resistance for extremely unstable stratification
# over grassland
PasquillClass <- "A"
RoughnessLength_m <- 0.03
WindSpeed_ms <- 1.5</pre>
AnemometerHeight_m <- 10
ReferenceHeight_m <- 10
ZeroPlaneDisplacementHeight_m <- 7 * RoughnessLength_m</pre>
MOL_m <- CalculateMoninObukhovLength(</pre>
 PasquillClass = PasquillClass,
 RoughnessLength_m = RoughnessLength_m
)
FrictionVelocity_ms <- CalculateFrictionVelocity(</pre>
 WindSpeed_ms = WindSpeed_ms,
 AnemometerHeight_m = AnemometerHeight_m,
 ZeroPlaneDisplacementHeight_m = ZeroPlaneDisplacementHeight_m,
 RoughnessLength_m = RoughnessLength_m,
 MoninObukhovLength_m = MOL_m
CalculateAerodynamicResistance(
 FrictionVelocity_ms = FrictionVelocity_ms,
 ReferenceHeight_m = ReferenceHeight_m,
 ZeroPlaneDisplacementHeight_m = ZeroPlaneDisplacementHeight_m,
 RoughnessLength_m = RoughnessLength_m,
 MoninObukhovLength_m = MOL_m
)
```

CalculateAirDensity CalculateAirDensity

Description

Calculates the density of air according to Seinfeld and Pandis (2006) page 735 eq. 16.36.

Usage

```
CalculateAirDensity(AirPressure_Pa, T_air_K)
```

Arguments

```
AirPressure_Pa Air pressure in Pa.

