



# Bulk Calculations – Solution

## BCS 3.0

Working Paper: Hydrogen (H<sub>2</sub>) High Pressure Quantity Conversions

## Notes

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This working paper supports certified QuantityWare BCG consultants in the implementation of the Advanced Development (AD) delivered with [note 000100](#) – High Pressure Hydrogen Quantity Conversions.

## Version History

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Version	Date	Description
01	2022-06-30	Initial Version
02	2023-11-30	Editorial revision and update

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# 1. Introduction

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QuantityWare BCS supports all bulk product quantity conversions in SAP Oil & Gas. Hydrogen quantity conversions have not been in scope of BCS until 2020; however, there is an increasing demand for such calculations, as expressed by the [Hydrogen Council](#) – “a global CEO-led initiative of leading companies with a united vision and long-term ambition: for hydrogen to foster the clean energy transition for a better, more resilient future”. Many major leading Oil & Gas companies already take part in this council which will play a decisive role in the coming decades.

The idea of a [hydrogen economy](#) is the guiding principle; however, “as of 2019, hydrogen is mainly used as an industrial feedstock, primarily for the production of [ammonia](#) and [methanol](#), and in petroleum refining (hydrogen cracking).”

Thus, the oil and gas industry has already a strong process knowledge of hydrogen production and “in-house” consumption, which requires quantity conversions for hydrogen (and ammonia) in existing SAP ERP systems.

Based upon the sources above, a strongly increasing demand of hydrogen production, transportation and storage is expected in the coming years.

Concerning hydrogen, an [ideal gas solution is already available since 2010 to all BCG](#) customers. For mixtures of natural gas and hydrogen, read the [FAQ on hydrogen mixtures](#).

For [hydrogen transportation and storage](#), three main options are in discussion, or currently utilized by the industry:

1. High-pressure storage & transportation in the gaseous form - **HPH**
2. Extremely low temperature storage & transportation in the liquid form - **LDH**
3. Hydride-based storage in the solid or liquid form – Liquid hydrogen carrier (LHC) technology - **LHC**

In this document, we focus on the implementation of the **high-pressure hydrogen quantity conversion solution**, delivered as an advanced development (AD) with [note 000100](#).

**This solution is defined for mass and volume calculations and represents the first phase of QuantityWare BCG hydrogen development “HPH 1” – see [note 000106](#) for the associated development roadmap.**

Note: All HPH and LDH Hydrogen implementations will become part of BCG. Hydrogen will appear as a new product in the BCG usage questionnaire. LHC implementations will become part of BCP.

## 2. Configuration Support – Advanced Development

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This working paper provides basic support to [certified BCS consultants](#), who wish to implement the high pressure hydrogen solution at customer site.

As noted above, the hydrogen solution is delivered as an Advanced Development (AD) with [note 000100](#). Thus, note 000100 must be implemented into the customer system landscape before the configuration can be implemented by a certified BCS consultant. With BCS 30A CSP03 30B CSP02, the AD is delivered to all BCG customers.

For additional clarifications, a consultant inquiry ticket (available to all certified BCS consultants) should be raised via the [QuantityWare Support Portal](#).

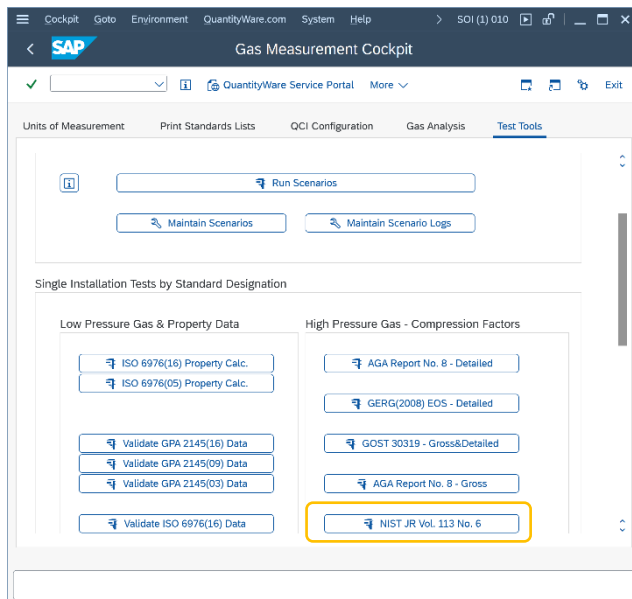
### 3. High Pressure Hydrogen – Measurement Standard

