DataApex Clarity™
CHROMATOGRAPHY SOFTWARE

NATURAL GAS ANALYSIS

Clarity Extension ENG

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Contents

To facilitate the orientation in the **Natural Gas Analysis** manual and **Clarity** chromatography station, different fonts are used throughout the manual. Meanings of these fonts are:

Open File (italics) describes the commands and names of fields in **Clarity**, parameters that can be entered into them or a window or dialog name.

WORK1 (capitals) indicates the name of the file and/or directory.

ACTIVE (capital italics) marks the state of the station or its part.

Chromatogram (blue underlined) marks clickable links referring to related chapters.

The bold text is sometimes also used for important parts of the text and the name of the **Clarity** station. Moreover, some sections are written in format other than normal text. These sections are formatted as follows:

Note: Notifies the reader of relevant information.

Caution: Warns the user of possibly dangerous or very important information.

Marks the problem statement or trouble question.

Description: Presents more detailed information on the problem, describes its causes, etc.

Solution: Marks the response to the question, presents a procedure how to remove it.

1 NGA - Natural Gas Analysis

The **NGA Extension** is an optional add-on for the **Clarity Chromatography Software**. It can expand any **Clarity** Instrument as well as **Clarity Offline**.

The **Clarity NGA Extension** is a tool for natural gas and liquefied petroleum gas data processing. It provides an interactive tool for calculations accordingly to supported norms, including options for measurement and reference conditions, ideal or real gas, and more.

2 Specification

The **NGA Extension** is an optional add-on for the **Clarity** software. It can be ordered as a part of a new software license or as an extension to an existing one (p/n A32).

It provides options for the calculation of gas properties in compliance with the following norms:

2.1 Natural Gas

- ISO 6976-16
  Calculation of calorific values, density, relative density, and Wobbe index from composition.
- ISO 6976-95 (outdated; replaced by ISO 6976-16)
  Calculation of calorific values, density, relative density, and Wobbe index from composition.
- ASTM D 3588-98
  The standard practice for calculating heating values, compressibility factor, and relative density of gaseous fuels.
- GPA 2172-09
  Calculation of gross/net heating values, relative density, and compressibility factor for natural gas mixtures from compositional analysis.

2.2 Liquefied Petroleum Gas

- ASTM D 2421-02
  The standard practice for interconversion of analysis of C_5 and lighter hydrocarbons to gas-volume, liquid-volume, or weight basis.
- ASTM D 2598-02
  The standard practice for calculation of certain physical properties of liquefied petroleum (LP) gases from compositional analysis.
- ISO 8973-97 / EN 589+A1
  Standards for calculation methods for density and vapor pressure in liquefied petroleum gases.

2.3 Calculated properties according to norms

The particular calculation details and equations used can be found in the chapter **"Appendix - Mathematical Formulas"** on pg. **22**.

ISO 6976-16

- Compression Factor
- Mean Molecular Weight
- Relative Density
- Density
- Gross Calorific Value
- Net Calorific Value
- Gross Wobbe Index
- Net Wobbe Index

ISO 6976-95 (outdated)

- Compression Factor
- Mean Molecular Weight
- Relative Density
- Density
- Superior Calorific Value
- Inferior Calorific Value
- Wobbe Index

ASTM D 3588-98 and GPA 2172-09

- Molar Mass
- Molar Mass Ratio
- Compressibility Factor
- Relative Density
- Ideal Heating Value (incl.calculations in BTU - British Thermal Units)
- Real Heating Value (incl.calculations in BTU - British Thermal Units)

ASTM D 2421-02 and ASTM D 2598-02

- Vapor Pressure
- Relative Density
- Motor Octane Number

ISO 8973-97 / EN 589+A1

- Absolute Vapor Pressure (for Molar and Mass Percent only)
- Gauge Vapor Pressure (for Molar and Mass Percent only)
- Octane Number

Additional calculations

- Methane Number is calculated if the LPG norms are selected (ASTM D 2421-02 and ASTM D 2598-02 or ISO 8973-97 / EN 589+A1). The calculation is based on the calculated (Motor) Octane Number according to KUBESH, John; KING, Steven R.; LISS, William E. *Effect of gas composition on octane number of natural gas fuels*. SAE Technical Paper, 1992

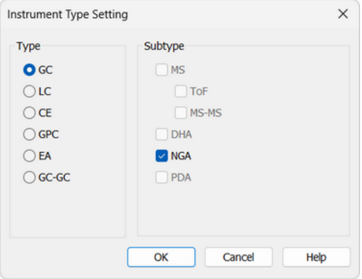
3 Installation

The NGA Extension is activated by entering an appropriate user code during the installation of **Clarity** or later using the *Help - User Code…* command from the *Clarity* main window.

To enable the NGA Extension on an *Instrument*, you have to set the corresponding instrument type. To set the instrument type, click the … button in the *System Configuration* dialog.

In the invoked *Instrument Type Setting* dialog, select the GC-NGA option.

Caution: The NGA Extension is available only on the **GC** instrument type.



Type
● GC
○ LC
○ CE
○ GPC
○ EA
○ GC-GC

Subtype
☐ MS
☐ ToF
☐ MS-MS
☐ DHA
☑ NGA
☐ PDA

Fig. 1: Enabling the NGA Extension on an Instrument

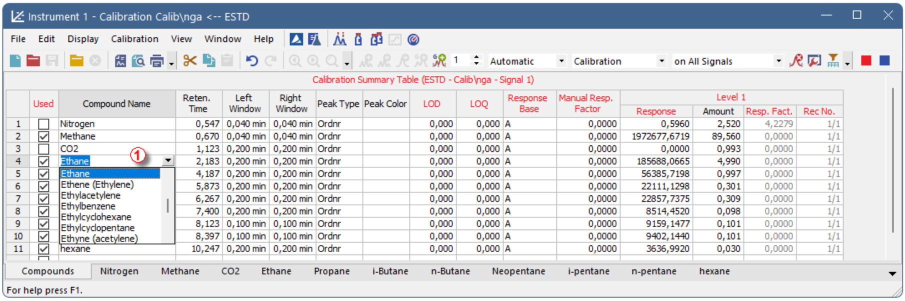
4 NGA Extension Description

This chapter lists and describes the features changed in or added into **Clarity** by the **NGA Extension**.

4.1 Calibration

For the accurate detection of compounds required for gas properties calculations, it is necessary to calibrate the peaks.

- Create a new calibration or open the NGA.CAL calibration from the DEMO_NGA project for demonstration.
- When adding new compounds to the calibration table, use the predefined compound names from the drop-down menu (① in the **Fig. 2** on pg. **5**.) which contains all compound names available in the supported norms. For more details see the chapter **Specification** on pg. **2**. If you use different compound names, they will not be recognized in the NGA calculations, but they can be later linked to the names in norms using the Link Table.
- The NGA Extension often uses multi-signal calibrations. This means that the peaks can be identified on different signals. The calibration table including *Compound Names*, *Response Times*, and *Amounts* is common for all signals. It is important that each compound is identified on one signal only to prevent warnings in the Result Calculations. Check the checkboxes in the *Used* column of the calibration table to use the *Compound Name* in the defined signal only. You can change the signal in the *Calibration - Set Signal* menu.



