Package 'ISO6976.2016'

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Title Calorific Values and Properties of Natural Gas per ISO 6976:2016

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LinkingTo Rcpp

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Suggests knitr, lintr, rmarkdown, testthat (>= 3.0.0)

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Description Calculates calorific values (gross and net), density, relative density, and Wobbe indices together with their standard uncertainties from natural gas composition, implementing the method of ISO 6976:2016 ``Natural Gas — Calculation of calorific values, density, relative density and Wobbe indices from composition". Uncertainty propagation follows Annex B of that standard.
Reference: International Organization for Standardization (2016) <https://www.iso.org/standard/55842.html>.

License GPL (>= 3)

URL https://github.com/RuedigerForster/ISO_6976

BugReports https://github.com/RuedigerForster/ISO_6976/issues

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VignetteBuilder knitr

NeedsCompilation yes

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Repository CRAN

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Contents

`ISO6976.2016-package` *ISO6976.2016: Calorific Values and Properties of Natural Gas per ISO 6976:2016*

Description

Calculates calorific values (gross and net, molar, mass and volumetric bases), density, relative density, and Wobbe indices together with their standard uncertainties from natural gas composition, following ISO 6976:2016 "Natural Gas — Calculation of calorific values, density, relative density and Wobbe indices from composition".

Details

Uncertainty propagation is implemented according to Annex B of that standard (variance-covariance method).

Application restrictions (ISO 6976:2016 §5): * Combustion temperature: 0, 15, 15.55 (60 °F), 20, or 25 °C. * Volume reference temperature: 0, 15, 15.55 (60 °F), or 20 °C. * Reference pressure: 90–110 kPa. * Compression factor Z must be > 0.9.

Author(s)

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References

ISO 6976:2016 "Natural Gas — Calculation of calorific values, density, relative density and Wobbe indices from composition".

See Also

Useful links:

- https://github.com/RuedigerForster/ISO_6976
- Report bugs at https://github.com/RuedigerForster/ISO_6976/issues

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`calculateProperties` *Calculate natural gas properties per ISO 6976:2016*

Description

Computes all combustion and volumetric properties of a natural gas mixture together with their standard (or expanded) uncertainties, following the method and tables of ISO 6976:2016 and the uncertainty propagation formulae of its Annex B.

Usage

```
calculateProperties(
  compositionArray,
  uncertaintyArray,
  correlationMatrix,
  combustionTemperature = 25,
  volumeTemperature = 15,
  pressure = 101.325,
  coverage = 1
)
```

Arguments

`compositionArray`	Numeric vector of length 60: mole fractions \[mol/mol\] in the component order of ISO 6976:2016 Table A.2. See `componentNames` for the ordering. If values are given in mol%, divide by 100 before passing them here.
`uncertaintyArray`	Numeric vector of length 60: standard uncertainties of the mole fractions (same units as `compositionArray`).
`correlationMatrix`	60x60 numeric matrix of correlation coefficients between component mole fractions. Use `diag(60)` when correlations are unknown or assumed to be zero.
`combustionTemperature`	Combustion reference temperature in °C. Permitted values: 0, 15, 15.55, 20, 25. Default: 25.
`volumeTemperature`	Volume reference temperature in °C. Permitted values: 0, 15, 15.55, 20. Default: 15.
`pressure`	Reference pressure in kPa. Must be in \[90, 110\]. Default: 101.325.
`coverage`	Coverage factor k; uncertainties are multiplied by k before being returned. Default: 1 (standard uncertainty).

Value

A named list with the following elements (all numeric scalars):