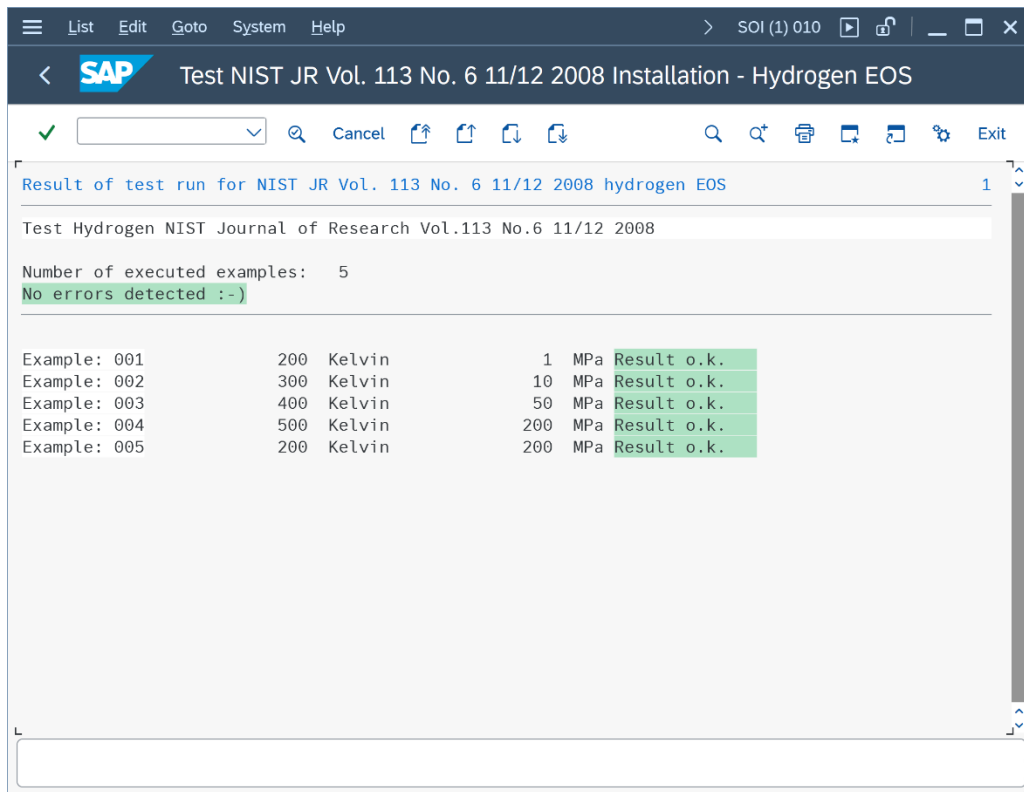
A complete and well defined measurement standard defining all required quantity conversions - including a precise implementation instruction – for high pressure H<sub>2</sub> calculations is not currently available. To provide a scientifically-based solution to meet the industries’ needs, QuantityWare thus implemented the NIST equation (3) calculation defined in *J. Res. Natl. Inst. Stand. Technol. 113, 341-350 (2008) - Revised Standardized Equation for Hydrogen Gas Densities for Fuel Consumption Applications*. The implementation is based on an equation of state with an expression (equation (3)) that allows calculation of H<sub>2</sub> compressibility factors and molar densities. It thus provides all required calculation parameters to convert mass and volume quantity values for high pressure hydrogen conversions within a newly developed real gas hydrogen calculation model.

This implementation is confirmed by [a new BCG test report](#), based on the examples given therein:

**Table 2.** Test points for validating computer code based on Eq. (3)

$T(K)$	$p(MPa)$	$Z$	$\rho(mol/l)$
200	1	1.00675450	0.59732645
300	10	1.05985282	3.78267048
400	50	1.24304763	12.09449023
500	200	1.74461629	27.57562673
200	200	2.85953449	42.06006952



