Hydrogen Metering uncertainty calculation tool met4h2

Contents

Application and related projects	2
Inputs, requirements and test run	2
General information	3
Configuration	3
ProcessData	5
Composition	6
Flow meter uncertainty	7
Temperature transmitter uncertainty	7
Pressure transmitter uncertainty	8
Composition uncertainty	8
Software overview	9
Meter	9
Process	9
Met4H2	10
Uncertainty analysis	10
Outputs	11
Raw gas property output	11
Raw uncertainty output	11
Main output	13
Gas Properties	13
References	14

Application and related projects

The met4h2-code is a python-tool for calculating uncertainty in metering stations for hydrogen gas flow. The uncertainty in volume, mass or energy flow are calculated from measured data (flow rates, temperatures, pressures and gas composition) and input uncertainties for the measured quantities. Calculation of energy and energy uncertainty is done according to ISO 15112 [1]. Gas properties at actual and reference conditions are calculated using third party equation of state tools such as REFPROP [2]. Uncertainties and correlations between variables are calculated using the Monte Carlo Method. More details on the functional relationships applied in the code is found in the best-practice guide [3] and the accompanying report with examples [4].

The code was developed in the project Met4H2 21GRD05 (met4h2.eu). This project received funding from the European Partnership on Metrology, co-financed from the European Union's Horizon Europe Research and Innovation Programme and by the Participating States.

The software development was started in February 2023. The code will be further developed in the research project SmartGasNet 24GRD10.

Inputs, requirements and test run

The main inputs to the met4H2-code are provided with an Excel document containing several sheets. The excel-file can have a filename of choice, but it is important that the layout of the input file is preserved. Inputs in the Excel-file that are not locked for editing may, however, be changed by the user. Each Excel sheet is explained in further detail in the following subsections.

When running the met4H2 code, the user must provide the full filename of the input file, this is given as an argument to a *run_it*-function. If the input file is in a folder different to the folder with the .py file, the full path should be specified in the optional argument of the *run_it* function.

The user must also provide the path to the refprop [5, 6] program files, as well as the path to the TREND dll location and file, if the user intends to use the TREND software [7]. These are also set using optional arguments in the *run_it*-function. If these are not set, the code will try to locate the refprop and TREND frameworks in folders that may not exist in the users' file system. An additional external framework is AGA8Detail [8].

An example of how to run the main parts of the software is shown in Figure 1.

```
m4h2 = met4H2()

filepath = os.getcwd()

unc, out_file = m4h2.run_it(
    filepath,
    'test_file.xlsx',
    refprop_path=refprop_path,
    trend_path=trend_path,
    trend_dll_path=trend_dll_path)
```

Figure 1: How to run the software, using the run_it-function.

It is recommended to create an environment with the .yml file located in the met4h2 repository. The software was developed using a 64-bit version of Windows.

Gas property calculations using the various frameworks (TREND, pyforfluids, AGA8Detail, and refprop) were validated against reference tables in ISO 20765-2 [9].

Key calculations have been performed in MatLab by Kjetil Folgerø, parallel to the main python-based code written by Lea Starck. Results have been compared to validate the python code. Federica Gugole reviewed an early version of the code, and Gregor Bobovnik has contributed towards validating against ISO-standard ISO 20765-2 [9].

Citation: Lea Starck, Kjetil Folgerø, Federica Gugole, Gregor Bobovnik, Met4H2 Software framework, https://github.com/vanswindenlaboratory/Met4H2, 2025.

General information

An overview of the Excel-sheets is given on the *Info-sheet*, as shown in Figure 2. The info-sheet is intended as a high-level overview for the user. All cells are locked for editing.

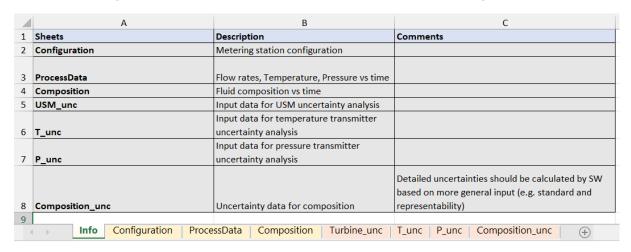


Figure 2: Info-sheet in the met4H2 input-file. All cells are locked for editing.

Configuration

Figure 3 shows the *Configuration*-sheet. The user may adjust several settings, but grey cells are locked for editing. Some of the locked cells are locked because the software does not yet support alternative settings than those given in the locked cells, functionality may be added in the future.