T_air_K Air temperature in K.
```

Value

Density of air in kg/m3.

References

Seinfeld JH, Pandis SN. Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. Wiley; 2006.

CalculateDepositionVelocity

CalculateDepositionVelocity

Description

Calculates the deposition velocity of particle according to the Zhang et al. (2001) and the Emerson et al. (2020) publications.

This is a wrapper function over the various dry deposition sub-processes. It is designed for use cases where information on wind speed is available for the same land use type where deposition velocities should be calculated (e.g. wind speed measured at 10 m anemometer height and concentrations at 1.5 m, both over grassland.) Use CalculateDepositionVelocity2() for situations where wind speed data is available for one land use but dry deposition velocities should be calculated for another land use.

Required inputs are:

- (1) basic meteorological data (wind speed, global ration, relative humidity, cloud cover, air temperature, air pressure, surface wetness)
- (2) information on the surface properties (land use class, roughness length and displacement height) and reference height (height of concentration measurements)

(3) particle properties (dry particle diameter, density, optional: aerosol type to calculate hygroscopic swelling)

The calculation steps in CalculateDepositionVelocity() are:

- 1. Calculate meteorological basics (e.g. viscosity and density of air) and whether its day of night (based on parameter SunAngle_degree).
- 2. Calculate the Pasquill class (general classification of atmospheric stability).
- 3. Calculate other meteorological parameters (Monin-Obukhov length, friction velocity, stability corrections).
- 4. Calculate the aerodynamic resistance (Ra) between the reference height and the effective height of the receptor (displacement height plus roughness length). Calculate surface resistance (Rs) and gravitation settling.
- 5. Calculate dry deposition velocity.

Usage

CalculateDepositionVelocity(InputTable)

Arguments

InputTable

A data frame with the following columns:

- SunAngle_degree: The sun angle in degree. Only used to determine if its "day" (> 0°) or "night" (< 0°) which is required for the determination of the Pasquill stability class (GetPasquillClass()). The sun angle can easily be calculated with oce::sunAngle().
- T_air_K: Air temperature in Kelvin.
- AirPressure_Pa: Air pressure in Pa. Required for the calculation of the mean free path of an air molecule, which is required for the calculation of the particle settling (sedimentation) velocity.
- GlobalRadiation_W_m2: Global radiation in W/m2. Required for the determination of the Pasquill stability class (GetPasquillClass()).
- CloudCover_percent: Cloud cover in percent. Required for the determination of the Pasquill stability class (GetPasquillClass()).
- WindSpeedAtAnemometerHeight_ms: Wind speed (m/s) at the the anemometer height. Required for GetPasquillClass() and CalculateFrictionVelocity().
- RoughnessLength_m: Roughness length (m) of the land cover for which the anemometer wind speed is provided. Required for multiple functions.
- ZeroPlaneDisplacementHeight_m: Zero plane displacement height (m) of the land cover for which the anemometer wind speed is provided. Required for multiple functions.
- AnemometerHeight_m: Height to which the wind speed data refers
- SurfaceIsWet_bool: Boolean indicating whether the surface is wet, in which case the particle rebound effect is disabled. Can be set e.g. depending on relative humidity and/or precipitation events.
- SurfaceIsVegetated_bool: Boolean indicating whether the surface is vegetated. Should be TRUE for all LUCs currently implemented in ddpart.

- LUCNames: Land use classes (character). See ?GetLandUseParameters for information.
- ReferenceHeight_m: Aeordynamic resistance is calculated between ReferenceHeight_m and the effective receptor height (RoughnessLength_m + Zero-PlaneDisplacementHeight_m).
- RoughnessLength_m: Roughness length of the land use class.
- Zero-PlaneDisplacementHeight_m: Zero-plane displacement height of the land use class.
- Season: Integer determining the season according to Zhang et al. (2001) table 2.
- DryParticleDiameter_m: Particle diameter in m before the growth particles due to water uptake is taken into account (see parameter "AerosolType").
- ParticleDensity_kgm3: Density of the particles in kg/m3.
- AerosolType: 'Set parameter AerosolType to "Dry" to disable calculation of hygroscopic swelling. Set parameter "AerosolType" to one of "SeaSalt", "Urban", "Rural", "AmmoniumSulfate" to enable hygroscopic swelling according to Zhang et al. (2001). See CalculateHygroscopicSwelling() for further details.
- RelHum_percent: Relativ humidty (particles.
- Parametrization: A character indicates which parametrization should be used. See ?GetLandUseParameters for allowed values.

Value

A data frame repeating the InputTable plus additional columns with calculated values.

References

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560. Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

Examples

See vignette.

CalculateDepositionVelocity2

CalculateDepositionVelocity2

Description

Calculates the deposition velocity of particle according to the Zhang et al. (2001) and the Emerson et al. (2020) publications.

This is a wrapper function over the various dry deposition sub-processes. It is designed for use cases where information on wind speed is available for one land use but dry deposition velocities should be calculated for another land use. For example, wind speed is available from modelled data for standard WMO conditions (10 m over grassland) but the dry deposition velocity should be calculated for forest. Use CalculateDepositionVelocity() for the more typical case where wind speed information is available for the sane land use type where dry deposition should be calculated.

The approach therefore differentiates between two sites:

- "anemometer site": Location/land use class where the wind speed measurements are available. Characterized by parameters "RoughnessLengthAnemometer_m" and "ZeroPlaneDisplacementHeightAnemometer m"
- "target land use site": Location/land use class where the dry deposition velocity should be calculated. Characterized by parameters "RoughnessLengthTargetLUC_m", "ZeroPlaneDisplacementHeightTargetLUC_m", "Season"

CalculateDepositionVelocity2() vertically extrapolates the wind speed at "anemometer site" the to a "blending height" (e.g. 50 m) where atmospheric conditions are somewhat independent of the underlying surface. From the blending height, the parameters relevant for particle dry deposition to the target land use site (friction velocity, aerodynamic resistance, etc.) are be calculated. The main calculation steps in CalculateDepositionVelocity() are:

- 1. Calculate meteorological basics (e.g. viscosity and density of air) and whether its day of night (based on parameter SunAngle degree)
- 2. Calculate the Pasquill class (general classification of atmospheric stability) based on data at the anemometer location (e.g. grassland land use class). This classification is also applied to the target land use type.
- 3. Calculate other meteorological parameters for the anemometer site (Obukhov length, friction velocity, stability corrections) and extrapolate wind speed to the blending height, using CalculateWindSpeedAtTargetHeight()
- 4. Calculate meteorological parameters for the target land use type (Obukhov length, friction velocity, stability corrections), based on the wind speed at blending height and the surface properties of the target land use type.
- 5. Calculate the aerodynamic resistance (Ra) between the reference height and the effective height of the receptor / target land use type. Calculate surface resistance (Rs) and gravitation settling.
- 6. Calculate dry deposition velocity to the target land use class.

Usage

CalculateDepositionVelocity2(InputTable)

Arguments

InputTable A data frame with the all columns required by CalculateDepositionVelocity(), but:

- RoughnessLengthAnemometer_m: Roughness length (m) of the land cover for which the anemometer wind speed is provided. Required for multiple functions.
- ZeroPlaneDisplacementHeightAnemometer_m: Zero plane displacement height (m) of the land cover for which the anemometer wind speed is provided. Required for multiple functions.
- WindSpeedBlendingHeight_m: Height in m to which the wind speed is extrapolated. At this height, the wind speed is assumed to be independent of the underlying land use.
- TargetLUCNames: Land use classes (character). See ?GetLandUseParameters for information.
- RoughnessLengthTargetLUC_m: Roughness length (m) of the land cover for which the dry deposition velocities are calculated.
- ZeroPlaneDisplacementHeightTargetLUC_m: Zero plane displacement height (m) of the land cover for which the dry deposition velocities are calculated.

Value

A data frame repeating the InputTable plus additional columns with calculated values.

References

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560. Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