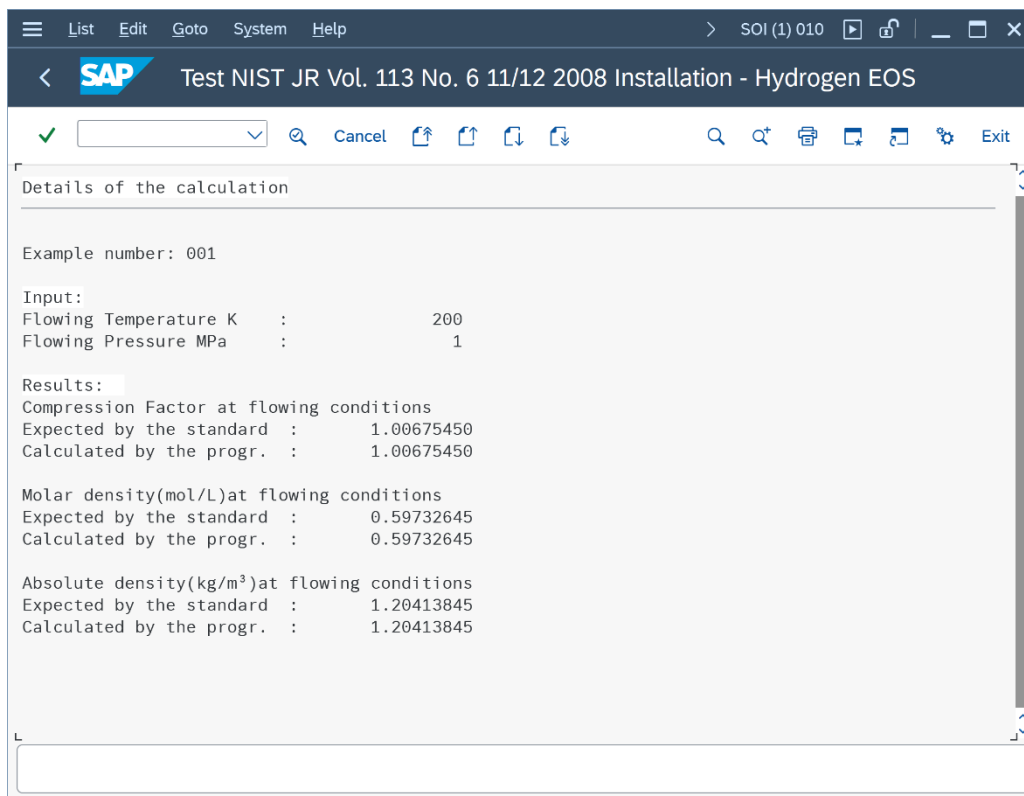


Result of test run for NIST JR Vol. 113 No. 6 11/12 2008 hydrogen EOS

Test Hydrogen NIST Journal of Research Vol.113 No.6 11/12 2008

Number of executed examples: 5  
**No errors detected :-)**

Example: 001	200 Kelvin	1 MPa	Result o.k.
Example: 002	300 Kelvin	10 MPa	Result o.k.
Example: 003	400 Kelvin	50 MPa	Result o.k.
Example: 004	500 Kelvin	200 MPa	Result o.k.
Example: 005	200 Kelvin	200 MPa	Result o.k.



Details of the calculation

Example number: 001

Input:

Flowing Temperature K	:	200
Flowing Pressure MPa	:	1

Results:

Compression Factor at flowing conditions

Expected by the standard	:	1.00675450
Calculated by the progr.	:	1.00675450

Molar density(mol/L)at flowing conditions

Expected by the standard	:	0.59732645
Calculated by the progr.	:	0.59732645

Absolute density(kg/m³)at flowing conditions

Expected by the standard	:	1.20413845
Calculated by the progr.	:	1.20413845

## 4. Configuration Details

- For hydrogen, the existing SAP QCI product type:

### B General Gases (Pure, Inert)

is utilized. This required extension of the natural gas/LNG conversion groups customizing transaction allows selection of this product types' conversion groups for maintenance and exclusion from the crude oil & products conversion group maintenance.

- For this product type, the natural gas/LNG customizing transaction is also used:

The image displays three screenshots of the SAP configuration transaction 'Change View "QCI: LNG, Natural Gas, Hydrogen Conversion Groups": Data'. The top-left screenshot shows the 'Basic Data' tab, including fields for 'Conversion group', 'Product type', 'Product class', 'Isobutanol formula', 'Calculator scenario', 'Use ISO tab formula', 'Heating value class', 'Source R, M (t)', 'Rounding pres. calc.', 'Summation fact. ind.', '(Pct.) density calc.', 'Z mix calc. (t-d)', 'Z mix usage (C/V)', 'Density type', 'Heating value type', 'Activate ISO 6976 2016 edition calculation', 'Poland range of standard interpolation', 'Melting & combustion reference conditions', and 'Vapor correction'.