| Name | Description | Unit | |—————|———————————————————————|—————| | M | Molar mass | kg/kmol | | Z | Compression factor | — | | G_o | Ideal-gas relative density | — | | D_o | Ideal-gas density | kg/m³ | | G, u_G | Real-gas relative density and uncertainty | — | | D, u_D | Real-gas density and uncertainty | kg/m³ | | Hcg, u_Hcg| Molar gross calorific value and uncertainty | kJ/mol | | Hcn, u_Hcn| Molar net calorific value and uncertainty | kJ/mol | | Hmg, u_Hmg| Mass-basis gross calorific value and uncertainty | MJ/kg | | Hmn, u_Hmn| Mass-basis net calorific value and uncertainty | MJ/kg | | Hvg_o, u_Hvg_o | Ideal-gas vol. gross CV and uncertainty | MJ/m³ | | Hvn_o, u_Hvn_o | Ideal-gas vol. net CV and uncertainty | MJ/m³ | | Hvg, u_Hvg| Real-gas vol. gross CV and uncertainty | MJ/m³ | | Hvn, u_Hvn| Real-gas vol. net CV and uncertainty | MJ/m³ | | Wg_o | Ideal-gas gross Wobbe index | MJ/m³ | | Wn_o | Ideal-gas net Wobbe index | MJ/m³ | | Wg, u_Wg | Real-gas gross Wobbe index and uncertainty | MJ/m³ | | Wn, u_Wn | Real-gas net Wobbe index and uncertainty | MJ/m³ |

References

ISO 6976:2016 "Natural Gas — Calculation of calorific values, density, relative density and Wobbe indices from composition"

See Also

GasComponents, componentNames

Examples

```
data("example1")
res <- calculateProperties(example1$fractionArray, example1$uncertaintyArray,
                           example1$correlationMatrix,
                           combustionTemperature = 15, volumeTemperature = 15)
res$M      # molar mass [kg/kmol]
res$Hvg    # real-gas vol. gross CV [MJ/m^3]
res$u_Wg   # standard uncertainty of gross Wobbe index
```

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componentIndex *Return the index of a gas component by name*

Description

Return the index of a gas component by name

Usage

```
componentIndex(name)
```

Arguments

name	Character string: component name (English). See componentNames for the full list.

Value

Integer index (1–60) into the composition vector.

---

componentName *Return the name of a gas component by index*

Description

Return the name of a gas component by index

Usage

```
componentName(index)
```

Arguments

index	Integer 1–60.

Value

Character string with the English component name.

---

componentNames *Return the names of all 60 gas components*

Description

Returns the ordered character vector of all 60 natural gas components recognised by ISO 6976:2016 (Table A.2). The position of each name corresponds to the index used in compositionArray, uncertaintyArray, and correlationMatrix.

Usage

```
componentNames()
```

Value

Character vector of length 60.

See Also

componentIndex, componentName

`example1` *ISO 6976:2016 Annex D.2 — Example 1 (5-component mixture, 15/15 °C)*

Description

A five-component natural gas mixture from Annex D.2 of ISO 6976:2016. Non-zero components: methane, ethane, propane, nitrogen, carbon dioxide.

Format

A named list with three elements:

fractionArray Numeric vector (length 60) of mole fractions [mol/mol].

uncertaintyArray Numeric vector (length 60) of standard uncertainties [mol/mol].

correlationMatrix 60×60 identity correlation matrix.

Source

ISO 6976:2016 Annex D.2, Table D.2.

`example2` *ISO 6976:2016 Annex D.3 — Example 2 (mixture with water vapour, 15.55/15.55 °C)*

Description

An eleven-component natural gas mixture including water vapour from Annex D.3 of ISO 6976:2016.

Format

A named list with three elements (same structure as `example1`).

Source

ISO 6976:2016 Annex D.3, Table D.3.

`example3` *ISO 6976:2016 Annex D — Example 3 (11-component mixture, identity matrix)*

Description

An eleven-component natural gas mixture from Annex D of ISO 6976:2016 with an identity correlation matrix (no inter-component correlations). Used to verify calculations at 15/15 °C and 25/0 °C.

Format

A named list with three elements (same structure as `example1`).

Source

ISO 6976:2016 Annex D.

`example3_ex` *ISO 6976:2016 Annex D — Example 3, full correlation matrix*

Description

The same eleven-component mixture as `example3` but with a full inter-component correlation matrix from a GC calibration covariance analysis, as given in Annex D of ISO 6976:2016.

Format

A named list with three elements (same structure as `example1`).

Source

ISO 6976:2016 Annex D (extended correlation case).

