QuantityWare

BCG 1.0A

Natural Gas Components – Physical Properties Data

Description of data sets provided by QuantityWare and important notes on fundamental data

Notes

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Introduction

BCG covers quantity conversion solutions for:

- All natural gases, natural-gas substitutes and similar fluids that are present in the gaseous phase (state) at normal(standard) ISO conditions as specified in ISO 13443 First edition –1996-12-15. The standard conditions are 101,325 kPa and 15 °C. By this definition, LNG (liquefied natural gas) is also included in the product definition range.
- Liquid hydrocarbons (NGL/LPG) having a vapour pressure greater then atmospheric pressure at 15°C, in which the standard pressure shall be equilibrium pressure at 15°C. The standard conditions are 101,325 kPa and 15 °C.

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With BCG 1.0A, we deliver a complete solution which covers all quantity conversion and measurement requirements for the relevant supply chain management business processes of natural gas (low and high pressure regime), NGL and LNG. With the conversion groups (270 conversion groups for natural gas, 50 for LNG) you are able to configure all your SAP Oil & Gas processes, such as inventory management, order-to-cash processes, procure-to-pay, as well as complex scheduling and transmission processes within the SAP Trader's & Schedulers Workbench (TSW).

> ⚠ *Common to all comprehensive natural gas conversions is the fact that such conversions require data sets containing physical property data for all components of the natural gas. Based on this data natural gas properties such as compression factors, heating values, molecular weight and densities can be calculated.*

QuantityWare delivers 16 data sets as required content for natural gas conversions. These data sets are based on three standards:

- DIN EN ISO 6976:2005 (English version of ISO 6976:1995 incl. Corrigendum 1:1997, Corrigendum 2:1997 and Corrigendum 3:1999)
- ISO 6578:1991, First edition 1991-12-01
- GPA 2145-03, Rev.02 (07/07)

- GPA 2145-09

LNG Contracts typically specify which data sets have to be applied for custody transfer measurements and calculations. QuantityWare has selected these data sets based on an analysis of publicly available contract data. If customers require data sets based on other standards or other versions of the standards noted above, QuantityWare can deliver such sets together with the relevant validation test reports as part of the maintenance agreement.

In this document, we describe the data sets delivered and how the correctness of the data can be validated using QuantityWare validation tools.

1. Installation

The technical implementation is provided as a part of the initial BCG 10A installation SAINT package.

Please follow the QuantityWare SAINT installation instructions for BCG 10A.

SAP Oil & Gas must be installed

Customizing settings are included in this package, which are needed in every client in which this solution will be used.
On releases 4.72 and below, the related customizing transport must be imported into all necessary clients, or distributed to them from client 000.
On releases ERP 2005 (ERP 6.0) or newer, BC Set /QTYW/BCG_10A must be activated in the relevant clients.

Please refer to the QuantityWare BCG 10A Installation Guide for more information.

2. Basic definitions of natural gas quantities and behaviour

Besides serving as basic feedstock for the chemical industry, natural gas is predominantly used for heat production as a fuel in large industry sites and millions of households worldwide.
In order to define a trading value for natural gas and to ensure natural gas interchangeability, certain quantities that characterize natural gas must be defined and recorded in business transactions for various processes e.g. inventory management, quality assurance, pricing and excise duty payments. For a comprehensive list of such quantities we recommend ISO standard ISO 6976 as a reference.
With BCG 1.0A QuantityWare delivers conversion groups that are designed for all globally known standard reference conditions for natural gas in the gas phase (high and low pressure regime (CNG), as well as conversion groups for NGL (Natural Gas Liquids). With the release of BCG 1.0A, LNG (Liquefied Natural Gas) support is also in scope.
In order to aid the comprehension of this documentation, we cite the most important definitions from standard ISO 6976 & ISO 6578.

Common definitions:

Superior calorific value:

The amount of heat which would be released by the complete combustion in air of a specified quantity of gas, in such a way that the pressure p_1 at which the reaction takes place remains constant, and all the products of combustion are returned to the same specified temperature t_1 as that of the reactants, all of these products being in the gaseous state except for water formed by combustion, which is condensed to the liquid state at t_1.

> ⚠ *A synonym for calorific value is the term **heating value**. Calorific values can be specified on a molar or mass basis. Then the calorific value depends on the combustion reference conditions t_1 and p_1. More commonly, calorific values are determined based upon a volumetric basis ;in this instance, the calorific value needs to be specified with the combustion reference conditions t_1 and p_1 as well as the volumetric reference conditions t_2 and p_2.*

Inferior calorific value:

The amount of heat which would be released by the complete combustion in air of a specified quantity of gas, in such a way that the pressure p_1 at which the reaction takes place remains constant, and all the products of combustion are returned to the same specified temperature t_1 as that of the reactants, all of these products being in the gaseous state.