```
if (require("tidyr")) {
# Define some standard conditions
Basics <- data.frame(</pre>
 SunAngle_degree = 30,
 T_{air}K = 293.15,
 AirPressure_Pa = 101325,
 SurfaceIsWet_bool = FALSE,
 SurfaceIsVegetated_bool = TRUE,
 GlobalRadiation_W_m2 = 100,
 RelHum_percent = 80,
 CloudCover_percent = 80,
 RoughnessLengthAnemometer_m = 0.03, # WMO grassland
 ZeroPlaneDisplacementHeightAnemometer_m = 0.21,
 AnemometerHeight_m = 10,
 WindSpeedAtAnemometerHeight_ms = 5,
 WindSpeedBlendingHeight_m = 50, # WS no longer dependent on LUC at 50m
 Season = 1,
 DryParticleDiameter_m = 5e-6,
 ParticleDensity_kgm3 = 2000,
 AerosolType = "Dry", # disable hygroscopic swelling
```

```
Parametrization = "GCNew",
  ReferenceHeight_m = 50 # assuming concentrations are known at blending height
)
# Define two land use classes for which to calculate dry deposition velocity
TargetLUCs <- data.frame(</pre>
  TargetLUCNames = c("Needleleaf", "DecBroadleaf"),
  RoughnessLengthTargetLUC_m = c(0.8, 2.65) # Zhang01 table 3
) %>%
  mutate(
    ZeroPlaneDisplacementHeightTargetLUC_m = 7 * RoughnessLengthTargetLUC_m
# Run calculations
InputTable <- merge(Basics, TargetLUCs)</pre>
Output <- CalculateDepositionVelocity2(
  InputTable = InputTable
}
# Show results.
print(Output %>% select(TargetLUCNames, V_d_RefHeight_ms))
```

CalculateDynamicViscosityOfAir

CalculateDynamicViscosityOfAir

Description

Calculates Dynamic viscosity of air according to Seinfeld and Pandis (2006) page 909.

Usage

CalculateDynamicViscosityOfAir(T_air_K)

Arguments

T_air_K Air temperature in Kelvin.

Value

Dynamic viscosity of air in kg/(m*s).

References

Seinfeld JH, Pandis SN. Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. Wiley; 2006.

CalculateFrictionVelocity

 ${\it CalculateFrictionVelocity}$

Description

Calculates friction velocity according to Erisman and Draaijers (1995) page 67 equation 3.25.

Usage

```
CalculateFrictionVelocity(
   WindSpeed_ms,
   AnemometerHeight_m,
   ZeroPlaneDisplacementHeight_m,
   RoughnessLength_m,
   MoninObukhovLength_m
)
```

Arguments

MoninObukhovLength_m

Monin-Obkukhiv length in m. Monin-Obkukhiv length for neutral stratification (Pasquill class D) is "infinity". This case is encoded by a value defined in GetConstants()\$InfLength in this package.

Value

A friction velocity value in m.

References

Erisman JW, Draaijers GPJ. Atmospheric Deposition In Relation to Acidification and Eutrophication. 1995.

```
# Friction velocity over grassland for extremely unstable stratification
# (Pasquill class A)
MOL_m <- CalculateMoninObukhovLength(
   PasquillClass = "A",</pre>
```

```
RoughnessLength_m = 0.03
)
CalculateFrictionVelocity(
 WindSpeed_ms = 1.5,
 AnemometerHeight_m = 10,
 ZeroPlaneDisplacementHeight_m = 0.21,
 RoughnessLength_m = 0.03,
 MoninObukhovLength_m = MOL_m
)
# Friction velocity over grassland for neutral stratification
# (Pasquill class D)
MOL_m <- CalculateMoninObukhovLength(</pre>
 PasquillClass = "D",
 RoughnessLength_m = 0.03
CalculateFrictionVelocity(
 WindSpeed_ms = 7,
 AnemometerHeight_m = 10,
 ZeroPlaneDisplacementHeight_m = 0.21,
 RoughnessLength_m = 0.03,
 MoninObukhovLength_m = MOL_m
)
```

CalculateHygroscopicSwelling

CalculateHygroscopicSwelling

Description

Calculates increase in particle diameter due to water update according to Zhang et al. (2001) eq. 10. All parameters must be vectors of same lengths. Note that a correction has been applied to Zhang et al. (2001) eq. 10: The whole equation is raised to the power of 1/3, following the original publication mentioned by Zhang: Gerber (1985). Without this correction, the wet diameter is often smaller compared to the dry diameter.

Usage

```
CalculateHygroscopicSwelling(
  DryParticleDiameter_m,
  AerosolType,
  RelHum_percent
)
```

Arguments

```
DryParticleDiameter_m
```

The diameter of the particles before application of hygroscopic swelling (dry) in m.