Project name: May be freely edited.
Project info: May be freely edited.

Quantity meter: Choose between Turbine, Ultrasonic or Coriolis meters from a drop-down

menu. In this example a Turbine-meter is chosen. If an Ultrasonic meter was chosen, the *Turbine_unc*-sheet would change to *USM_unc*. Similarly, if a Coriolis meter is chosen the *Turbine_unc*-sheet would change to

Coriolis_unc.

Quantity meter: Currently, only a single quantity meter is supported. In the future this may

be updated to a drop-down menu where serial or parallel meters can be

chosen.

No of meters: Currently, only a single quantity meter is supported.

Correlation

coefficient metering: As only a single quantity meter is currently supported, there is no

correlation between quantity meters.

Process analyzer: OnlineGC, sampling and calorie-meter can be chosen from a drop-down

menu as the method by which the gas composition is found. At present this does not affect the calculations, as uncertainties are always found in the *Composition_unc*-sheet. However, in the future, this choice may

trigger default composition uncertainties.

Sampling: NA.

Performance

requirements: The software conforms to the OIML R 140-standard.

EoS: The GERG-2008 or the AGA-8 equations of state (EoSs) can be chosen from

a drop-down menu.

EoS-tool: One of four frameworks for implementing the EoS can be selected from a

dropdown menu; refprop, pyforfluids, TREND, and AGA8Detail. These frameworks differ greatly in calculation speed. refprop is recommended.

Note that if the AGA-8 EoS was chosen previously, only TREND and

AGA8Detail support this EoS.

Pipe diameter: At present, this is an unused parameter, however, if the software is

expanded to include pressure drop meters, this variable will become

relevant.

Composition

uncertainty: The composition is read from the Composition_unc-sheet. If default

uncertainties are added to the software, this may be changed to a

drop-down menu.

Normalize all

components: Drop-down menu with choices 'yes' and 'no'. The mol-fractions of the

composition must sum to 1. This sum may be upset by the Latin-

Hypercube-Sampling, since the variables are drawn individually. If 'yes' is chosen all components are normalized by dividing their value by the sum of components. If 'no' is chosen, the composition samples from the Latin-Hypercube-sampling are accepted, and only one component is

adjusted by-difference such that the composition sums to 1.

By difference component

analysis: Select the gas component to be adjusted by difference from a drop-down

menu.

Gross calorific

value temperature: Select the temperature from a drop-down menu, at which to extract the

calorific value.

Gross calorific

value H2 only: Select 'yes' or 'no' from a drop-down menu. If 'yes' is selected the

calorific value is calculated for the H2 component only. If 'no' is selected

the calorific value is calculated for the entire gas.

Number of Monte

Carlo draws: Set an integer for the number of draws to be made for the Latin

Hypercube samplings to create parameter distributions corresponding

to the uncertainty specifications that will be given in the following

sheets.

	Α	В	С	D							
1	Configuration	Setting	Unit	Comment							
2	Project name	Testcase		1							
3	Project info	Test-config		2							
4	Quantity meter	Turbine		3							
5	Meter configuration	Single		4							
6	No of meters	1		5							
7	Correlation coefficient metering	0		6							
8	Process analyzer	OnlineGC		7							
9	Sampling	NA		8							
10	Performance requirements	OIML R 140		9							
11	EoS	GERG-2008		10							
12	EoS tool	refprop		11							
13	Pipe diameter	10	inch	12							
14	Base conditions	Normal		13							
15	Composition uncertainty	From input sheet		14							
16	Normalize all components	no		15							
17	By difference component analysis	H2		Only applies if 'Normalize all components'> 'No' is selected.							
18	Gross calorific value temperature	20	°C	17							
19	Gross calorific value H2 only	yes		18							
20	Number of Monte Carlo draws	100		If set to zero, only nominal values are computed.							
4	Info Configuration ProcessData Composition Turbine_unc T_unc P_unc Composition_unc										

Figure 3: Configuration-sheet in the met4H2 input-file. Grey cells are locked for editing.

