Package ‘ddpart’

October 14, 2022

Type Package

Title Simulation of particle dry deposition

Version 0.1.0

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Description Implementation of the particle dry deposition model of Zhang et al. (2001) including the parametrization from Emerson et al. (2020).

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Encoding UTF-8

LazyData true

Suggests devtools,
ggplot2,
knitr,
rmarkdown,
scales,
tidyr

VignetteBuilder knitr

RoxygenNote 7.1.2

Depends dplyr,
R (>= 2.10)

R topics documented:

`CalculateAerodynamicResistance`

CalculateAerodynamicResistance

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.

Examples

```
# Aerodynamic resistance for extremely unstable stratification
# over grassland
PasquillClass <- "A"
RoughnessLength_m <- 0.03
WindSpeed_ms <- 1.5
AnemometerHeight_m <- 10
ReferenceHeight_m <- 10
ZeroPlaneDisplacementHeight_m <- 7 * RoughnessLength_m

MOL_m <- CalculateMoninObukhovLength(
  PasquillClass = PasquillClass,
  RoughnessLength_m = RoughnessLength_m
)
FrictionVelocity_ms <- CalculateFrictionVelocity(
  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 + ZeroPlaneDisplacementHeight_m).

- RoughnessLength_m: Roughness length of the land use class.

- ZeroPlaneDisplacementHeight_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.

Examples

```
if (require("tidyr")) {

# Define some standard conditions
Basics <- data.frame(
  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(
  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)
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`

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

`WindSpeed_ms` Wind speed in m/s.

`AnemometerHeight_m` Height in m to which WindSpeed_ms refers.

`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

A friction velocity value in m.

References

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

Examples

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

```
  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(
  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

Examples

```
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(
  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.

`CalculateLossEfficiencyBrownianDiffusion`
CalculateLossEfficiencyBrownianDiffusion

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()

`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.

`CalculateLossEfficiencyInterception`
CalculateLossEfficiencyInterception

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.

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). 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.

Examples

```
# 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
```

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.

Examples

```
# 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*

Description

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

Usage

```
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.

Examples

```
# 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,
```

```
    #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 %>%
        mutate(
          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.

`MeanFreePathOfAirMolecule_m`
: Mean free path of an air molecule in m. E.g. provided by CalculateMeanFreePath().

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

Value

Gravitation settling velocity in m/s.

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.

CalculateStokesNumber *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

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.

CalculateSurfaceResistance *CalculateSurfaceResistance*

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.

Value

Surface resistance in s/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.

`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

`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 subprocesses 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.

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.

`diffusion_validation` *Data for validation of the diffusion term*

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.

`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) 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.

Examples

```
if (require("tidyr")) {

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

```
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.

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.

Examples

```
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.

`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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