```
AerosolType Hygroscopic swelling differs depending on aerosol type. Implemented types are (1) "Dry" for no swelling, (2) "SeaSalt", (3) "Urban", (4) "Rural" and (5) "AmmoniumSulfate".
```

RelHum_percent Relative humidity in percent.

Value

A vector of particle diameters after accounting for hygroscopic swelling in m.

References

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560.

Gerber HE. 1985. Relative - Humidity Parameterization of the Navy Aerosol Model (NAM). NAVAL RESEARCH LAB WASHINGTON DC; December 30, 1985. Available at: https://apps.dtic.mil/sti/citations/ADA16

```
DryParticleDiameter_m <- c(0.01, 1, 5, 10) * 1e-6
AerosolType <- c("SeaSalt", "Rural", "Dry")
RelHum_percent <- seq(60, 100, by = 0.5)
Input <- expand.grid(</pre>
  DryParticleDiameter_m = DryParticleDiameter_m,
  AerosolType = AerosolType,
  RelHum_percent = RelHum_percent
)
Output <- Input %>%
  mutate(
    WetParticleDiameter_m = CalculateHygroscopicSwelling(
      DryParticleDiameter_m = DryParticleDiameter_m,
      AerosolType = AerosolType,
      RelHum_percent = RelHum_percent
   )
  )
if (require("ggplot2")) {
ggplot(
  data = Output,
  mapping = aes(
   x = RelHum_percent,
   y = WetParticleDiameter_m,
    color = as.factor(DryParticleDiameter_m),
    linetype = AerosolType
) +
  geom_line()
}
```

CalculateKinematicViscosityOfAir

CalculateKinematicViscosityOfAir

Description

Calculates kinematic viscosity of air according to Dixon (2007) appendix B

Usage

CalculateKinematicViscosityOfAir(DynamicViscosityAir_kgms, AirDensity_kgm3)

Arguments

```
DynamicViscosityAir_kgms

Dynamic viscosity of air in kg/(m*s).

AirDensity_kgm3

Density of air in kg/m3.
```

Value

Kinematic viscosity of air in kg/(m*s).

References

Dixon JC. The Shock Absorber Handbook. John Wiley & Sons; October 22, 2007.

 $\label{lem:calculateLossEfficiencyBrownianDiffusion} Calculate Loss \textit{EfficiencyBrownianDiffusion}$

Description

Calculates loss efficiency by brownian diffusion according to Emerson et al. (2020) eq. 3.

Usage

```
CalculateLossEfficiencyBrownianDiffusion(
   SchmidtNumber,
   BrownianDiffusionParameterGamma,
   Parametrization
)
```

Arguments

SchmidtNumber Schmidt number. E.g. provided by CalculateSchmidtNumber()

 ${\tt BrownianDiffusionParameterGamma}$

Empirical parameter. Land use specific in Zhang et al. (2001) and constant at a

value of 2/3 in Emerson et al. (2020)

Parametrization

A character defining which parametrization to use. See ?GetLandUseParameters for a list of valid values.

Value

Loss efficiency by brownian diffusion

References

Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

CalculateLossEfficiencyImpaction

CalculateLossEfficiencyImpaction

Description

Calculates loss efficiency by impaction according to Emerson et al. (2020) eq. 4.

Usage

```
CalculateLossEfficiencyImpaction(
   StokesNumber,
   ImpactionParameterAlpha,
   Parametrization
)
```

Arguments

StokesNumber Stokes number ImpactionParameterAlpha

A land-use specific empirical paramete

Parametrization

A character defining which parametrization to use. See ?GetLandUseParameters for details.

Value

Stokes number

References

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560.

 $\label{loss} Calculate Loss Efficiency Interception \\ {\it Calculate Loss Efficiency Interception}$

Description

Calculates the loss efficiency by interception (E_In) according to Emerson et al. (2020)

Usage