ProcessData

The *ProcessData*-sheet contains four columns: DateTime, Flow Rate, Temperature (T), and Pressure (P). The flow rate unit can be set in the green column header from a drop-down menu. If a volume flow meter (e.g., Turbine or USM) is used, a volume flow rate should be chosen. Possible reported units could be at Standard Conditions (T = 15 °C), Normal conditions (T = 0 °C), or actual conditions. If a mass flow meter (Coriolis) is used, mass flow rate should be chosen. Temperatures should be given in units of degrees Celsius, if the unit displayed in the column header is also given in degrees Celsius. Similarly, pressure should be given in bara if the unit displayed in the corresponding column header is bara.

Process variables are defined as flow rate, temperature and pressure, as well as composition. Composition is given on a separate input-sheet.

	Α	В	С	D	Е	F	G	Н	1
1	DateTime	Normal volume flow rate [Nm3/h]	T [°C]	P [bara]					
2	07.04.2022 00:00	0.000	9.44	18.72					
3	07.04.2022 01:00	0.000	9.55	18.88					
4	07.04.2022 02:00	0.000	9.39	18.74					
5	07.04.2022 03:00	0.000	9.04	18.11					
6	07.04.2022 04:00	38.201	8.80	17.50					
7	07.04.2022 05:00	875.400	8.87	17.02					
8	07.04.2022 06:00	2 410.693	9.19	16.95					
9	07.04.2022 07:00	3 302.049	9.01	16.86					
10	07.04.2022 08:00	2 968.828	8.94	16.72					
11	07.04.2022 09:00	3 498.891	8.87	16.46					
12	07.04.2022 10:00	4 454.197	8.95	16.34					
	Info	Configuration ProcessData Con	npositio	n Turb	ine_unc	T_unc	P_unc	Composition	n_unc

Figure 4: ProcessData-sheet in the met4H2 input-file.

Composition

The Composition-sheet contains columns for DateTime, Unit and a column for each component in the gas composition. The DateTime column should match the DateTime column in the ProcessData-sheet. Units can be given as in the example as cmol/mol, (mol %) or as molar fractions (mol/mol). Write the units as cmol_mol-1 or mol_mol-1 in order for the software to be able to interpret it.

When entering the composition, more components can be added by adding columns to the right in the table. Column headings for the composition can be edited to achieve this. However, note that if component names that are not recognized by the software are used, the software will crash. Recognized component names are given in Table 1.

Table 1: Recognized component names.

H2	C1	n-C7	Ethylene	Ethylcyclopentane
N2	C2	n-C8	Propene	Cyclohexane
CO2	C3	n-C9	1-Butene	Methylcyclohexane
H2O	n-C4	n-C10	cis-2-Butene	Ethylcyclohexane
H2S	i-C4	n-C11	trans-2-Butene	Benzene
NH3	n-C5	n-C12	2-Methylpropene	Toluene
HCN	i-C5	n-C13	1-Pentene	Ethylbenzene
CO	neo-C5	n-C14	Propadiene	o-Xylene
COS	n-C6	n-C15	1,2-Butadiene	Methanol
CS2	2-Methylpentane		1,3-Butadiene	Methanetiol
He	3-Methylpentane		Acetylene	Ethylcyclopentane
O2	2,2-		Cyclopentane	
	Dimethylbutane			
Ar	2,3-		Methylcyclopentane	
	Dimethylbutane			

	Α	В	С	D	E	F	G	Н
1	DateTime	Unit	N2	O2	C1	H2		
2	07.04.2022	cmol_mol-1	0.00359221	7.04E-05	5.20012E-05	99.99629		
3	07.04.2022	cmol_mol-1	0.00385408	6.28E-05	5.22919E-05	99.99603		
4	07.04.2022	cmol_mol-1	0.00469253	7.71E-05	5.23818E-05	99.99518		
5	07.04.2022	cmol_mol-1	0.00759444	0.000109	5.20682E-05	99.99224		
6	07.04.2022	cmol_mol-1	0.00760266	0.000106	5.18324E-05	99.99224		
7	07.04.2022	cmol_mol-1	0.00395738	0.000104	5.12041E-05	99.99589		
8	07.04.2022	cmol_mol-1	0.00295639	9E-05	5.1099E-05	99.9969		
9	07.04.2022	cmol_mol-1	0.00265353	8.67E-05	5.11979E-05	99.99721		
10	07.04.2022	cmol_mol-1	0.00270925	8.68E-05	5.12619E-05	99.99715		
11	07.04.2022	cmol_mol-1	0.00334101	8.74E-05	5.14334E-05	99.99652		
12	07.04.2022	cmol_mol-1	0.00399759	8.75E-05	5.1327E-05	99.99586		
4	▶ Info Configuration	ProcessDat	a Composi	tion Tur	bine_unc T_	unc P_u	nc Comp	osition_unc

Figure 5: Composition-sheet in the met4H2 input-file.