Density:

The density is the mass of a gas sample divided by its volume at specified conditions of pressure and temperature.

Relative density:

The density of a gas divided by the density of dry air of standard composition (see Annex B ISO 6976:1995 for a definition of dry air) at the same specified conditions of pressure and temperature.

Wobbe index:

The superior calorific value on a volumetric basis at specified reference conditions, divided by the square root of the relative density at the same specified metering reference conditions.

> ⚠ *The Wobbe index is an important quality designation for natural gas, which is commonly used to determine trade prices and the interchangeability of natural gas.*
>
> ⚠ *The SAP QCI does not calculate the Wobbe index for natural gas. BCG contains functions to perform these calculations within the delivered global templates.*

Gas interchangeability:

An important business requirement when trading natural gas is that natural gas combustion is kept at a defined quality levels that are e.g. required by burners. The Wobbe index (sometimes also referred to as Wobbe number) can serve as one important quality number to ensure interchangeability of natural gas batches with e.g. an apparent different composition.

Ideal gas and real gas:

An ideal gas is one that obeys the ideal gas law:

$p \cdot V_m = R \cdot T$ …(1)

where

p is the absolute pressure

T is the thermodynamic temperature

V_m is the volume per mole of gas

R is the molar gas constant, in coherent units.

No real gas obeys this law. For real gases, equation (1) must be rewritten as

$p \cdot V_m = Z(T,p) \cdot R \cdot T$ …(2)

where Z(T,p) is a variable often close to unity, and is known as the compression factor.

Compression factor:

The actual (real) volume of a given mass of a gas at specified pressure and temperature divided by its volume, under the same conditions, as calculated by the ideal gas law.

Combustion reference conditions:

The specified temperature t_1 and pressure p_1. These are the conditions at which the fuel (natural gas) is notionally burned.

Metering reference conditions:

The specified temperature t_2 and pressure p_2. These are the conditions at which the amount of the fuel to be burned is notionally determined; there is no a priori reason for these to be the same as the combustion reference conditions.

> ⚠ *A range of reference conditions is in use throughout the world. In order to ensure ease of trade, exact conversions of natural gas quantities between different sets of reference conditions is required, based on international standards. This range of different reference conditions is also one of the main reasons why natural gas quantity conversions are complex, even in the low pressure regime.*

Standard reference conditions of selected countries:

Country	t_1	p_1	t_2	p_2
Argentina	-	101,325 kPa	15 °C	101,325 kPa
Australia	15 °C	101,325 kPa	0 °C	101,325 kPa
Austria	25 °C	101,325 kPa	0 °C	101,325 kPa
Belgium	25 °C	101,325 kPa	0 °C	101,325 kPa
Brazil	-	101,325 kPa	0 °C	101,325 kPa
Canada	15 °C	101,325 kPa	15 °C	101,325 kPa
China	20 °C	101,325 kPa	20 °C	101,325 kPa
Czechoslovakia	25 °C	101,325 kPa	20 °C and 0 °C	101,325 kPa
Denmark	25 °C	101,325 kPa	0 °C	101,325 kPa
Egypt	-	101,325 kPa	15 °C	101,325 kPa
Finland	-	101,325 kPa	15 °C	101,325 kPa
France	0 °C	101,325 kPa	0 °C	101,325 kPa
Germany	25 °C	101,325 kPa	0 °C	101,325 kPa
Hong Kong	-	101,325 kPa	15 °C	101,325 kPa
Hungary	-	101,325 kPa	0 °C	101,325 kPa
India	-	101,325 kPa	0 °C	101,325 kPa
Indonesia	-	101,325 kPa	0 °C	101,325 kPa
Iran	-	101,325 kPa	15 °C	101,325 kPa
Ireland	15 °C	101,325 kPa	15 °C	101,325 kPa
Italy	25 °C	101,325 kPa	0 °C	101,325 kPa
Japan	0 °C	101,325 kPa	0 °C	101,325 kPa
Netherlands	25 °C	101,325 kPa	0 °C	101,325 kPa
New Zealand	-	101,325 kPa	15 °C	101,325 kPa
Norway	-	101,325 kPa	15 °C	101,325 kPa
Pakistan	-	101,325 kPa	15 °C	101,325 kPa
Romania	25 °C	101,325 kPa	15 °C and 0 °C	101,325 kPa
Russia	25 °C	101,325 kPa	20 °C and 0 °C	101,325 kPa
Spain	0 °C	101,325 kPa	0 °C	101,325 kPa
Sweden	-	101,325 kPa	0 °C	101,325 kPa
United Kingdom	15 °C	101,325 kPa	15 °C	101,325 kPa
USA	15 °C	101,325 kPa	15 °C	101,325 kPa
Yugoslavia	0 °C	101,325 kPa	0 °C	101,325 kPa