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Level 1			
												Response	Amount	Resp. Fact.	Rec No.
1	☐	Nitrogen	0,547	0,040 min	0,040 min	Ordnr		0,000	0,000	A	0,0000	0,5960	2,520	4,2279	1/1
2	☑	Methane	0,670	0,040 min	0,040 min	Ordnr		0,000	0,000	A	0,0000	1972677,6719	89,560	0,0000	1/1
3	☐	CO2	1,123	0,200 min	0,200 min	Ordnr		0,000	0,000	A	0,0000	0,0000	0,993	0,0000	1/1
4	☑	Ethane	2,183	0,200 min	0,200 min	Ordnr		0,000	0,000	A	0,0000	185688,0665	4,990	0,0000	1/1
5	☑		4,187	0,200 min	0,200 min	Ordnr		0,000	0,000	A	0,0000	56385,7198	0,997	0,0000	1/1
6	☑		5,873	0,200 min	0,200 min	Ordnr		0,000	0,000	A	0,0000	22111,1298	0,301	0,0000	1/1
7	☑		6,267	0,200 min	0,200 min	Ordnr		0,000	0,000	A	0,0000	22857,7375	0,309	0,0000	1/1
8	☑		7,400	0,200 min	0,200 min	Ordnr		0,000	0,000	A	0,0000	8514,4520	0,098	0,0000	1/1
9	☑		8,123	0,100 min	0,100 min	Ordnr		0,000	0,000	A	0,0000	9159,1477	0,101	0,0000	1/1
10	☑		8,397	0,100 min	0,100 min	Ordnr		0,000	0,000	A	0,0000	9402,1440	0,101	0,0000	1/1
11	☑	hexane	10,247	0,200 min	0,200 min	Ordnr		0,000	0,000	A	0,0000	3636,9920	0,030	0,0000	1/1

Fig. 2: Calibration window with a Compound Name drop-down menu

For detailed information about the Calibration, see the chapter "Calibration".

4.2 Chromatogram window

A new NGA and NGA Summary tabs are available in the *Chromatogram* window (opened by clicking the icon). Furthermore, there is a new *NGA* menu at the top of the window.

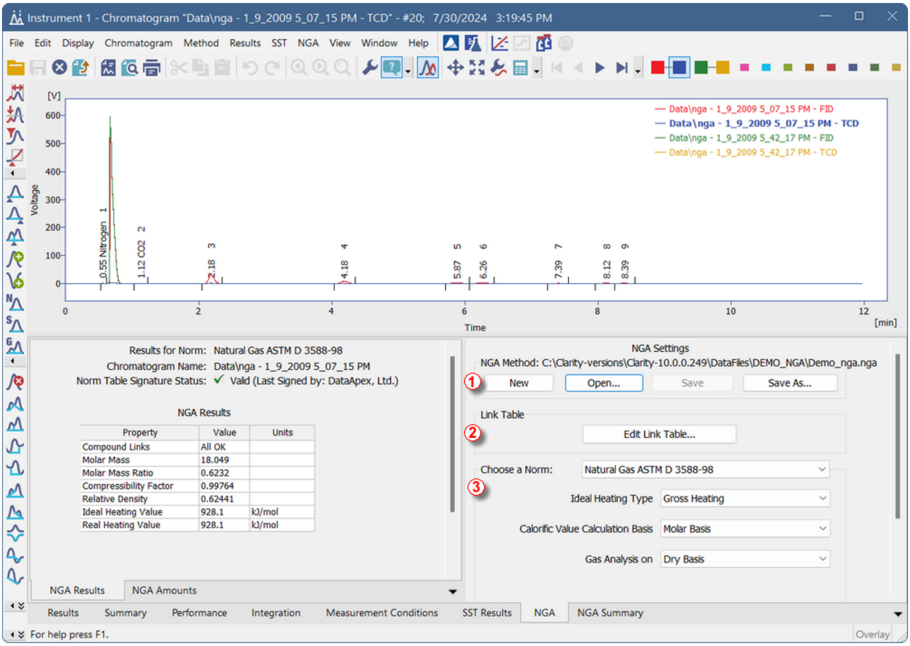
4.2.1 NGA tab

The *NGA* tab is divided into two panes:

- Left pane: includes the NGA Results and NGA Amounts subtabs.
- Right Pane: includes the NGA Settings.

4.2.1.1 NGA Settings

In this pane, you can set up the *NGA Method* - choose a norm and edit its parameters.



Results for Norm: Natural Gas ASTM D 3588-98
Chromatogram Name: Data\nga - 1_9_2009 5_07_15 PM
Norm Table Signature Status: ✓ Valid (Last Signed by: DataApex, Ltd.)

NGA Results

Property	Value	Units
Compound Links	All OK	
Molar Mass	18.049	
Molar Mass Ratio	0.6232	
Compressibility Factor	0.99764	
Relative Density	0.62441	
Ideal Heating Value	928.1	kJ/mol
Real Heating Value	928.1	kJ/mol

NGA Settings
NGA Method: C:\Clarity-versions\Clarity-10.0.0.249\DataFiles\DEMO_NGA\Demo_nga.nga
Choose a Norm: Natural Gas ASTM D 3588-98
Ideal Heating Type: Gross Heating
Calorific Value Calculation Basis: Molar Basis
Gas Analysis on: Dry Basis

Fig. 3: Chromatogram window - NGA Results - NGA Settings

NGA Method ①

Displays the currently opened *NGA Method*. All settings in the *NGA Method* are saved in a *.NGA file, which is independent on the method opened from the *Instrument* window.

New

Creates a new *NGA Method* with default settings.

Open

Displays the *Open NGA Method* dialog where you can select NGA method you want to use.

Save

Saves the settings of the current *NGA Method*.

Save As…

Opens the *Save NGA Method As* dialog for saving the *NGA Method* into a new file.

Link Table ②

The *Compound Names* for the NGA Results are retrieved from the *Calibration Summary Table*. In calibrations, it is possible to use multi-signal chromatograms. However, it is necessary to set the detection of each compound to one signal only, otherwise you will see warnings in the NGA Results pane (this can be specified by the *Used* checkbox; the selected signal can be switched using *Calibration - Set Signal*).

Compounds with the same names in calibrations as in the norms are automatically included in NGA calculations. If the compound names in norms differ from the names set in the calibration, you can use the *Link Table* for linking those compound names to ensure that all compounds are included in the calculations. For more details see the chapter **Link Table** on pg. **10**.

Edit Link Table…

Opens the Link Table dialog, where you can create and edit links between compound names in calibrations and norms.

Choose a Norm ③

Select the norm you want to use for your calculations. Each norm has a specific list of parameters that can be changed:

- **ISO 6976-16**

Source Amount

Determines that the *Amount* is in mole fractions (only option supported by ISO 6976-16).

Calorific Value Calculation Basis

Determines the units in which to calculate the *Gross* and *Net Calorific Values*.

Combustion Temperature

Selects the combustion temperature.

Metering Temperature

Selects the metering temperature.

Ideal / Real Gas

Determines whether the calculations are for *Ideal* or *Real Gas*. For the *Real Gas*, the *Compression Factor* is added to the results.

Gas Analysis on

Only calculations on dry gas basis are supported by ISO 6976-16 (effects introduced by water are considered in calculations only if the water content is determined in the chromatogram).

Metering Pressure [kPa]

Specifies the metering pressure (the valid range is between 90 and 110 kPa).

- **ISO 6976-95**

Source Amount

Determines whether the *Amount* is in mole fractions or in volume fractions. *Volume* fractions are converted to mole fractions if selected.

Calorific Value Calculation Basis

Determines the units in which to calculate the *Superior* and *Inferior Calorific Values*.

Temperatures

Selects the combustion and metering temperatures.

Ideal / Real Gas

Determines whether the calculations are for *Ideal* or *Real Gas*. For the *Real Gas*, the *Compression Factor* is added to the results.