The top-right screenshot shows the 'Base conversion units of measure' tab, which includes settings for 'Heating value (volume) Unit', 'Heating value (mass) Unit', 'Density (absolute) Unit', 'Webbe index Unit', 'Base conversion units of measure' (Energy, Mass, Volume, Molar mass), and 'LNG settings' (Base temperature, Base density, Vapor correction, Vapor data, and LNG comp. data).

The bottom screenshot shows the 'Rounding settings for model' and 'Quantity tolerance levels' tabs. The 'Rounding settings for model' includes options for 'Round base source quantity within model', 'Round intermediate quantity within model', 'Round base target quantity within model', and 'Round quantities and parameters within model using destination's rounding'. The 'Quantity tolerance levels' tab includes 'Tolerance group' and 'Quantity error % high/low' settings.





Gas Measurement Cockpit: Display Conversion Groups by Calc. Scenario

### Conversion Groups for Natural Gas/LNG/Hydrogen Scenario

D  
HPH COMP - flowing p, T - 100% hydrogen NIST JR VOL 113

...	C.Grp	Rdg. gro...	Ran...	QCI	Set...	Description	P.t.	Qty.EL...	Qty.WL...	Qty.WH...	Qty.EH...
1	QTH0	QTH0	QTH0	QTYW	QX	HYDROGEN HIGH PRESA 15 °C / 101.325 KPA B	B	0.50	0.10	0.10	0.50
2	QTH1	QTH0	QTH0	QTYW	QX	HYDROGEN HIGH PRESG 15 °C / 101.325 KPA B	B	0.50	0.10	0.10	0.50
3	QTH2	QTH2	QTH2	QTYW	QY	HYDROGEN HIGH PRESA 60 °F / 14.696 PSI B	B	0.50	0.10	0.10	0.50
4	QTH3	QTH2	QTH2	QTYW	QY	HYDROGEN HIGH PRESG 60 °F / 14.696 PSI B	B	0.50	0.10	0.10	0.50

Four new template conversion groups are defined (and are delivered with the BCS 3.0 CSP in Q4 2023); two for the ISO base conditions (either absolute or gauge pressure input) and two for the U.S. customary base conditions (either absolute or gauge pressure input).

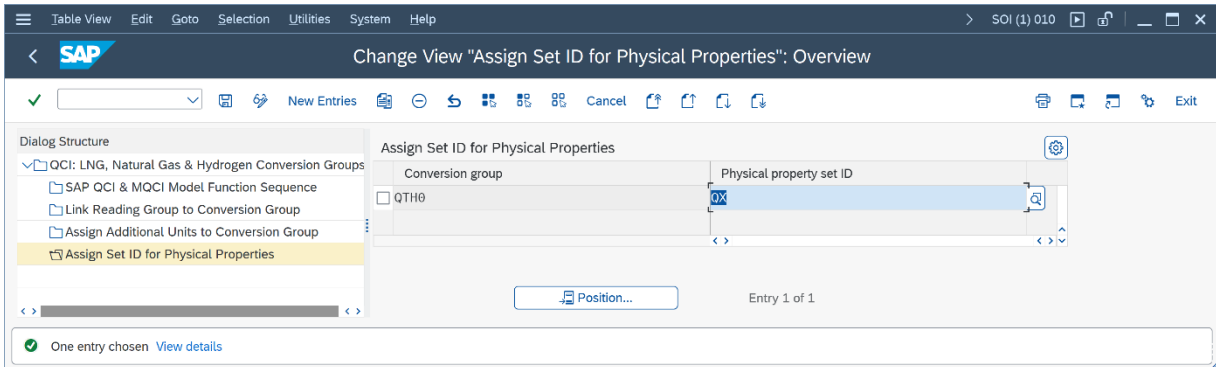
Configuration Example: 7 new hydrogen MQCI model functions have been developed:

Change View "SAP QCI MQCI Model Function Sequence": Overview

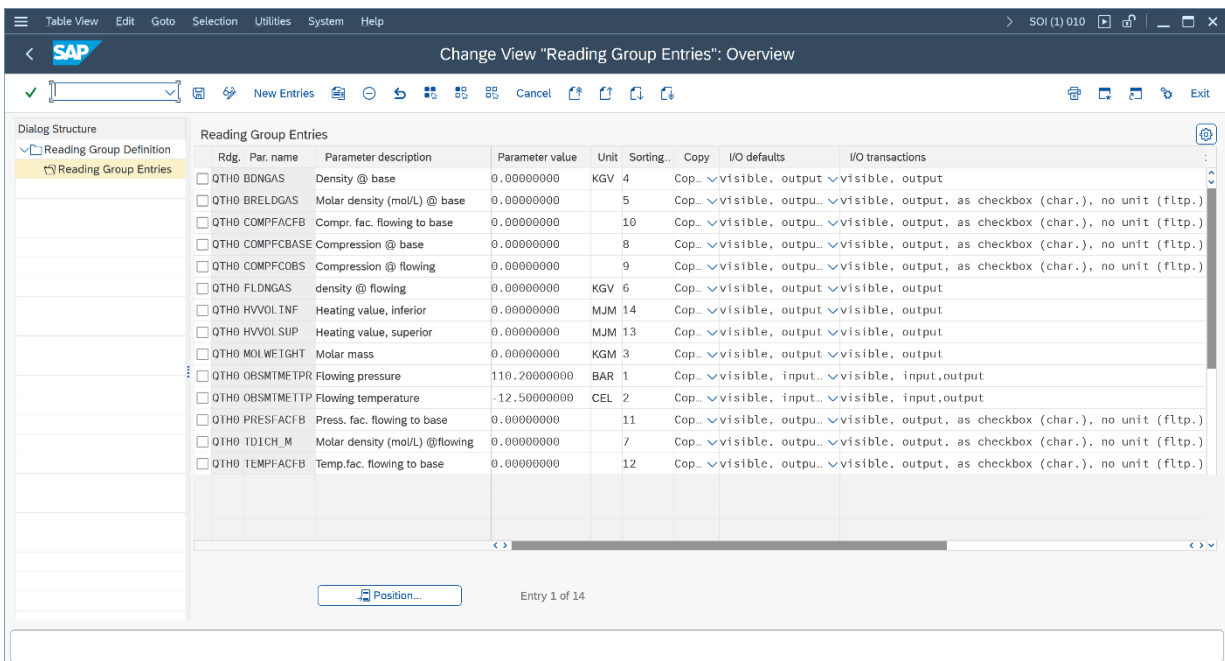
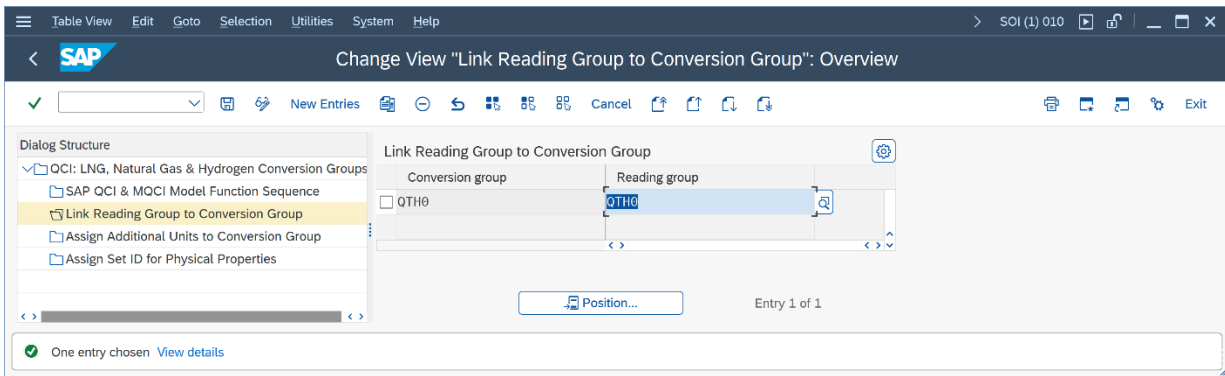
SAP QCI & MQCI Model Function Sequence