Source: ISO 13443 and ISO 12213.
On the other hand, ISO 6976 specifies six sets of reference conditions for heating values on a volumetric basis (Table 5 therein), which can be extracted from the above table, and one additional set (25/15) is apparently in usage in some countries. QuantityWare thus defines a global template for the SI system based on seven sets of combustion and metering reference conditions, plus an additional three sets of U.S. customary conditions.

Additional LNG specific definitions:

Liquefied natural gas (LNG):

Liquids composed predominantly of methane.

Orthobaric density:

The mass of the liquid occupying unit volume at a given temperature, the liquid being in equilibrium with its vapour.

3. High level description of the basic measurement principles

Natural gas – gaseous state:

In the gaseous state, natural gas is transmitted through pipeline systems that easily span thousands of miles. Storage for demand buffering and fluctuating seasonal demand is organised through the use of large underground caverns or special high pressure storage pipe systems.

After extraction, natural gas typically flows at low pressures to gas processing (gas plant) facilities, where it is “cleaned” (removal of unwanted components e.g. corrosives such as Hydrogen Sulphide, Water etc. and extraction of high value components e.g. Butane, Propane etc.). In order to transmit commercially relevant quantities over large distances, high pressure pipelines are then fed with pipeline quality gas, where compressor stations along the line ensure that the gas flows at high pressures to the destination locations (e.g. large utility companies or industrial consumers).

From a measurement and quantity conversion point of view, we distinguish here the low and high pressure regime for natural gas. The definitions of these two regimes vary according to the literary source. We have decided to utilize the ISO standard 13443:1996(E) temperature and pressure range given therein in Annex B (informative) to define the low pressure range, where the pressure range for reference condition conversions is given as

$95 < p/kPa < 105$

Equal to: $13.78 < p/PSI < 15.23$.

The temperature range is given as $270 < T/K < 300$

Equal to: $26 < T/°F < 80$.

Within that range, the ideal gas law and the correction formulas for real gases can be applied as given in ISO 13443.

High pressure transmission introduces additional calculation complexity.

Gas interchangeability:

An important business requirement when trading natural gas is that natural gas combustion is kept at defined quality levels (e.g. burner requirements). The Wobbe index can serve as one important quality value to ensure interchangeability of natural gas batches which, for example, have an apparent different composition.

LNG:

While natural gas in the gaseous state is transmitted through pipelines, LNG (Liquefied Natural Gas) offers the possibility to supply global locations via special LNG tankers that cannot be reached via pipelines, e.g. Japan, South Korea and Taiwan. In addition LNG composition, due to the liquefaction process where components are removed, results in the delivery of a higher quality product to the market.

Simply put, LNG is natural gas with a specified composition (high methane content, low levels of corrosive components and components that would solidify during liquefaction) that is cooled down to cryogenic temperatures (typically at, or slightly below the melting point of methane - approximately minus 161°C). At such low temperatures the gas condenses into a liquid and experiences a volume reduction to approx. 1/600 when compared to the same amount in gaseous form. Using special tankers with insulated tanks, LNG can be shipped across oceans to reach locations where pipelines are not feasible, due to geographical, political or environmental obstacles. At present (2007) approx. 190 LNG tankers are available world wide, however the LNG market is expected to show high growth rates within the next decades. The rising demand for clean and reliable energy from LNG at an increasing number of locations justifies large investments – in liquefaction, storage and regasification sites, as well as LNG tankers. As an example of increasing interest and investment, tanker capacities are growing; the latest plans include tankers with 250.000 Cubic Meter capacity, at initial investments of approx. 200 Mio US Dollars for one tanker.

From a measurement point of view, during custody transfer of the liquid (LNG), the LNG's density, molar composition and heating value are required; typically, molar composition is determined from several samples taken during transfer. Using the transfer samples, gas chromatography is applied to determine the composition (e.g. mol % of all components) of LNG, which can then be utilised to calculate the LNG density and heating values, as well as the density of the gaseous state at any desired reference condition. The document **"BCG 10A ISO LNG"** describes the QuantityWare solution for LNG processing. With this LNG conversion package, LNG processes (transfer shore to ship, ship to shore), using the SAP Trader's & Schedulers Workbench (TSW), are fully supported from a measurement and quantity conversion point of view, including corrections for gas/vapour phase quantities, as well as transmission processes for pipeline via TSW, based on the solutions described above.