Flow meter uncertainty

The flow meter uncertainty is set according to the example given in Figure 6. Grey cells are locked for editing. In the example, the flowmeter of choice is a Turbine meter, as specified in the configuration-sheet. The pattern is the same for a USM or a Coriolis meter.

There are three flow rates defined, Q_{min} , Q_{t} , and Q_{max} . Their values are defined in the *Range* column. If a flow rate Q falls between Q_{min} and Q_{t} , the uncertainty takes on the value given in row 4 in the *Uncertainty* column. If a flow rate Q falls between Q_{t} and Q_{max} , the uncertainty takes on the value in row 3 in the *Uncertainty* column. If a flow rate Q is larger than Q_{max} , the uncertainty takes on the value of row 2 in the *Uncertainty* column. Units can be given either as a percentage value (as shown in this example), or the absolute units of the flow as defined in the <u>ProcessData</u> sheet can be used. In the latter case, make sure that the units are identical to the units defined in the <u>ProcessData</u> sheet. The confidence intervals can be set using drop-down menus.

	Α	В	С	D	E	F	G	Н	I	J	k
1	Input variable	Range	Uncertainty	Unit	Confidence interval	Distribution					
2	Qv_max	1600	0.5	%	95 %	Normal					
3	Qv_t	320	1	%	95 %	Normal					
4	Qv_min	80	2	%	95 %	Normal					
5											
4	Info Configuration ProcessData Composition Turbine_unc T_unc P_unc Composition_unc										

Figure 6: Flowmeter uncertainty sheet in the met4H2 input-file. Grey cells are locked for editing.

Temperature transmitter uncertainty

The temperature uncertainty is set according to the example given in Figure 7. Grey cells are locked for editing.

There are defined three temperatures, T_{min} , T_{t} , and T_{max} . Their values are defined in the *Range* column. If a temperature T falls between T_{min} and T_{t} , the uncertainty takes on the value given in row 4 in the *Uncertainty* column. If a temperature T falls between T_{t} and T_{max} , the uncertainty takes on the value in row 3 in the *Uncertainty* column. If a temperature T is larger than T_{max} , the uncertainty takes on the value of row 2 in the *Uncertainty* column. Units can be given as absolute units matching the units in the <u>ProcessData</u> sheet, alternatively relative (%) units can be used. The confidence intervals can be set using drop-down menus.

	Α	В	С	D	E	F	G	Н	I	J	K
1	Input variable	Range	Uncertainty	Unit	Confidence interval	Distribution					
2	T_max	1600	0.2	့	95 %	Normal					
3	T_i	320	0.2	°C	95 %	Normal					
4	T_min	-50	0.2	°C	95 %	Normal					
5											
4	Info Configuration ProcessData Composition Turbine_unc T_unc P_unc Composition_unc										

Figure 7: Temperature transmitter uncertainty sheet in the met4H2 input-file. Grey cells are locked for editing.

Pressure transmitter uncertainty

The pressure uncertainty is set according to the example given in Figure 8. Grey cells are locked for editing.

There are defined three pressures, P_{min} , P_{t} , and P_{max} . Their values are defined in the *Range* column. If a pressure P falls between P_{min} and P_{t} , the uncertainty takes on the value given in row 4 in the *Uncertainty* column. If a pressure P falls between P_{t} and P_{max} , the uncertainty takes on the value in row 3 in the *Uncertainty* column. If a pressure P is larger than P_{max} , the uncertainty takes on the value of row 2 in the *Uncertainty* column. Units can be given as absolute units matching the units in the <u>ProcessData</u> sheet, alternatively relative (%) units can be used. The confidence intervals can be set using drop-down menus.

	Α	В	С	D	E	F	G	Н	1	J	
1	Input variable	Range	Uncertainty	Unit	Confidence interval	Distribution					
2	P_max	100000000	0.1	bar	95 %	Normal					
3	P_i	50	0.1	bar	95 %	Normal					
4	P_min	1	0.1	bar	95 %	Normal					
5											
4	Info Configuration ProcessData Composition Turbine_unc T_unc P_unc Composition_unc										

Figure 8: Pressure transmitter uncertainty sheet in the met4H2 input-file. Grey cells are locked for editing.