GasComponents *R6 class for natural gas composition input*

Description

R6 class for natural gas composition input

R6 class for natural gas composition input

Details

`GasComponents` holds the mole fractions, their standard uncertainties, and the inter-component correlation matrix for a natural gas mixture. All three quantities are required as input to `calculateProperties`.

Components are identified either by their integer index (1–60, matching ISO 6976:2016 Table A.2) or by English name (see `componentNames`).

Public fields

`fractions` Numeric vector (length 60) of mole fractions [mol/mol].

`uncertainties` Numeric vector (length 60) of standard uncertainties.

`correlations` 60x60 correlation matrix (default: identity matrix).

Methods

Public methods:

- `GasComponents$new()`
- `GasComponents$getFraction()`
- `GasComponents$getUncertainty()`
- `GasComponents$getCorrelation()`
- `GasComponents$setFraction()`
- `GasComponents$setUncertainty()`
- `GasComponents$setCorrelation()`
- `GasComponents$setFractionArray()`
- `GasComponents$setUncertaintyArray()`
- `GasComponents$setCorrelationMatrix()`
- `GasComponents$clone()`

Method `new()`**:** Create a new GasComponents object. Initialises fractions and uncertainties to zero and correlations to the 60x60 identity matrix.

Usage:

```
GasComponents$new()
```

Method `getFraction()`**:** Get the mole fraction of a single component.

Usage:

```
GasComponents$getFraction(name)
```

Arguments:

`name` Component name (English) or integer index 1–60.

Returns: Numeric scalar.

Method `getUncertainty()`**:** Get the standard uncertainty of a single component.

Usage:

```
GasComponents$getUncertainty(name)
```

Arguments:

`name` Component name (English) or integer index 1–60.

Returns: Numeric scalar.

Method `getCorrelation()`**:** Get the correlation between two components.

Usage:

```
GasComponents$getCorrelation(name1, name2)
```

Arguments:

`name1` First component name or index.

`name2` Second component name or index.

Returns: Numeric scalar in \[-1, 1\].

Method `setFraction()`**:** Set the mole fraction of a single component.

Usage:

```
GasComponents$setFraction(name, value)
```

Arguments:

`name` Component name or index.

`value` Mole fraction [mol/mol].

Method `setUncertainty()`**:** Set the standard uncertainty of a single component.

Usage:

```
GasComponents$setUncertainty(name, value)
```

Arguments:

`name` Component name or index.

`value` Standard uncertainty.

Method `setCorrelation()`**:** Set the correlation between two components.

Usage:

```
GasComponents$setCorrelation(name1, name2, value)
```

Arguments:

`name1` First component name or index.

`name2` Second component name or index.

`value` Correlation coefficient in \[-1, 1\].

Method `setFractionArray()`**:** Set all mole fractions at once.

Usage:

```
GasComponents$setFractionArray(x)
```

Arguments:

`x` Numeric vector of length 60.

Method `setUncertaintyArray()`**:** Set all uncertainties at once.

Usage:

```
GasComponents$setUncertaintyArray(u)
```

Arguments:

`u` Numeric vector of length 60.

Method `setCorrelationMatrix()`**:** Set the full correlation matrix.

Usage:

```
GasComponents$setCorrelationMatrix(r)
```

Arguments:

`r` 60x60 numeric matrix; values must lie in \[-1, 1\].

Method `clone()`**:** The objects of this class are cloneable with this method.

Usage:

```
GasComponents$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

`iso6976_calc` *Calculate all ISO 6976:2016 properties and their uncertainties*

Description

Calculate all ISO 6976:2016 properties and their uncertainties

Usage

```
iso6976_calc(x, u_x, r_x, t1, t2, p2, k = 1)
```

Arguments

`x`	Numeric vector of length 60: mole fractions [mol/mol]
`u_x`	Numeric vector of length 60: standard uncertainties
`r_x`	Numeric matrix 60x60: correlation matrix
`t1`	Combustion temperature [°C]: 0, 15, 15.55, 20, or 25
`t2`	Volume reference temperature [°C]: 0, 15, 15.55, or 20
`p2`	Reference pressure [kPa]: 90–110
`k`	Coverage factor (default 1)

Value

Named list of properties and uncertainties

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