Both LNG and natural gas (gaseous) measurement and conversion are typically based on the molar composition analysis of the natural gas' individual components. The physical properties of these components must be known before accurate calculations can be attempted.

4. Physical properties - data set description

The following data sets are contained in BCG 10A, SP01:

- Q0 QW: GPA 2172-96, 60°F/14.696 PSI
- Q1 QUANTITYWARE: 25°C / 0°C ISO 6976 DATA
- Q2 QUANTITYWARE: 15°C / 15°C ISO 6976 DATA
- Q3 QUANTITYWARE: 0°C / 0°C ISO 6976 DATA
- Q4 QUANTITYWARE: 15°C / 0°C ISO 6976 DATA
- Q5 QUANTITYWARE: 20°C / 20°C ISO 6976 DATA
- Q6 QUANTITYWARE: 25°C / 20°C ISO 6976 DATA
- Q7 QUANTITYWARE: 25°C / 15°C ISO 6976 DATA
- Q8 QUANTITYWARE: 15°C / 15°C ISO 6578 DATA
- QA QW: GPA 2145-03, REV.2, 60°F/14.696 PSI
- QB QW: GPA 2145-09 60°F/14.696 PSI
- QC QW: GPA 2145-09 15 °C/101.325 KPA
- QD QW: GPA 2145-03, REV.2,15°C/15°C/101,325
- QE QW: GPA 2145-09 BASED 60°F/15.025 PSI
- QF QW: GPA 2145-09 BASED 60°F/14.730 PSI
- QG QW: GPA 2145-09 BASED 60°F/14.650 PSI

Data set Q0 contains data defined in GPA 2172-96.
Data sets Q1 to Q7 are based on ISO 6976. Each set contains the relevant physical properties for the 55 components defined in ISO 6976. The molar heating values are maintained as given in ISO 6976.
Data set Q8 contains data for 13 components defined in ISO 6578. The mass based heating values are maintained as given in ISO 6578.
Sets QA to QG contain the data as defined in GPA 2145. The volume based heating values are maintained as given in GPA 2145.

In detail, the following data is maintained by QuantityWare:

- Molecular weight (molar mass)
- Summation factor
- Inferior heating value

- Superior heating value
- Relative density (only QB, QC, QE, QF; QG)

The definition of the summation factor is different in ISO standards and GPA standards. QuantityWare supports both summation factor definitions. If you define your own data set, you have to declare which definition you intend to use for the data you maintain. The sets Q0 to QG are maintained using either definition.

5. Fundamental constants and properties of dry air

Fundamental constants:

Natural gas quantity conversions need to utilize the proper value of the molar gas constant R. The value of this constant changes due to progress made in scientific research. CODATA publish data in a consistent way on a regular basis (see http://www.codata.org/ for details). The accepted value of the molar gas constant R is 8.314 472 J mol^{-1} K^{-1}(at the time of writing). This value can also be found at http://physics.nist.gov/cuu/Constants/Table/allascii.txt and is published in GPA 2145-03. ISO 6976 on the other hand, still references the older value of 8.314 510 J mol^{-1} K^{-1}. The SAP QCI also utilizes that value based on ISO 6976.

> ⚠ *Within BCG 10A, QuantityWare utilizes the value 8.314 510 J mol^{-1} K^{-1}, to be consistent with SAP QC for the SAP QCI conversion groups for the gas constant R. If you utilize the MQCI conversion groups, you can configure a conversion group to use any required value for R*

Properties of dry air:

Molar mass:

Natural gas quantity conversions utilize compression factors of dry air at various conditions and the molar mass of dry air for conversion calculations.
Dry air:
ISO 6976 defines the proper value of these constants. For the molar mass of dry air, it defines the value to be 0.0289626 kg/mol. GPA 2145-03, Rev.02 and GPA 2145-09 define a value of 0.0289625 kg/mol.
Within BCG 10A QuantityWare utilizes the value 0.0289626 kg/mol to be consistent with the SAP QCI for the SAP QCI conversion groups. If you use the MQCI conversion groups, you can configure a conversion group to use any desired value.