Composition uncertainty

Figure 9 shows how the composition uncertainty is set. Grey cells are locked for editing. The components are the same and appearing in the same order as the components that are given in the <u>composition</u>-sheet. The uncertainty magnitude can be edited. The composition uncertainty is given in absolute units, the units will be the same as the units given in the <u>composition</u>-sheet. The uncertainty distribution is set to normal. The confidence level can be edited.

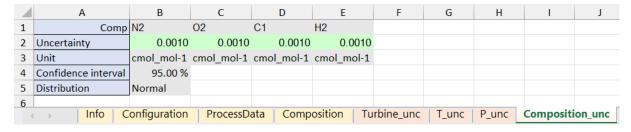


Figure 9: Composition uncertainty sheet in the met4H2 input-file. Grey cells are locked for editing.

Software overview

The code is based on four classes, as shown in Figure 10. Meter and process information as read from the input file are stored on the *meter* and *process* objects. The *met4h2* class produces parameter distributions (parameters: flow rates, temperatures, pressures, gas compositions). The gas property distributions are then fed to *ucalc*, which is a class responsible for computing the uncertainty of any given functional relationship, in this application functional relationships for volume, reference volume and mass flows. Input and output uncertainties are written to an output file. The most important methods in these classes will be described in the following sections.



Figure 10: Python-classes. meter: storing general meter information, transmitter uncertainties, and configuration settings, process: storing process related values, such as flow rates, temperatures, pressures, and gas compositions, met4H2: producing variable distributions and calculating gas properties, ucalc: performing uncertainty calculations and correlation estimates.

Meter

General information and metering <u>configurations</u> are stored on the *meter* object. A few tests are run to check that for example the EoS that is chosen is supported by the chosen framework for gas property calculations.

Transmitter uncertainties (flow, temperature, and pressure) are also stored on the *meter* object, as well as the composition uncertainties. Together with the uncertainties, the confidence level, uncertainty distribution (currently only the normal distribution is supported), and unit are also stored on the object.

All values are converted to SI-units.

Process

Process data, as defined in input sheets <u>ProcessData</u> and <u>Composition</u>.

All values are converted to SI-units.

Met4H2

The met4h2 class has two main functions: (1) producing uncertainty distributions from the input variables and corresponding uncertainty distributions, and (2) computing gas properties.

Uncertainty distributions

Based on the input <u>process variables</u>' values, distributions, confidence intervals and standard deviations, a distribution is drawn using a Latin Hypercube Sampling. Currently, only normal distributions are supported. The distribution can be truncated, for instance, when drawing distributions for gas components, the molar fraction of a component is limited between 0 and 1.

Calorific value tables for the various components and reference temperatures 15, 15.55, 20, and 25 °C, are hardcoded in a dictionary, along with the corresponding uncertainties, in accordance with ISO 6976:2016 [10]. For each component given in the input data, as well as reference temperature, the distributions of calorific values are also drawn using Latin Hypercube sampling.

Compute gas properties

If met4H2 is run in nominal mode, only nominal values will be computed. Data frames with the gas properties can be accessed on the object as a dictionary: self.main_nominal_m4h2_output.

If met4H2 is run in normal mode, both nominal values, as well as a distribution of gas properties will be computed based on the distribution of input parameters produced by the Montecarlo draws. Data frames with the gas distributions can be accessed on the object as a dictionary self.main_m4h2_output.

Gas properties are computed using the specified method and EoS, temperatures, pressures, and gas composition.

Model uncertainty for the compressibility factor is modelled by adding noise to the compressibility distributions, using Latin Hypercube sampling to generate the noise.

The gas property distributions are checked for normality using the Shapiro test, the test-result is printed in the terminal and the distributions are plotted as histograms and saved to file.

Gas properties will be printed to .xlsx files, cf. Outputs.

Uncertainty analysis

The uncertainty analysis is performed using a separate class called *UncertaintyCalculator*, which was written outside this project. Uncertainties are calculated according to Guide to the expression of uncertainty (GUM) [11]. *UncertaintyCalculator* is <u>initialized</u> from <u>Met4H2</u> and produces the combined uncertainties of the target measurands; mass, volume, and/or energy, as well as all information needed to produce complete and traceable uncertainty budgets. These outputs are written to file, cf. <u>Outputs</u>.