Conversion group	FSQ	Function module name	Fun...
<input type="checkbox"/> QTH0	1	/QTYW/MQCI_CALL_BCG	5
<input checked="" type="checkbox"/> QTH0	2	/QTYW/MQCI_HYD_UOM_DIM_CHECK	5
<input type="checkbox"/> QTH0	3	/QTYW/MQCI_BCG_CALC_ABS_PRESS2	7
<input checked="" type="checkbox"/> QTH0	5	/QTYW/MQCI_BCG_HYDCOND_DEFAULT	9
<input type="checkbox"/> QTH0	15	/QTYW/CHECK_PARAM_RANGES	9
<input checked="" type="checkbox"/> QTH0	20	/QTYW/MQCI_BCG_ROUND_INP_HYD	7
<input checked="" type="checkbox"/> QTH0	25	/QTYW/MQCI_BCG_CONVERT_INP_HYD	5
<input checked="" type="checkbox"/> QTH0	30	/QTYW/MQCI_BCG_HYDROGEN_HP_PT	5
<input checked="" type="checkbox"/> QTH0	35	/QTYW/MQCI_BCG_ROUND_RES_HYD	5
<input checked="" type="checkbox"/> QTH0	40	/QTYW/ALT_HYD_OBS_TO_ALT_QUAN	5
<input type="checkbox"/> QTH0	45	/QTYW/MQCI_ROUND_ALT_QUANTITY	5
<input type="checkbox"/> QTH0	50	/QTYW/MQCI_SAP_OVERFLOW_CHECK	5
<input type="checkbox"/> QTH0	55	/QTYW/MQCI_SAP_QUANTITY_CHECK	5
<input type="checkbox"/> QTH0	90	/QTYW/MQCI_SYNC_EXT_VALUES	C