```
CalculateLossEfficiencyInterception(
  ParticleDiameter_m,
  CharacteristicRadius_m,
  Parametrization
)
```

Arguments

ParticleDiameter_m

Particle diameter in m.

CharacteristicRadius_m

Characteristic radius of the receptor surfaces in m.

Parametrization

A character defining which parametrization to use. See ?GetLandUseParameters for a list of valid values.

Value

Loss efficiency by interception.

References

Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

16 CalculateMeanFreePath

CalculateMeanFreePath CalculateMeanFreePath

Description

Calculates the mean free path of an air molecule according to Seinfeld and Pandis (2006) page 399 eq. 9.6.

Usage

```
CalculateMeanFreePath(T_air_K, AirPressure_Pa, DynamicViscosityAir_kgms)
```

Arguments

```
T_air_K Air temperature in Kelvin.

AirPressure_Pa Air pressure in Pa.

DynamicViscosityAir_kgms

Dynamic viscosity of air in kg/(m*s) F.g. provided by CalculateDynamicViscosity.
```

Dynamic viscosity of air in kg/(m*s). E.g. provided by CalculateDynamicViscosityOfAir().

Value

Mean free path of an air molecule in m.

References

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560.

```
# Validation against example Seinfeld and Pandis eq 9.7 page 399
T_air_K <- 298
AirPressure_Pa <- 101325
DynamicViscosityAir_kgms <- 1.8e-5
MeanFreePath_m <- CalculateMeanFreePath(T_air_K, AirPressure_Pa, DynamicViscosityAir_kgms)
MeanFreePath_um <- MeanFreePath_m * 1e6
print(MeanFreePath_um)
# 0.0651 um as given in SP06</pre>
```

CalculateMoninObukhovLength

CalculateMoninObukhovLength

Description

Calculates Monin-Obukhov length according to Seinfeld and Pandis (2006) page 751 eq. 16.83.

Usage

CalculateMoninObukhovLength(PasquillClass, RoughnessLength_m)

Arguments

PasquillClass A single character indicating the Pasquill stability class. For example according to Seinfeld and Pandis (2006) page 750 as implemented in GetPasquillClass().

RoughnessLength_m

Roughness length in m.

Value

A numeric value for Monin-Obukhov length. Monin-Obkukhiv length for neutral stratification (Pasquill class D) is "infinity". This case is encoded by a value defined in GetConstants()\$InfLength in this package.

References

Seinfeld JH, Pandis SN. Atmospheric Chemistry and Physics: From Air Pollution to Climate Change 2006.

```
# For Pasquill class A ("extremely unstable" conditions) and grassland
CalculateMoninObukhovLength(
   PasquillClass = "A",
   RoughnessLength_m = 0.03
)

# For Pasquill class D ("neutral" conditions) and grassland
CalculateMoninObukhovLength(
   PasquillClass = "D",
   RoughnessLength_m = 0.03
)
GetConstants()$InfLength
```

CalculateSchmidtNumber

CalculateSchmidtNumber

CalculateSchmidtNumber

Description

Calculates the Schmidt number according to Seinfeld and Pandis (2006) page 574

Usage

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```
CalculateSchmidtNumber(
   DynamicViscosityAir_kgms,
   KinematicViscosityOfAir_m2s,
   T_air_K,
   ParticleDiameter_m
)
```

Arguments

DynamicViscosityAir_kgms

Dynamic viscosity of air in kg/(m*s). E.g. provided by CalculateDynamicViscosityOfAir().

KinematicViscosityOfAir_m2s

Kinematic viscosity of air in m2/2. E.g. provided by CalculateKinematicViscosityOfAir().

T_air_K Air temperature in Kelvin.

ParticleDiameter_m

Particle diameter in m.

Value

Schmidt number

References

Seinfeld JH, Pandis SN. Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. Wiley; 2006.

```
# Reproduce relation between brownian diffusivity and particle diameter as shown
# in Seinfeld and Pandis (2006) page 417 Figure 9.8

data(diffusion_validation)
PlotData <- data.frame(
    # Set standard atmospheric conditions
    T_air_K = 20,
    AirPressure_Pa = 101325,</pre>
```