Gas Analysis on

Determines whether to include a mole fraction of water or not. If water is included in calculations, it is also added to the NGA Amounts.

- **ASTM D 3588-98** and **GPA 2172-09**

Ideal Heating Type

Determines whether to calculate *Gross Heating Value* or *Net Heating Value*. For gross calculations, the water condenses to liquid, and, for net calculations, the water remains in the vapor state.

Calorific Value Calculation Basis

Determines the units in which to calculate the *Heating Value*.

Gas Analysis on

Determines whether to include a mole fraction of water or not. If water is included in calculations, it is also added to the NGA Amounts (but not for **GPA 2172-09**).

- **LPG ASTM D 2598-02 / 2421-02**

Original Basis

Determines the source *Amount* type. It can be *Liquid, Mole*, *Gas*, or *Weight* type. Other types are converted to *Liquid* type.

- **LPG ISO 8973-97 / EN 589+A1**

Original Basis

Determines the source *Amount* type. Both *Molar* and *Mass* fractions are required for calculations (one is converted into another). If *Volume* fractions are selected, only the *Octane Number* can be calculated.

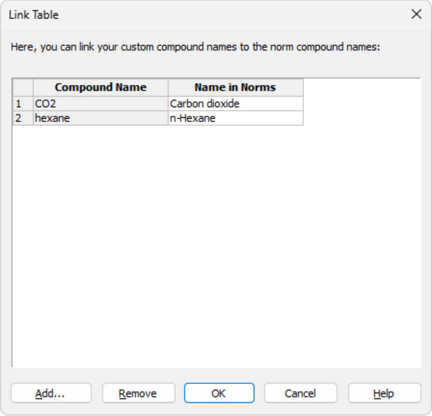
Temperature of Liquid

The approximate temperature of liquid.

4.2.1.2 Link Table

This dialog can be used to edit the *Link Table* in the NGA Extension. The *Link Table* is used when you have unresolved compound names in the NGA Amounts. For example, you are using compound names specific to your language, but there is a different name for the same compound in the selected norm. The *Link Table* allows you to link the different compound names so you can use your custom compound names in calibrations and chromatograms as needed.

After you add some link to the *Link Table*, you can also add them to the calibration using the drop-down menu in the ***Calibration*** window.



Link Table

Here, you can link your custom compound names to the norm compound names:

	Compound Name	Name in Norms
1	CO2	Carbon dioxide
2	hexane	n-Hexane

Fig. 4: Link Table dialog

1st column in the table

Number of the *Link Table* row.

Compound Name

The compound name in the ***Calibration*** that is linked to the one in norm, and thus to be included in the NGA Results.

Name in Norms

The compound name as given by the norms (if the name is in multiple norms, only one occurrence is displayed).

Add…

Displays the Add Link dialog for adding a new record to the *Link Table*.

Remove

Removes the selected record from the *Link Table*.

OK

Saves settings to the *Link Table* and exits the dialog.

Cancel

Exits the dialog without saving any changes to the *Link Table*.

4.2.1.3 Add Link

The *Add Link* dialog serves for adding new record to the Link Table.

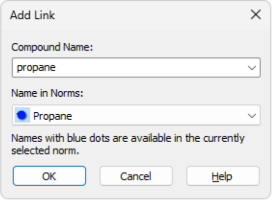


Fig. 5: Add Link dialog

Compound Name

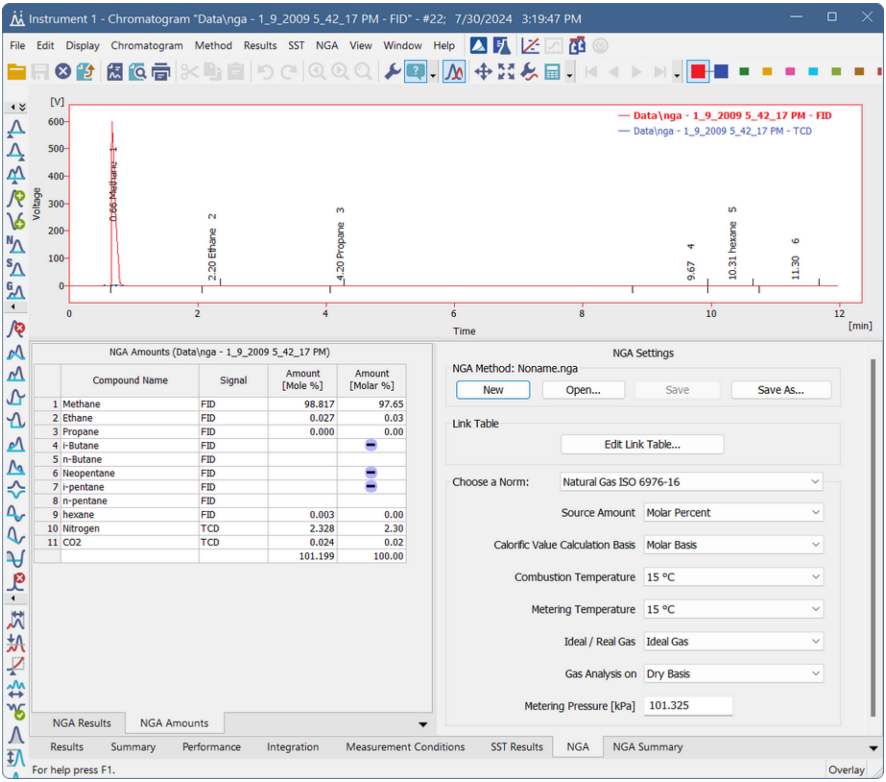
Enter the compound name you want to link to a name in norms. Unresolved compounds in the chromatogram are suggested in the drop-down menu.

Name in Norms

Select the appropriate compound name in norms. Names from all supported norms are available in the drop-down menu. For better orientation, blue dots are displayed on the compounds applicable to the norm selected in the NGA Settings.

4.2.1.4 NGA Amounts

The *NGA Amounts* table contains some of the columns from the standard ***Result Table***, but it also contains additional columns specific for the NGA Extension.



NGA Amounts (Data\nga - 1_9_2009 5_42_17 PM)

	Compound Name	Signal	Amount [Mole %]	Amount [Molar %]
1	Methane	FID	98.817	97.65
2	Ethane	FID	0.027	0.03
3	Propane	FID	0.000	0.00
4	i-Butane	FID		⊖
5	n-Butane	FID		
6	Neopentane	FID		⊖
7	i-pentane	FID		⊖
8	n-pentane	FID		
9	hexane	FID	0.003	0.00
10	Nitrogen	TCD	2.328	2.30
11	CO2	TCD	0.024	0.02
			101.199	100.00

NGA Settings

NGA Method: Noname.nga

Link Table

Choose a Norm: Natural Gas ISO 6976-16
Source Amount: Molar Percent
Calorific Value Calculation Basis: Molar Basis
Combustion Temperature: 15 °C
Metering Temperature: 15 °C
Ideal / Real Gas: Ideal Gas
Gas Analysis on: Dry Basis
Metering Pressure [kPa]: 101.325

Fig. 6: Chromatogram window - NGA Results

Compound Name

If the chromatogram contains calibrated peaks or groups, the names are shown in the *Compound Name* column. The table contains compounds from all signals of the chromatogram.

Signal

Displays the *Signal* on which the compound was detected.

Amount [Mole %]

This column shows the same data as the *Amount* column in the ***Result Table*** (*Results* tab in the ***Chromatogram*** window). This columns is only informational and it is not used in the NGA calculations.