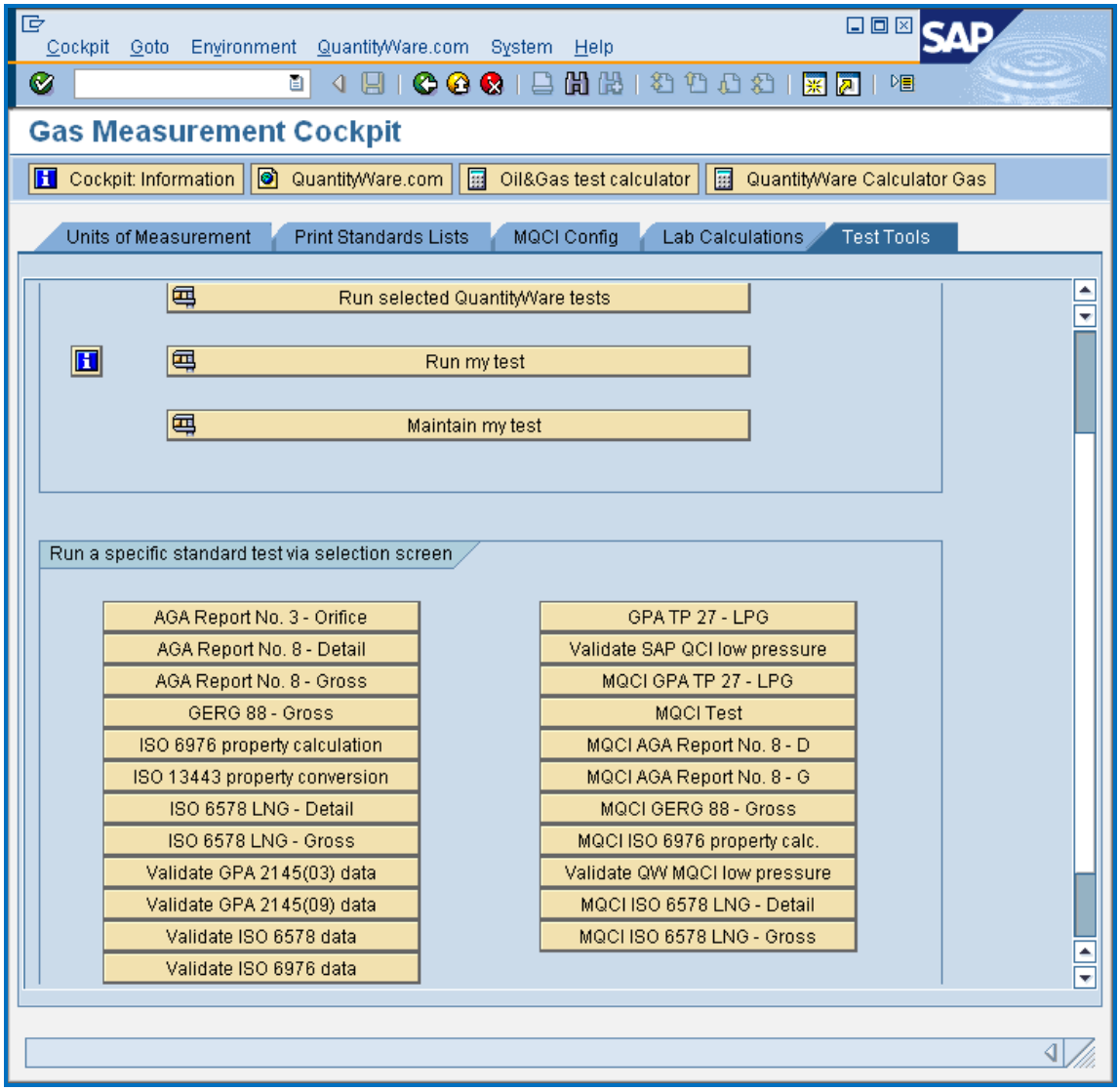
Compression factors:

ISO 6976 defines a compression factor of 0.99958 at 15 °C and 101.325 kPa. GPA 2145-03 Rev.02 defines a summation factor of 0.00201 which transforms to a compression factor of 0.99959 (rounded value to five decimal places).

> ⚠ *Within BCG 10A QuantityWare utilizes the value 0.99958 to be consistent with SAP QCI for SAP QCI conversion groups. This value can also be reproduced in the same way as the other relevant values utilizing the virial equation defined in AGA Report No.8, equation C3-12 (page 131). QuantityWare has built function /QTYW/CALC_ZAIR based on that equation to calculate compression factors of dry air with an accuracy of 5 decimal places. If you utilize MQCI conversion groups, you can define in customizing any desired value.*

6. Test reports for physical property data

Along with the package BCG 1.0A QuantityWare provides test & validation programs that can be used to test the installation and also to validate the SAP QCI for natural gas conversions. The reports are accessible from the Gas Measurement Cockpit:



The validation reports check that each component value is identical to the four hard coded values within the report datasets.

- molecular weight
- summation factor (ISO format)

- inferior(net) heating value,
- superior(gross) heating value
- relative density (where maintained)