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```
# Set particle diameter according to Seinfeld and Pandis (2006)
 ParticleDiameter_m = 10^seq(-9, -5, length.out = 50)
) %>%
 # Calculation of quantities related to diffusion
 mutate(
   DynamicViscosityAir_kgms = CalculateDynamicViscosityOfAir(T_air_K),
   AirDensity_kgm3 = CalculateAirDensity(
     AirPressure_Pa = AirPressure_Pa,
     T_air_K = T_air_K
   ),
   KinematicViscosityOfAir_m2s = CalculateKinematicViscosityOfAir(
     DynamicViscosityAir_kgms = DynamicViscosityAir_kgms,
     AirDensity_kgm3 = AirDensity_kgm3
    SchmidtNumber = CalculateSchmidtNumber(
     DynamicViscosityAir_kgms = DynamicViscosityAir_kgms,
     KinematicViscosityOfAir_m2s = KinematicViscosityOfAir_m2s,
     T_air_K = T_air_K,
     ParticleDiameter_m = ParticleDiameter_m
   ),
    # Calculate brownian diffusivity from intermediate results
   BrownianDiffusivity_m2s = KinematicViscosityOfAir_m2s / SchmidtNumber,
    # For plotting:
   BrownianDiffusivity_cm2s = BrownianDiffusivity_m2s * 1e4,
   ParticleDiameter_um = ParticleDiameter_m * 1e6,
   Type = "Results from ddpart"
# Plot
if (require("ggplot2")) {
 ggplot() +
   geom_line(
     data = diffusion_validation %>%
          Type = "Validation data from Seinfeld and Pandis (2006)"
       ),
     mapping = aes(
       x = log10(ParticleDiameter_um),
       y = log10(DiffusionCoefficient_cm2s),
       color = Type
     )
   ) +
    geom_point(
     data = PlotData,
     mapping = aes(
       x = log10(ParticleDiameter_um),
       y = log10(BrownianDiffusivity_cm2s),
       color = Type
     ),
     shape = "x"
    ) +
    annotate(
      geom = "text",
```

```
x = -0,
y = -3,
label = "Small differences likely related\nto errors from extraction of
validation data from PDF figure."
) +
theme(
legend.position = "bottom"
)
}
```

CalculateSettlingVelocity

CalculateSettlingVelocity

Description

Calculates settling velocity of particles by gravitation according to Zhang et al. (2001).

Usage

```
CalculateSettlingVelocity(
   ParticleDensity_kgm3,
   ParticleDiameter_m,
   MeanFreePathOfAirMolecule_m,
   DynamicViscosityAir_kgms
)
```

Arguments

ParticleDensity_kgm3

Particle density in kg/m3.

ParticleDiameter_m

Particle diameter in m.

 ${\tt MeanFreePathOfAirMolecule_m}$

Mean free path of an air molecule in m. E.g. provided by CalculateMean-FreePath().

DynamicViscosityAir_kgms

Dynamic viscosity of air in kg/(m*s). E.g. provided by CalculateDynamicViscosityOfAir().

Value

Gravitation settling velocity in m/s.

References

CalculateStokesNumber 21

 ${\tt CalculateStokesNumber} \ \ {\tt CalculateStokesNumber}$

Description

Calculates the stokes number according to Zhang et al. (2001)

Usage

```
CalculateStokesNumber(
  FrictionVelocity_ms,
  SettlingVelocity_ms,
  CharacteristicRadius_m,
  KinematicViscosityOfAir_m2s,
  SurfaceIsVegetated
)
```

Arguments

```
FrictionVelocity_ms
Friction velocity in m/s

SettlingVelocity_ms
Settling velocity in m/s

CharacteristicRadius_m
Characteristic radius of receptor surface in m

KinematicViscosityOfAir_m2s
```

Kinematic viscosity of air in m2/s

SurfaceIsVegetated

Boolean value indicating whether the receptor surface is a vegetation surface

Value

Stokes number

References

CalculateSurfaceResistance

 ${\it Calculate Surface Resistance}$

Description

Calculates the surface resistance (R_s) according to Zhang et al. (2001).

Usage

```
CalculateSurfaceResistance(
   SurfaceIsWet,
   FrictionVelocity_ms,
   StokesNumber,
   E_b,
   E_Im,
   E_In,
   ParticleDiameter_m,
   Parametrization
)
```

Arguments

SurfaceIsWet Indicator whether the receptor surface is wet (for bounce correction term), boolean.

FrictionVelocity_ms

Friction velocity in m/s.

StokesNumber Stokes number.

E_b Loss efficiency by brownian diffusion.

E_Im Loss efficiency by impaction.E_In Loss efficiency by interception.

ParticleDiameter_m

Particle diameter in m.

Parametrization

A character defining which parametrization to use. See ?GetLandUseParameters for a list of valid values.

Tor a fist or varie

Value

Surface resistance in s/m.

References

 ${\tt CalculateWindSpeedAtTargetHeight}$

CalculateWindSpeedAtTargetHeight

Description

Calculate wind speed according to stability-corrected log wind profile. This function is rearrangement of the formula for friction velocity after Erisman and Draaijers (1995) page 67. It is in line with https://en.wikipedia.org/wiki/Log_wind_profile

Usage

