

Package ‘ISO6976.2016’

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

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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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ISO6976.2016-package	<i>ISO6976.2016: Calorific Values and Properties of Natural Gas per ISO 6976:2016</i>
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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

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 $\backslash[\text{mol/mol}\backslash]$ 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 <code>diag(60)</code> 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 $\backslash[90, 110\backslash]$. 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/m ³
G, u_G	Real-gas relative density and uncertainty	—
D, u_D	Real-gas density and uncertainty	kg/m ³
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/m ³
Hvn_o, u_Hvn_o	Ideal-gas vol. net CV and uncertainty	MJ/m ³
Hvg, u_Hvg	Real-gas vol. gross CV and uncertainty	MJ/m ³
Hvn, u_Hvn	Real-gas vol. net CV and uncertainty	MJ/m ³
Wg_o	Ideal-gas gross Wobbe index	MJ/m ³
Wn_o	Ideal-gas net Wobbe index	MJ/m ³
Wg, u_Wg	Real-gas gross Wobbe index and uncertainty	MJ/m ³
Wn, u_Wn	Real-gas net Wobbe index and uncertainty	MJ/m ³

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
```

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	<i>ISO 6976:2016 Annex D.2 — Example 1 (5-component mixture, 15/15 °C)</i>
----------	--

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	<i>ISO 6976:2016 Annex D.3 — Example 2 (mixture with water vapour, 15.55/15.55 °C)</i>
----------	--

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	<i>ISO 6976:2016 Annex D — Example 3 (11-component mixture, identity matrix)</i>
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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	<i>ISO 6976:2016 Annex D — Example 3, full correlation matrix</i>
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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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