Amount [Molar %]

Contains mole fractions (in percent) or some other fraction type as specified in the *NGA Settings*. The fractions are to the total amount of 100%. If a compound is not found in the norms, its mole fraction is set to *zero* for NGA calculations.

Amounts of compounds with the same names in calibrations and in norms are automatically linked. A compound with a compound name different from the name in norms can be included in the calculations by linking it to a compound in norms using the "Link Table" on page 10,

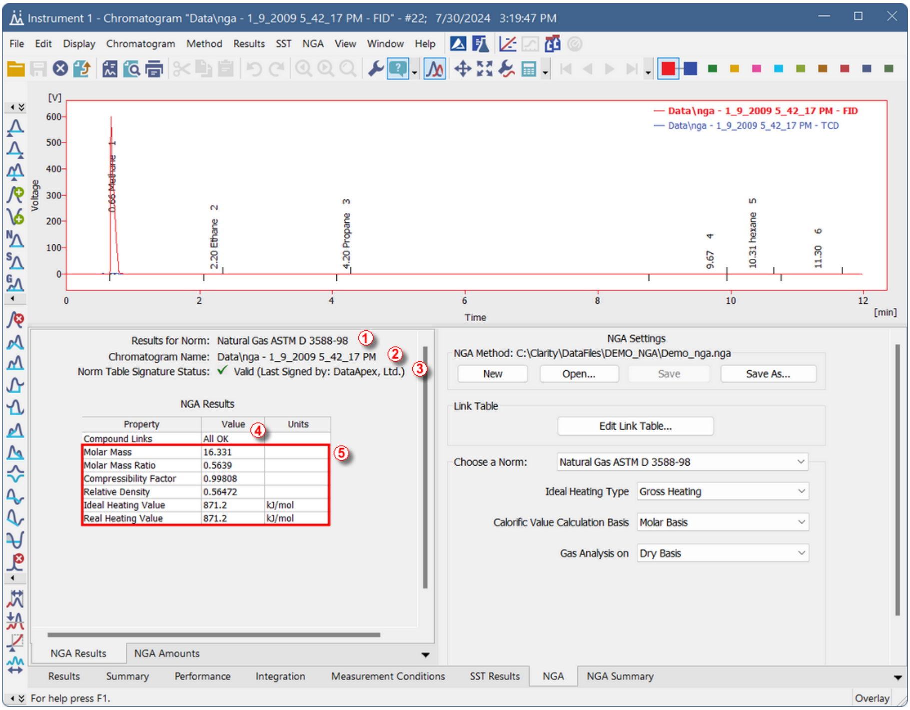
The table can contain a virtual compound *Water*. This one is added when you select *Wet Basis* in the NGA Settings.

⊖ The "minus" icon means, that the *Compound Name* from the *NGA Results* was not found in the selected norm and it will not be considered in the calculations.

? The "question mark" icon means, that the *Compound Name* cannot be found neither in the norms nor in the *Link Table*. Click the *Edit Link Table…* button, and link the compound name with requested name in norms in the Link Table dialog. This icon may appear in such situations, when the *Compound Name* is present two or more times in the *NGA Results*. This is caused mostly when you have compound detected and calibrated in more then one signal in the *Calibration* window. Since the NGA calculations are performed on all signals in the *Chromatogram*, each compound should be calibrated in one signal only (see the chapter **"Calibration"** on pg. **5**.

4.2.1.5 NGA Results

In the *NGA Results* tab, you can find the table containing results of calculations for the selected norm. Results are automatically recalculated each time you open or change the chromatogram or select different norm (or its parameters).



Instrument 1 - Chromatogram "Data\nga - 1_9_2009 5_42_17 PM - FID" - #22; 7/30/2024 3:19:47 PM

Results for Norm: Natural Gas ASTM D 3588-98 ①
Chromatogram Name: Data\nga - 1_9_2009 5_42_17 PM ②
Norm Table Signature Status: ✓ Valid (Last Signed by: DataApex, Ltd.) ③

NGA Results

Property	Value ④	Units
Compound Links	All OK	
Molar Mass	16.331	
Molar Mass Ratio	0.5639	
Compressibility Factor	0.99808	
Relative Density	0.56472	
Ideal Heating Value	871.2	kJ/mol
Real Heating Value	871.2	kJ/mol

⑤

NGA Settings
NGA Method: C:\Clarity\DataFiles\DEMO_NGA\Demo_nga.nga
Choose a Norm: Natural Gas ASTM D 3588-98
Ideal Heating Type: Gross Heating
Calorific Value Calculation Basis: Molar Basis
Gas Analysis on: Dry Basis

Fig. 7: Chromatogram window - NGA Results

Results for Norm ①

Displays the name of the norm according to which the calculations are performed.

Chromatogram Name ②

Displays the name of the chromatogram for which the results are present (this is helpful especially if you have multiple chromatograms opened in the *OVERLAY MODE*).

Norm Table Signature Status ③

Information about the validity of the *Norms Table* file, where the data required for the calculations are saved. This file is provided by **DataApex** and is digitally signed. If any changes are done to the file, the signature will be no longer valid.

Note: For any update request in the *Norm Table* (e.g., adding support for a new norm), contact the DataApex Support at www.dataapex.com.

NGA Results

Compound Links ④

Information about the compounds present in the *Result Table*(for more details see the chapter **NGA Amounts** on pg. **12**). The field may contain:

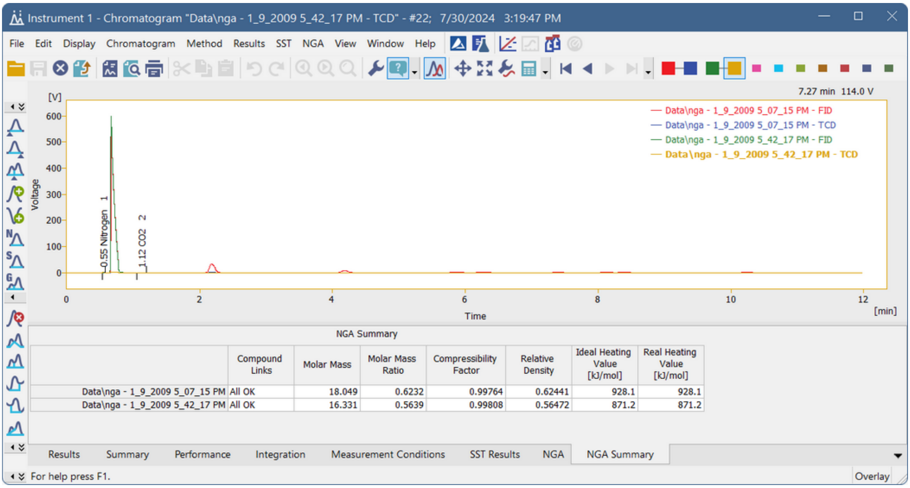
- *All OK*: There are no errors and warnings in the *NGA Results*.
- *X Errors*: The *X* is number of the unresolved *Compound Names* in the *NGA Results*.
- *X Warnings*: The *X* is number of the compounds not found in *Norms Table* nor in the *Link Table*. This warning may occur if you have set the detection of the same compound in more then one signal. For more details, see also the chapter Calibration.

The other rows in the table are respective to the selected norm ⑤

What parameters are calculated in each norm you can find in the chapter **"Specification"** on pg. **3**.

4.2.2 NGA Summary

Displays the NGA results for all chromatograms opened in the *OVERLAY MODE* (for more details see the chapter **NGA Results** on pg. **14**).