```
CalculateWindSpeedAtTargetHeight(
   FrictionVelocity_ms,
   TargetHeight_m,
   ZeroPlaneDisplacementHeight_m,
   RoughnessLength_m,
   MoninObukhovLength_m
)
```

Arguments

```
FrictionVelocity_ms
```

Friction velocity in m/s.

TargetHeight_m Height at which the wind speed should be calculated in m.

ZeroPlaneDisplacementHeight_m

Zero-plane displacement height in m.

RoughnessLength_m

Roughness length in m.

MoninObukhovLength_m

Monin-Obukhov-length in m.

Value

Wind speed at target height in m/s.

References

Erisman JW, Draaijers GPJ. Atmospheric Deposition In Relation to Acidification

24 dd_validation

dd_subprocess_validation

Data for validation of dry deposition subprocesses

Description

Data extracted from Emerson et al. (2020) fig. 2. Shows the dependency of dry deposition sub-processes to particle size according to the old and the old and the revised parametrization of the GEOS-Chem model. Note that the old parametrization is not identical to the Zhang et al. (2001) parametrization although it is termed "Zhang (2001)" in the Emerson et al. (2020) paper. See ?GetLandUseParameters for details.

Usage

data(dd_subprocess_validation)

Format

A data frame with 153 rows and 4 columns:

ParticleDiameter_um Particle diameter in um

DepositionVelocity_cms Dry deposition velocity resulting from the respective dry-deposition subprocess in cm^2/s

Process Dry-deposition sub-process

Parametrization Parametrization (GEOS-Chem old (GCOld) or GEOS-Chem new (GCNew))

References

Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560.

dd validation

Data for validation of dry deposition

Description

Data extracted from Emerson et al. (2020) fig. 1. Shows the dependency of dry deposition velocity to particle size for different land use types according to the old and the revised parametrization of the GEOS-Chem model. Note that the old parametrization is not identical to the Zhang et al. (2001) parametrization although it is termed "Zhang (2001)" in the Emerson et al. (2020) paper. See ?GetLandUseParameters for details.

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Usage

```
data(dd_validation)
```

Format

A data frame with 106 rows and 4 columns:

ParticleDiameter_um Particle diameter in um

DepositionVelocity_cms Dry deposition velocity in cm^2/s

Parametrization Parametrization (GEOS-Chem old (GCOld) or GEOS-Chem new (GCNew))

LUCName Land use class name

References

Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560.

Description

Shows the dependency of the diffusion coefficient and particle diameter. Data extracted from Seinfeld and Pandis (2006) page 417 fig. 9.8.

Usage

```
data(diffusion_validation)
```

Format

A data frame with 38 rows and 2 columns:

ParticleDiameter_um Particle diameter in um

DiffusionCoefficient_cm2s Diffusion coefficient in cm^2/s

References

Seinfeld JH, Pandis SN. Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. Wiley; 2006.

26 GetLandUseParameters

GetConstants

GetConstants

Description

This function returns some constants.

Usage

GetConstants()

Value

A named list of constants.

Examples

GetConstants()

GetLandUseParameters

GetLandUseParameters

Description

Get land use parameters according to Zhang et al. (2001) table 3 or Emerson et al. (2020). There are 4 variants of parametrization for the Zhang01 approach:

- A) "Zhang01": The original model according to Zhang et al. (2001). Not used for the figures in Emerson et al. (2020). Implemented in ddpart as parametrization "Zhang01".
- B) "GEOS-Chem old": This is what Emerson et al. (2020) refer to as "Zhang et al. (2001)" in their Fig. 1 and 2. Implemented in ddpart as parametrization "GCOld". It is an adaption of parametrization A) with two differences:

First, the land use classes in the GEOS-Chem model differ from those in A). The mapping between land use classes is not always straightforward. For example, "Grassland" in B) uses parameters for "shrubs and interrupted woodland" from A). The complete mapping of LUCs is defined in file "drydep_mod.F90" starting in lines 3143: https://github.com/geoschem/geos-chem/blob/main/GeosCore/drydep_mod.F90.

For the LUCs relevant for ddpart, the mapping Emerson20 <-> Zhang01 is as follows:

- "Needleleaf" <-> "Needleleaf" (LUC1)
- "Broadleaf" <-> "Deciduous broadleaf" (LUC4)
- "Grassland" <-> "Shrubs and interrupted wood-lands" (LUC10)

Second, no differentiation according to seasons exists. Instead, the average over seasons 1-5 is used for each parameter. See for example "drydep_mod.F90" line 3226.

C) "GEOS-Chem new": This is the "revised parametrization" in Emerson et al. (2020) Fig. 1 and 2. Implemented in ddpart as parametrization "GCNew". It uses the same assignment of LUCs as in B)

GetLandUseParameters 27

and also averages land use parameters over seasons, but some parameters have been re-calibrated by Emerson et al. to better match measurement data. Note that although the parameters for "Shrubs and interrupted wood-lands" (LUC10 from Zhang01) are used for grassland, the parametrization is valid for grassland. This is because Emerson20 *calibrated* the other parameters, such that the resulting dry deposition velocity matches measurement data for grassland.

D) "GCNewSeason": Same as C) but with season-specific land use parameters. E.g. parameter "characteristic receptor radius" (A in mm) varies between seasons for deciduous broadleaf forest. This is implemented in ddpart as parametrization "GCNewSeason".

Usage