Entry 1 of 14

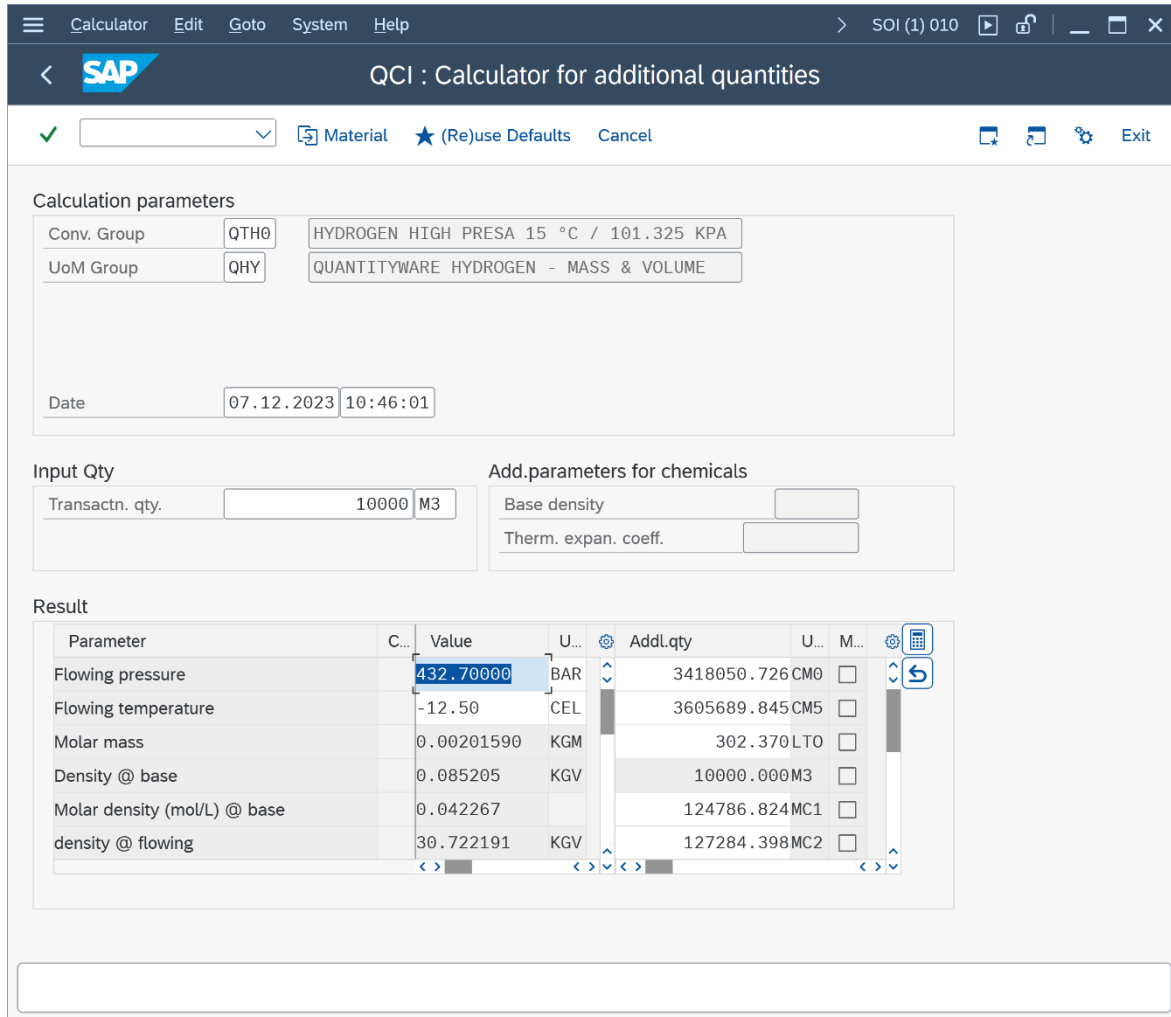


Note: The Physical property set contains hydrogen data only – e.g. from GPA 2145-16 (or other sources, depending on customer requirements)



## 5. Calculation Scenario HPH 1 - Details

The high-pressure calculation scenario requires the input of a flowing pressure and a flowing temperature; pressure values may be absolute (PRESA) or gauge (PRESG) values:



**Calculation parameters**

Conv. Group: QTH0    HYDROGEN HIGH PRESA 15 °C / 101.325 KPA  
 UoM Group: QHY    QUANTITYWARE HYDROGEN - MASS & VOLUME

Date: 07.12.2023 10:46:01

**Input Qty**

Transactn. qty.: 10000 M3

**Add.parameters for chemicals**

Base density:   
 Therm. expan. coeff.:

**Result**

Parameter	C...	Value	U...	Add.Qty	U...	M...
Flowing pressure		432.70000	BAR	3418050.726	CM0	<input type="checkbox"/>
Flowing temperature		-12.50	CEL	3605689.845	CM5	<input type="checkbox"/>
Molar mass		0.00201590	KGM	302.370	LTO	<input type="checkbox"/>
Density @ base		0.085205	KGV	10000.000	M3	<input type="checkbox"/>
Molar density (mol/L) @ base		0.042267		124786.824	MC1	<input type="checkbox"/>
density @ flowing		30.722191	KGV	127284.398	MC2	<input type="checkbox"/>