NGA Summary

	Compound Links	Molar Mass	Molar Mass Ratio	Compressibility Factor	Relative Density	Ideal Heating Value [kJ/mol]	Real Heating Value [kJ/mol]
Data\nga - 1_9_2009 5_07_15 PM	All OK	18.049	0.6232	0.99764	0.62441	928.1	928.1
Data\nga - 1_9_2009 5_42_17 PM	All OK	16.331	0.5639	0.99808	0.56472	871.2	871.2

For help press F1.

Fig. 8: Chromatogram window - NGA Summary

NGA Summary Table

In this table, you can find the NGA results transformed into rows per chromatogram.

1st column

Name of the chromatogram

Other columns

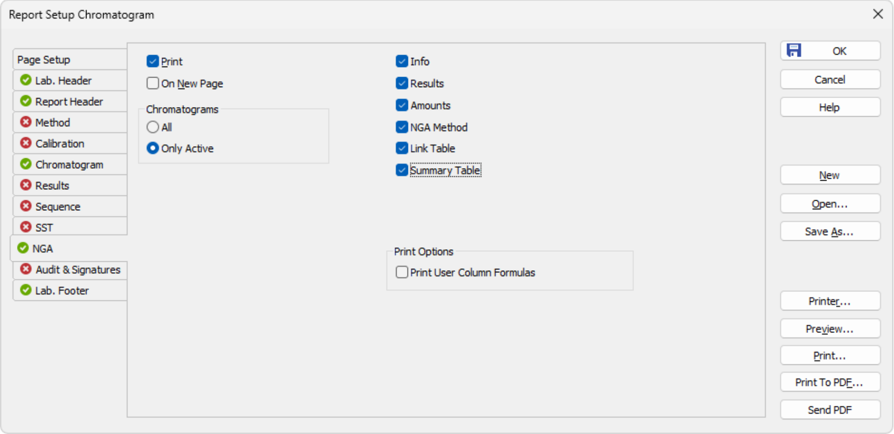
List of columns is identical to NGA Results, but the results are present for all chromatograms opened in the *OVERLAY MODE*. You can find detailed description of the calculated properties in the chapter **"Specification"** on pg. **3**.

User Columns

You can create *User Columns* by clicking the right button of the mouse and selecting the *User Columns - Add...* option. For more details, see also chapter Setup Columns… in the **Clarity Reference Guide**.

4.3 Report Setup

In the *Report Setup* dialog, tab *NGA*, you can set the printing options for the data in the **NGA Extension**.



Report Setup Chromatogram

☑ Print

☐ On New Page

Chromatograms

○ All

● Only Active

☑ Info

☑ Results

☑ Amounts

☑ NGA Method

☑ Link Table

☑ Summary Table

Print Options

☐ Print User Column Formulas

Fig. 9: Report Setup dialog

Print

Enable/disable the printing of the NGA details. If checked, the symbol ✓ will be shown before the tab name, and other fields on the tab will be enabled.

On New Page

If checked, the **NGA Section** is printed on a new page.

Chromatograms section

All

Prints the *NGA Amounts* and *NGA Results* of all chromatograms opened in the *OVERLAY MODE*.

Only Active

Prints the *NGA Amounts* and *NGA Results* of the *ACTIVE Chromatogram* only.

Info

If checked, prints the *NGA Info* including the *Norm Name* and the *Norm Table Signature Status*.

Results

If checked, prints the NGA Results.

Amounts

If checked, prints the NGA Amounts.

NGA Method

If checked, prints the NGA Method Settings.

Link Table

If checked, prints the Link Table.

Summary Table

If checked, prints the NGA Summary.

Print Options

Defines additional options of the printed report.

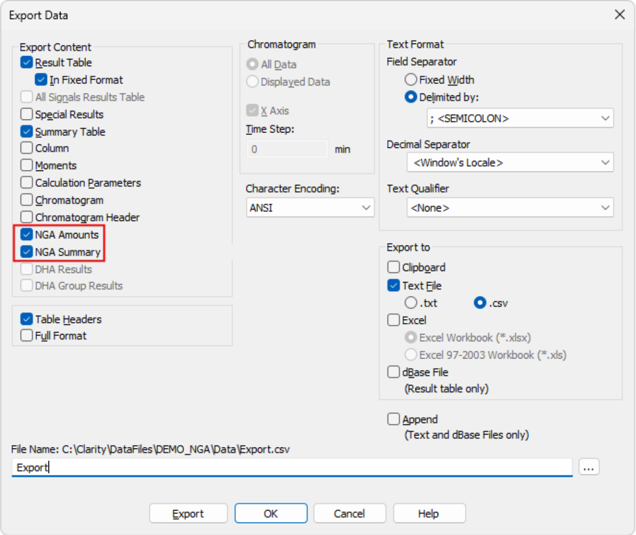
Print User Column Formulas

Adds calculation formulas used in the User Columns including *User Variables* at the end of the appropriate table to be printed.

Note: In the GLP mode, formulas are printed automatically, even if the checkbox is unchecked.

4.4 Export Data

In the *Export Data* dialog, you can set whether the *NGA Results* and *NGA Summary* will be included in the exported data. For more details, see also chapter Export Data in the **Clarity Reference Guide**.



Export Data

Export Content
☑ Result Table
☑ In Fixed Format
☐ All Signals Results Table
☐ Special Results
☑ Summary Table
☐ Column
☐ Moments
☐ Calculation Parameters
☐ Chromatogram
☐ Chromatogram Header
☑ NGA Amounts
☑ NGA Summary
☐ DHA Results
☐ DHA Group Results

☑ Table Headers
☐ Full Format

Chromatogram
● All Data
○ Displayed Data
☑ X Axis
Time Step: 0 min

Character Encoding: ANSI

Text Format
Field Separator
○ Fixed Width
● Delimited by: ; <SEMICOLON>
Decimal Separator: <Window's Locale>
Text Qualifier: <None>

Export to
☐ Clipboard
☑ Text File
○ .txt ● .csv
☐ Excel
● Excel Workbook (*.xlsx)
○ Excel 97-2003 Workbook (*.xls)
☐ dBase File
(Result table only)

☐ Append
(Text and dBase Files only)

File Name: C:\Clarity\DataFiles\DEMO_NGA\Data\Export.csv
Export

Fig. 10: Export Data dialog

5 How to try the NGA Extension

5.1 How to perform first calculations

In this chapter, you can find instructions on how to try the NGA Extension using the NGA demo project for the first time.

Step 1

In the *System Configuration* window (menu *Clarity - Configuration…*), select the *NGA* option in the *Instrument Type Setting* dialog, for example on *Instrument 1*.

For more details see the chapter **Installation** on pg. **4**.

Step 2

After closing the *System Configuration* window, open the appropriate *Instrument*. Now, open the NGA demo project: in the *Login Dialog*, select **DEMO_NGA** in the *Select Project* drop-down list, and click the *OK* button.

Step 3

Open the *Chromatogram* window. In the lower part of the *Chromatogram* window, you can see the new *NGA* and *NGA Summary* tabs. Open any chromatogram from the **DEMO_NGA** project using the *File - Open Chromatogram…* menu.

Step 4

Click the *NGA* tab, and on the right side of the pane, you can see the *NGA Settings*. There you can choose a norm and set the calculations parameters. The settings are saved in a special .NGA file, which can be used for multiple chromatograms.

Click the *Open…* button to browse the **Clarity Installation** directory (by default C:\CLARITY\DATAFILES). In the DEMO_NGA subdirectory, select the DEMO_NGA.NGA file. *NGA Method* will be loaded, and the active chromatogram results will be automatically recalculated according to the set norm and parameters.

For more details see the chapter **NGA Settings** on pg. **6**.