```
GetLandUseParameters(LUCNames, Seasons, Parametrizations, TargetParameter)
```

Arguments

LUCNames A vector of land use class names (character). Currently, allowed values are

- "Grassland"

- "Needleleaf"

- "DecBroadleaf" (deciduous broadleaf)

Seasons A vector of season codes (integer values 1-5).

Parametrizations

A character, one of "GCNewSeason", "Zhang01", "GCOld", "GCNew".

TargetParameter

A character indicating which parameter to return ("z_0_m", "A_mm", "alpha" or "gamma").

Value

A vector of values for parameter "TargetParameter".

References

Zhang L, Gong S, Padro J, Barrie L. A size-segregated particle dry deposition scheme for an atmospheric aerosol module. Atmospheric Environment 2001;35:549–560.

Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

```
if (require("tidyr")) {
GetLandUseParameters(
   LUCNames = c("Grassland", "Needleleaf", "DecBroadleaf"),
   Seasons = rep(x = 4, times = 3),
   Parametrizations = rep(x = "Zhang01", times = 3),
   TargetParameter = "A_mm"
)
```

28 GetParameters

```
GetLandUseParameters(
   LUCNames = c("Grassland", "Needleleaf", "DecBroadleaf"),
   Seasons = rep(x = 4, times = 3),
   Parametrizations = rep(x = "GCNewSeason", times = 3),
   TargetParameter = "A_mm"
)
```

GetParameters

GetParameters

Description

This function returns empirical constants for dry deposition sub-processes according to Zhang et al. (2001) or according to the re-paramtrization by Emerson et al. (2020). This function covers only parameters that are not land-use specific (see GetLandUseParameters()).

Usage

GetParameters(Parametrization, TargetParameter)

Arguments

Parametrization

A character defining which parametrization to use. See ?GetLandUseParameters for a list of valid values.

TargetParameter

A character indicating which parameter value to return. Valid options are "C_b", "beta", "C_Im", "nu", "C_In" and "epsilon_0". See Emerson et al. (2020) table S1.

Value

A named list of parameters.

References

Emerson EW, Hodshire AL, DeBolt HM, Bilsback KR, Pierce JR, McMeeking GR, Farmer DK. Revisiting particle dry deposition and its role in radiative effect estimates. Proceedings of the National Academy of Sciences 2020;117:26076–26082.

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Examples

```
if ( require("tidyr") ) {
  GetParameters(Parametrization = "Zhang01", TargetParameter = "C_b")
  GetParameters(Parametrization = "GCNewSeason", TargetParameter = "C_b")
}
```

GetPasquillClass

GetPasquillClass

Description

Calculates Pasquill stability class according to Seinfeld and Pandis (2006) page 750.

Usage

```
GetPasquillClass(
   SurfaceWindSpeed_ms,
   DayOrNight,
   IncomingSolarRadiation_Wm2,
   CloudCover_percent
)
```

Arguments

```
SurfaceWindSpeed_ms
Wind speed at surface in m/s.

DayOrNight Boolean indicating whther it is day or night.

IncomingSolarRadiation_Wm2
Solar radiation in W/m2.

CloudCover_percent
Cloud cover in percent.
```

Value

Chracter string indicating the Pasquill stability class (A - F)

References

Seinfeld JH, Pandis SN. Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. 2006.

30 meteo_time_series

meteo_time_series

Example 48 h meteorological time series

Description

Meteorological data required for dry deposition modelling (e.g. to determine atmospheric stability via Pasquill classes). Hourly data is for example available from the ERA5 model.

Usage

data(meteo_time_series)

Format

A data frame with 48 rows and 11 columns

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