Calculator Edit Goto System Help > SOI (1) 010

**SAP** QCI : Calculator for additional quantities

Material (Re)use Defaults Cancel

Exit

**Calculation parameters**

Conv. Group: QTH0 HYDROGEN HIGH PRESA 15 °C / 101.325 KPA

UoM Group: QHY QUANTITYWARE HYDROGEN - MASS & VOLUME

Date: 07.12.2023 10:46:01

**Input Qty** Transactn. qty. 10000 M3

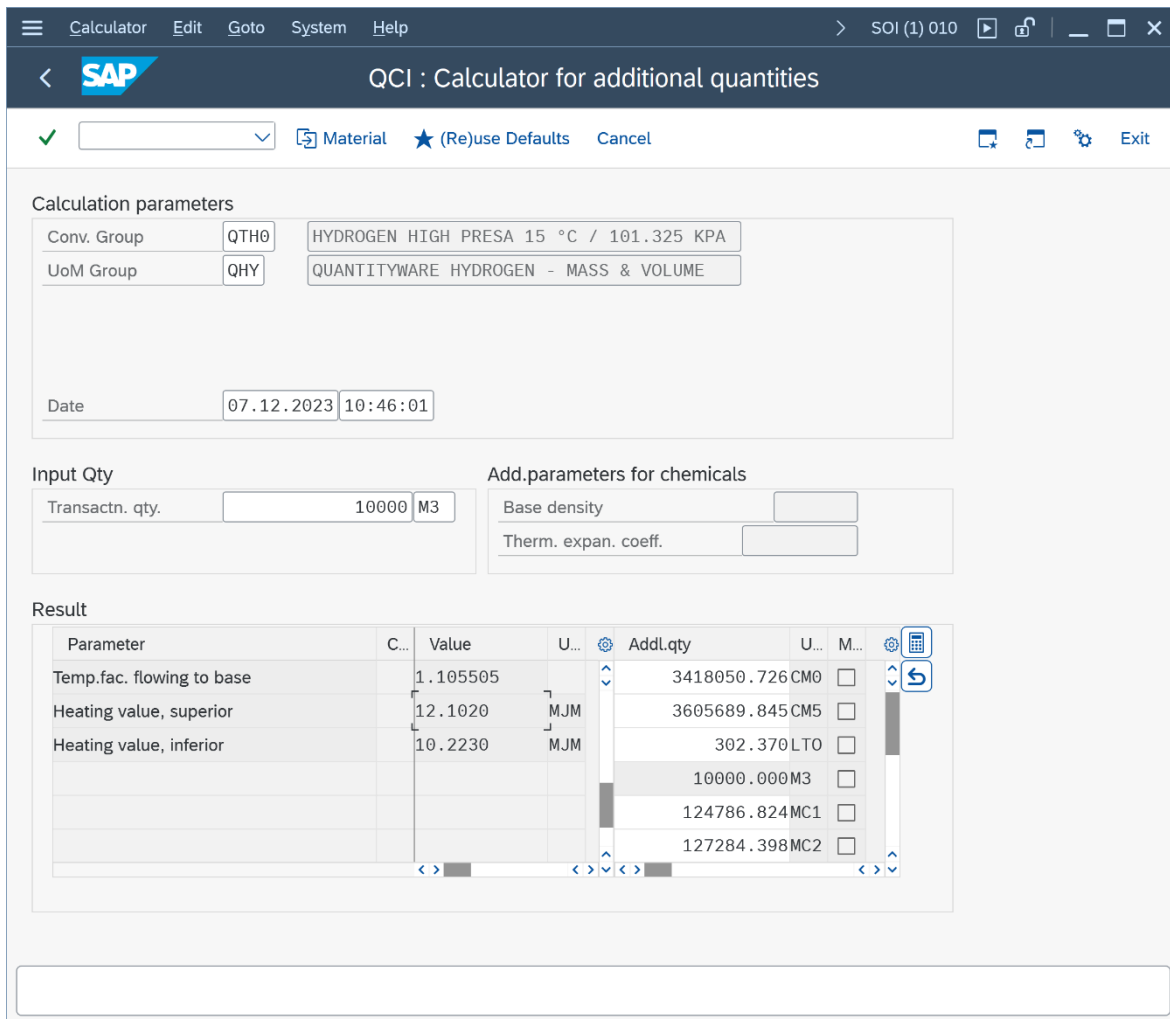
**Add.parameters for chemicals**

Base density:

Therm. expan. coeff.:

**Result**

Parameter	C...	Value	U...	Add.qty	U...	M...
Molar density (mol/L) @flowing		15.240089		3418050.726	CM0	<input type="checkbox"/>
Compression @ base		1.000608		3605689.845	CM5	<input type="checkbox"/>
Compression @ flowing		1.310108		302.370	LT0	<input type="checkbox"/>
Compr. fac. flowing to base		0.763760		10000.000	M3	<input type="checkbox"/>
Press. fac. flowing to base		427.041698		124786.824	MC1	<input type="checkbox"/>
Temp.fac. flowing to base		1.105505		127284.398	MC2	<input type="checkbox"/>



Calculator Edit Goto System Help > SOI (1) 010

**SAP** QCI : Calculator for additional quantities

Material (Re)use Defaults Cancel

Calculation parameters

Conv. Group QTH0 HYDROGEN HIGH PRESA 15 °C / 101.325 KPA

UoM Group QHY QUANTITYWARE HYDROGEN - MASS & VOLUME

Date 07.12.2023 10:46:01

Input Qty Transactn. qty. 10000 M3

Add.parameters for chemicals

Base density

Therm. expan. coeff.

Result

Parameter	C...	Value	U...	Addl.qty	U...	M...
Temp.fac. flowing to base		1.105505		3418050.726	CM0	<input type="checkbox"/>
Heating value, superior		12.1020	MJM	3605689.845	CM5	<input type="checkbox"/>
Heating value, inferior		10.2230	MJM	302.370	LTO	<input type="checkbox"/>
				10000.000	M3	<input type="checkbox"/>
				124786.824	MC1	<input type="checkbox"/>
				127284.398	MC2	<input type="checkbox"/>

- Calculation of molar densities and compression factors is achieved via the NIST function described above.
- Masses and volumes may be calculated & converted; volume UoM need to be either at observed conditions (no temperature and no pressure value assigned to the UoM) or at defined standard reference conditions (temperature and pressure value assigned to UoM).
- Typically, the volume at flowing conditions is the transaction quantity. However, any UoM of SAP Dimension ID MASS or VOLUME may be used as transaction UoM (symmetric model implementation), if the requirement described in (b) for volume UoM is considered.
- The molar mass and the heating values are read from the assigned physical property data set. The density value is calculated from the molar density value.

## Legal Notices

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