Step 5

In the *NGA Results* subtab of the *NGA* tab, you can see the results for the active chromatogram. The results depend on the norm selected in the *NGA Settings*, and whether all calibrated compounds are found in the norm. You can find detailed description of the norms supported by this Extension in the chapter **"Specification"** on pg. **2**.

More details can be found in the chapter **"NGA Results"** on pg. **14**. and in the chapter **"NGA tab"** on pg. **6**.

Step 6

Calculation data for all compounds covered by the norms are saved in the *Norm Table*. In case the calibration and chromatogram use different names for the same compounds as in the norm (for example compound names in your language), you can link them together to add them to the calculations: In the *NGA Settings* click the *Edit Link Table…* button to open the *Link Table* dialog. Here you can link the calibrated compound name with the compound name in the norm. The *Link Table* is used for all chromatograms, so you need to set it only once.

For more details see the chapter **Link Table** on pg. **10**.

Step 7

In case you need to process several chromatograms to conclude the analysis, open them in the *OVERLAY* mode and go to the *NGA Summary* tab, where you can see the NGA calculations results for all the opened chromatograms in one table.

For more details see the chapter **NGA Summary** on pg. **16**.

5.2 How to print and export results from the NGA Extension

Ensure that you have selected the *NGA Instrument Type* in the *System Configuration* window as described in the chapter **"How to try the NGA Extension"** on pg. **20**.

Print

To print the data from the NGA Extension, open the *Report Setup* window by clicking the menu *File* - *Report Setup…* in the *Chromatogram* window.

On the left side, select the *NGA* tab. By checking the *Print* checkbox, other controls on that pane are enabled. You can configure what information will be printed by choosing the corresponding options.

Settings from the *Report Setup* are used in the print output and preview, accessible from the *File* menu of the *Chromatogram* window.

You can also use the prepared NGA report styles: in the *Report Setup*, click *Open…*, and select the NGA_RESULT.STY or NGA_SUMMARY.STY report style.

For more details see the chapter **Report Setup** on pg. **17**.

Export

Open the *Export Data* dialog via the *Setting* - *Export Data…* menu of the *Instrument* window. Check the *NGA Amounts* and *NGA Summary* checkboxes to include them in the exports.

For more details see the chapter **Export Data** on pg. **19**.

6 Appendix - Mathematical Formulas

6.1 ISO 6976-16

6.1.1 Compression Factor

$$Z(t_2, p_2) = 1 - \frac{p_2}{p_0} \cdot \left[\sum_{j=1}^{N} x_j \cdot s(t_2, p_0) \right]^2$$

where the summation is taken over all *N* components of the mixture and:

$Z(t_2,p_2)$ is the compression factor at metering temperature t_2 and metering pressure p_2

p_0 is the atmospheric pressure (101.325 kPa)

p_2 is the metering pressure

x_j is the mole fraction of component *j*

$s(t_2,p_0)$ is the summation factor for component *j* at metering temperature t_2 and atmospheric pressure p_0

6.1.2 Mean Molecular Weight

$$M = \sum_{j=1}^{N} x_j \cdot M_j$$

where the summation is taken over all *N* components of the mixture and:

M is the mean molecular weight

x_j is the mole fraction of component *j*

M_j is the molar mass of component *j*

6.1.3 Gross Calorific Value

- Molar basis (real gas property is calculated as ideal)

$$(Hc)_G^0(t_1) = \sum_{j=1}^{N} x_j \cdot [(Hc)_G^0]_j(t_1)$$

where the summation is taken over all *N* components of the mixture and:

$(Hc)^0{}_G(t_1)$ is the ideal molar gross calorific value of the mixture at combustion temperature t_1

$[(Hc)^0{}_G]_j(t_1)$ is the ideal molar gross calorific value of the component *j* at combustion temperature t_1

x_j is the mole fraction of component *j*

- Mass basis (real gas property is calculated as ideal)

$$(Hm)_G^0(t_1) = \frac{(Hc)_G^0(t_1)}{M}$$

where:

$(Hm)^0{}_G(t_1)$ is the ideal mass gross calorific value of the mixture at combustion temperature t_1

$(Hc)^0{}_G(t_1)$ is the ideal molar gross calorific value of the mixture at combustion temperature t_1

M is the mean molecular weight

- Volumetric basis - ideal gas

$$(Hv)_G^0(t_1;t_2,p_2) = (Hc)_G^0(t_1) \cdot \frac{p_2}{R \cdot T_2}$$

where:

$(Hv)^0{}_G(t_1;t_2,p_2)$ is the ideal volumetric gross calorific value of the mixture at combustion temperature t_1

$(Hc)^0{}_G(t_1)$ is the ideal molar gross calorific value of the mixture at combustion temperature t_1

p_2 is the metering pressure

R is the molar gas constant

T_2 is the absolute metering temperature in kelvins

- Volumetric basis - real gas

$$(Hv)_G(t_1;t_2,p_2) = \frac{(Hv)_G^0(t_1;t_2,p_2)}{Z(t_2,p_2)}$$

where:

$(Hv)_G(t_1;t_2,p_2)$ is the real volumetric gross calorific value of the mixture at combustion temperature t_1

6.1.4 Net Calorific Value

- Molar basis (real gas property is calculated as ideal)

$$(Hc)_N^0(t_1) = (Hc)_G^0(t_1) - \sum_{j=1}^{N} x_j \cdot \frac{b_j}{2} \cdot L^0(t_1)$$

where the summation is taken over all N components of the mixture and:

$(Hc)^0{}_N(t_1)$ is the ideal molar net calorific value of the mixture at combustion temperature t_1

$(Hc)^0_G(t_1)$ is the ideal molar gross calorific value of the mixture at combustion temperature t_1

x_j is the mole fraction of component j

b_j is the hydrogen index of component j

$L^0(t_1)$ is the standard enthalpy of vaporization of water at combustion temperature t_1

- Mass basis (real gas property is calculated as ideal)

$$(Hm)^0_N(t_1) = \frac{(Hc)^0_N(t_1)}{M}$$

where:

$(Hm)^0_N(t_1)$ is the ideal mass net calorific value of the mixture at combustion temperature t_1

$(Hc)^0_N(t_1)$ is the ideal molar net calorific value of the mixture at combustion temperature t_1

M is the mean molecular weight

- Volumetric basis - ideal gas

$$(Hv)^0_N(t_1;t_2,p_2) = (Hc)^0_N(t_1) \cdot \frac{p_2}{R \cdot T_2}$$

where:

$(Hv)^0_N(t_1;t_2,p_2)$ is the ideal volumetric net calorific value of the mixture at combustion temperature t_1

$(Hc)^0_N(t_1)$ is the ideal molar net calorific value of the mixture at combustion temperature t_1

p_2 is the metering pressure

R is the molar gas constant

T_2 is the absolute metering temperature in kelvins

- Volumetric basis - real gas

$$(Hv)_N(t_1;t_2,p_2) = \frac{(Hv)^0_N(t_1;t_2,p_2)}{Z(t_2,p_2)}$$

where:

$(Hv)_N(t_1;t_2,p_2)$ is the real volumetric net calorific value of the mixture at combustion temperature t_1

6.1.5 Relative Density

- Ideal gas

$$G^0 = \frac{M}{M_{air}}$$

where:

G^0 is the relative density of the ideal gas

M is the mean molecular weight

M_{air} is the molar mass of dry air of standard composition (28.96546 kg·kmol^{-1})

- Real gas

$$G(t_2, p_2) = \frac{G^0 \cdot Z_{air}(t_2, p_2)}{Z(t_2, p_2)}$$

where:

$G(t_2, p_2)$ is the relative density of the real gas at t_2 and p_2

$Z(t_2, p_2)$ is the compression factor of the gas mixture at t_2 and p_2

$Z_{air}(t_2, p_2)$ is the compression factor of dry air of standard composition at t_2 and p_2 calculated as:

$$Z_{air}(t_2, p_2) = 1 - \frac{p_2}{p_0} \cdot \left[1 - Z_{air}(t_2, p_0)\right]$$

where $Z_{air}(t_2, p_0)$ is the compression factor of the dry air of standard composition at t_2 and p_0

6.1.6 Density

- Ideal gas

$$D^0(t_2, p_2) = \frac{M \cdot p_2}{R \cdot T_2}$$

where:

$D^0(t_2, p_2)$ is the density of the ideal gas at t_2 and p_2

M is the mean molecular weight

R is the molar gas constant

T_2 is the absolute metering temperature in kelvins

- Real gas

$$D(t_2, p_2) = \frac{D^0(t_2, p_2)}{Z(t_2, p_2)}$$

where:

$D(t_2, p_2)$ is the density of the real gas at t_2 and p_2

$Z(t_2,p_2)$ is the compressibility factor of the gas mixture at t_2 and p_2

6.1.7 Wobbe Index (Gross and Net)

- Ideal gas

$$W^0_{G/N}(t_1;t_2,p_2) = \frac{(Hv)^0_{G/N}(t_1;t_2,p_2)}{\sqrt{G^0}}$$

where:

$W^0_{G/N}(t_1;t_2,p_2)$ is the gross or net Wobbe index of the ideal gas at combustion temperature t_1

$(Hv)^0_{G/N}(t_1;t_2,p_2)$ is the ideal volumetric gross or net calorific value of the mixture at combustion temperature t_1

G^0 is the relative density of the ideal gas

- Real gas

$$W_{G/N}(t_1;t_2,p_2) = \frac{(Hv)_{G/N}(t_1;t_2,p_2)}{\sqrt{G}}$$

where:

$W_{G/N}(t_1;t_2,p_2)$ is the gross or net Wobbe index of the real gas at combustion temperature t_1

$(Hv)_{G/N}(t_1;t_2,p_2)$ is the real volumetric gross or net calorific value of the mixture at combustion temperature t_1

G is the relative density of the real gas

6.2 ISO 6976-95

6.2.1 Compression Factor

$$Z_{mix} = 1 - \left[\sum_{j=1}^{N} x_j \cdot \sqrt{b_j}\right]^2$$

where the summation is taken over all N components of the mixture and:

Z_{mix} is the compression factor

x_j is the mole fraction of component j

$\sqrt{b_j}$ is the summation factor for component j

6.2.2 Mean Molecular Weight

$$M = \sum_{j=1}^{N} x_j \cdot M_j$$

where the summation is taken over all *N* components of the mixture and:

M is the mean molecular weight

x_j is the mole fraction of component *j*

M_j is the molar mass of component *j*

6.2.3 Superior and Inferior Calorific Value

- Molar basis (real gas property is calculated as ideal)

$$\overline{H}^0(t_1) = \sum_{j=1}^{N} x_j \cdot \overline{H}_j^0(t_1)$$

where the summation is taken over all *N* components of the mixture and:

$\overline{H}^0(t_1)$ is the ideal molar calorific value of the mixture (superior or inferior)

$\overline{H}_j^0(t_1)$ is the ideal molar calorific value of the component *j* (superior or inferior)

x_j is the mole fraction of component *j*

- Mass basis (real gas property is calculated as ideal)

$$\hat{H}^0(t_1) = \frac{\overline{H}^0(t_1)}{M}$$

where:

$\hat{H}^0(t_1)$ is the ideal calorific value on a mass basis of the mixture (superior or inferior)

$\overline{H}^0(t_1)$ is the ideal molar calorific value of the mixture (superior or inferior)

M is the mean molecular weight

- Volumetric basis - ideal gas

$$\tilde{H}^0[t_1, V(t_2, p_2)] = \overline{H}^0(t_1) \cdot \frac{p_2}{R \cdot T_2}$$

where:

$\tilde{H}^0[t_1, V(t_2, p_2)]$ is the ideal calorific value on a volumetric basis, for a combustion temperature t_1, of the mixture (superior or inferior), metered at a temperature t_2 and pressure p_2

$\overline{H}^0(t_1)$ is the ideal molar calorific value of the mixture (superior or inferior)

R is the molar gas constant

T_2 is the absolute temperature in kelvins

- Volumetric basis - real gas

$$\tilde{H}[t_1,V(t_2,p_2)]=\frac{\tilde{H}^0[t_1,V(t_2,p_2)]}{Z_{mix}(t_2,V(t_2,p_2)}$$

where:

$H[t_1,V(t_2,p_2)]$ is the real-gas calorific value on a volumetric basis, for a combustion temperature t_1, of the mixture (superior or inferior), metered at a temperature t_2 and pressure p_2

$Z_{mix}(t_2,p_2)$ is the compression factor at the metering reference conditions

6.2.4 Relative Density

- Ideal gas

$$d^0=\sum_{j=1}^{N}x_j\cdot\frac{M_j}{M_{air}}$$

where the summation is taken over all N components of the mixture and:

d^0 is the relative density of the ideal gas

M_j is the molar mass of component j

M_j is the molar mass of dry air of standard composition

- Real gas

$$d(t,p)=\frac{d^0\cdot Z_{air}(t,p)}{Z_{mix}(t,p)}$$

where the summation is taken over all N components of the mixture and:

d is the relative density of the real gas

Z_{mix} is the compression factor of the gas mixture

Z_{air} is the compression factor of dry air of standard composition

6.2.5 Density

- Ideal gas

$$\rho^0(t,p)=(\frac{p}{R\cdot T})\sum_{j=1}^{N}x_j\cdot M_j$$

where the summation is taken over all *N* components of the mixture and:

ρ^0(t,p) is the density of the ideal gas

R is the molar gas constant

T is the absolute temperature in kelvins

x_j is the mole fraction of component *j*

M_j is the molar mass of component *j*

- Real gas

$$\rho(t,p) = \frac{\rho^0(t,p)}{Z_{mix}(t,p)}$$

where:

ρ(t,p) is the density of the real gas

Z_{mix} is the compressibility factor of the gas mixture

6.2.6 Wobbe Index

- Ideal gas

$$W^0[t_1,V(t_2,p_2)] = \frac{\tilde{H}_S^0[t_1,V(t_2,p_2)]}{\sqrt{d^0}}$$

where:

$W^0[t_1,V(t_2,p_2)]$ is the Wobbe index of the ideal gas

$H_S{}^0[t_1,V(t_2,p_2)]$ is the superior calorific value on a volumetric basis, for a combustion temperature t_1, of the ideal gas, metered at a temperature t_2 and pressure p_2

d^0 is the relative density of the ideal gas

- Real gas

$$W[t_1,V(t_2,p_2)] = \frac{\tilde{H}_S[t_1,V(t_2,p_2)]}{\sqrt{d(t_2,p_2)}}$$

where:

$W[t_1,V(t_2,p_2)]$ is the Wobbe index of the real gas

$\tilde{H}_S[t_1,V(t_2,p_2)]$ is the superior calorific value on a volumetric basis, for a combustion temperature t_1, of the real gas, metered at a temperature t_2 and pressure p_2

$d(t_2,p_2)$ is the relative density of the real gas

6.3 ASTM D 3588-98 and GPA 2172-09

6.3.1 Molar Mass

$$M = \sum_{j=1}^{N} x_j \cdot M_j$$

where the summation is taken over all *N* components of the mixture and:

M is the molar mass of the mixture

x_j is the mole fraction of component *j*

M_j is the molar mass of component *j*

6.3.1.1 Molar Mass Ratio

$$G^{id} = \sum_{j=1}^{N} x_j \cdot G_j^{id} = \frac{M}{M_a}$$

where the summation is taken over all *N* components of the mixture and:

G^{id} is the molar mass ratio of the mixture

x_j is the mole fraction of component *j*

G_j^{id} is the molar mass ratio of the compound *j*

M is the molar mass of the mixture

M_a is the molar mass of air

6.3.2 Compressibility Factor

$$Z(T,P) = 1 - P \cdot \left[\sum_{j=1}^{N} x_j \cdot \sqrt{\beta_j} \right]^2$$

where the summation is taken over all *N* components of the mixture and:

$Z(T,P)$ is the compression factor

P is the pressure

x_j is the mole fraction of component *j*

$\sqrt{\beta_j}$ is the summation factor for component *j*

6.3.3 Relative Density

- Ideal gas

$$d^{id} = \frac{M}{M_a}$$

where:

d^{id} is the relative density of the ideal gas

M is the molar mass of the mixture

M_a is the molar mass of air

- Real gas

$$d = \frac{M \cdot Z_a}{M_a \cdot Z}$$

where:

d is the relative density of the real gas

Z is the compression factor of the gas mixture

Z_a is the compression factor of dry air

M is the molar mass of the mixture

M_a is the molar mass of air

6.3.4 Heating Value

According to ASTM D 3588-98, the real heating value is not given by division of the ideal heating value by the compressibility factor (Z). Real gas heating values differ from the ideal gas values by less than the order of the accuracy of the heating values. Thus, the real heating value is calculated as ideal. Furthermore, according to GPA 2172-09, dividing the ideal volumetric heating value by the compressibility factor provides the energy transferred in an ideal gas reaction per volume of real gas fuel (in Clarity, printed as Ideal Heating Value per Real Gas Volume).

- Molar basis

$$H_n^{id} = \sum_{j=1}^{N} x_j \cdot H_{n,j}^{id}$$

where the summation is taken over all N components of the mixture and:

H_n^{id} is the heating value of the gas mixture on molar basis (gross or net)

x_j is the mole fraction of component j

$H_{n,j}^{id}$ is the molar heating value of component j (gross or net)

- Mass basis

$$H_m^{id} = \frac{\sum_{j=1}^{N} x_j \cdot M_j \cdot H_{m,j}^{id}}{\sum_{j=1}^{N} x_j \cdot M_j}$$

where the summation is taken over all *N* components of the mixture and:

H_m^{id} is the heating value of the gas mixture on mass basis (gross or net)

x_j is the mole fraction of component *j*

M_j is the molar mass of component *j*

$H_{m,j}^{id}$ is the heating value per unit mass of component *j* (gross or net)

- Volumetric basis

$$H_V^{id} = \sum_{j=1}^{N} x_j \cdot H_{V,j}^{id}$$

where the summation is taken over all *N* components of the mixture and:

H_V^{id} is the heating value of the gas mixture on volumetric basis (gross or net)

x_j is the mole fraction of component *j*

$H_{V,j}^{id}$ is the heating value per unit volume of component *j* (gross or net)

6.4 ASTM D 2421-02 and D 2598-02

6.4.1 Vapor Pressure

$$p_V = \sum_{j=1}^{N} x_{V,j} \cdot vp'_j$$

where the summation is taken over all *N* components of the mixture and:

p_V is the liquified petroleum (LP) gas vapor pressure of the sample at 37.8 °C

$x_{V,j}$ is the liquid volume percent of component *j* in the mixture

vp_j' is the vapor pressure factor of component *j* at 37.8 °C

6.4.2 Relative density

$$d = \sum_{j=1}^{N} \frac{x_{V,j} \cdot sg'_j}{100}$$

where the summation is taken over all *N* components of the mixture and:

d is the relative density of the mixture

$x_{V,j}$ is the liquid volume percent of component *j* in the mixture

sg_j' is the relative density of component *j* at 15.6 °C

6.4.3 Motor Octane Number

$$MON = \sum_{j=1}^{N} \frac{x_{V,j} \cdot mon_j}{100}$$

where the summation is taken over all *N* components of the mixture and:

MON is the calculated motor octane number of the mixture

$x_{V,j}$ is the liquid volume percent of component *j* in the mixture

mon_j is the motor octane number of component *j*

6.5 ISO 8973-97 and EN 589+A1

6.5.1 Density

$$\rho = \frac{1}{\sum_{j=1}^{N} \frac{W_j}{\rho_j}}$$

where the summation is taken over all *N* components of the mixture and:

ρ is the density of the mixture at 15 °C

ρ_j is the density factor of component *j* in the mixture at 15 °C

W_j' is the mass fraction of component *j* in the mixture, calculated as:

$$W_j = \frac{x_j \cdot M_j}{\sum_{j=1}^{N} x_j M_j}$$

where the summation is taken over all *N* components of the mixture and:

x_j is the mole fraction of component *j*

M_j is the relative molecular mass of component *j*

6.5.2 Absolute Vapor Pressure

$$p_v = \sum_{j=1}^{N} x_j \cdot p_{v,j}$$

where the summation is taken over all *N* components of the mixture and:

p_V is the absolute vapor pressure of the LPG sample

x_j is the mole fraction of component *j* in the mixture

$p_{V,j}$ is the vapor pressure factor of component *j*

6.5.3 Gauge Vapor Pressure

$$p_{ve} = p_v - \text{local atmospheric pressure (101.325 kPa)}$$

where:

p_{ve} is the gauge vapor pressure

6.5.4 Octane Number

$$ON = \sum_{j=1}^{N} x_j \cdot pon_j$$

where the summation is taken over all N components of the mixture and:

ON is the calculated octane number of the mixture

x_j is the molar fraction of component j in the mixture

pon_j is the partial octane number of component j

6.6 Additional notes

6.6.1 Methane Number

According to KUBESH, John; KING, Steven R.; LISS, William E. *Effect of gas composition on octane number of natural gas fuels*. SAE Technical Paper, 1992, equation (4):

$$MN = 1.624 \cdot ON - 119.1$$

where:

MN is the calculated methane number of the mixture

ON is the octane number of the mixture

1.624 and 119.1 are the coeficients obtained via regression as described in the Article

6.6.2 Calculation on wet basis

For calculations of gas properties on wet basis according to norms ISO 6976-95, ASTM D 3588-98, and GPA 2172-09, the mole fraction of water in natural gas saturated with water is added to the resulting NGA Amounts. For ASTM D 3588-980 and GPA 2172-09, the base temperature is defined as 60 °F (corresponding to the saturated mole fraction of water equal to 0.01744). In ISO 6976-95, the available metering temperatures are 0, 15, and 20 °C. The mole fractions of water vapor in saturated gas at these temperatures were calculated according to the following equation:

$$x_W(T) = \frac{p_{sat}(T)}{p_{atm}}$$

where:

$x_w(T)$ is the mole fraction of water vapor in saturated gas at temperature T

p_{atm} is the atmospheric pressure (101.325 kPa).

$p_{sat}(T)$ is the saturation vapor pressure of water at temperature T, obtained from the NIST database, Saturation water properties, P.J. Linstrom and W.G. Mallard, Eds., NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg MD, 20899, https://doi.org/10.18434/T4D303, (retrieved February 15, 2024).