Outputs

Five raw output Excel files can be produced. <u>Two of these</u> pertain to the computed gas properties. <u>Three of them</u> pertain to the uncertainties of the target measurands; mass, volume and/or energy.

Finally, the most important output is summarized in a main output file.

Raw gas property output

Gas property files

A file with filename beginning with 'nominal_output_' will always be generated. If the code was run in normal mode, cf. <u>Configuration</u>, a file with filename beginning with 'output_' will also be generated.

Sheets common to both raw gas property output files are:

input: Summarizes the inputs for the computation in separate columns for timestamps,

quantity (volume, mass, or energy), temperature, pressure, and composition.

Units are converted to SI-units.

output: Nominal, and if relevant, average gas properties. Nominal gas properties are

computed directly from input measurements, whereas average gas properties are computed from distributions of properties arising from Latin Hypercube

sampling simulations of the input uncertainty distributions.

Sheets unique to the normal mode file are:

input

uncertainties: Uncertainties of input variables defined in the input-sheet. The uncertainties are

given with units, level of confidence, and distributions.

MCA

uncertainties: MCA uncertainties of the input variables are given as standard deviations of the

Monte Carlo modelled input variable distributions. These will depend on the

number of draws, as well as on whether components are normalized or

or computed by-difference, cf. Configuration. A column for noise is also added.

This noise distribution corresponds to the model uncertainty of the

compressibility Z.

output

uncertainties: Standard deviations of the output distributions of gas properties.

configurations: Input configurations.

Raw uncertainty output

Unique uncertainty output .xlsx files are generated for mass, volume, and energy. Which files are generated depends on which output variables *UncertaintyCalculator* was initialized for. In default mode all three output files are generated. The output files summarize how *uncertaintyCalculator* was initialized, well as the information needed to generate traceable uncertainty budgets.

Sheets in the uncertainty output files are:

settings: Specifies the functional relationship, method of computation (which in this

project is always Latin Hypercube sampling), and whether there are correlations

between the input variables.

inputs: Specifies labels and units of the input variables.

outputs: Specifies labels and units of the output variable and its calculated uncertainty.

values: Shows the calculated measurand at each time stamp.

uncertainties: Shows the calculated absolute standard uncertainty of the measurand at each

time stamp.

rel

uncertainties: Shows the calculated relative standard uncertainty of the measurand at each

time stamp.

input

uncertainties: Shows the absolute values of the uncertainties of the input variables. These are

the standard deviations of the Monte Carlo distributions that were generated in

Met4H2 and then inherited by uncertaintyCalculator.

input

uncertainty

confidences: Shows the confidence of the uncertainties of the input variables.

input

uncertainty

distributions: Shows the distributions of the input variables.

sensitivity

coefficients: Shows the calculated sensitivity coefficients for the input variables.

coverage

interval: Shows the coverage interval of the measurand.

correlation

matrix: Shows the correlation coefficients between the input variables at each time

stamp.

Main output

The main output file summarizes the most important information contained in the raw gas property output file and the raw uncertainty output file. The main output filename is called 'results'.

Sheets in the main output file are:

input: Summarizes the inputs for the computation in separate columns for timestamps,

quantity (volume, mass, or energy), temperature, pressure, and composition.

Units are converted to SI-units.

input

uncertainties: Uncertainties of input variables defined in the input-sheet. The uncertainties are

given with units, level of confidence, and distributions.

gas

properties: Nominal and average gas properties. Nominal gas properties are computed

directly from input measurements, whereas average gas properties are computed from distributions of properties arising from Latin Hypercube

sampling simulations of the input uncertainty distributions.

mass/ volume/

energy: Shows the calculated measurand, the calculated absolute and relative standard

uncertainties of the measurand, and the sensitivity coefficients of and

correlations between the input variables at each time stamp.

Gas Properties

The gas properties which are written to the output files, are produced in the following manner:

Z [-]: output from method/framework

Z0 [-]: output from method/framework at reference conditions

MM [kg/mol]: output from method/framework

DM [mol/kg]: output from method/framework

DM0 [mol/kg]: output from method/framework at reference conditions

D [kg/m³]: DM*MM

D0 [kg/m³]: DM0*MM

Hg [J/mol]: The calorific values are given by ISO 6976:2016 [10] and are hardcoded.

Hv [J/m³]: Hmol/(MM/D0)

Hm [J/kg]: Hmol/MM

References

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