Bulk Calculations – Solution BCS 3.0

Working Paper: Hydrogen (H_2) High Pressure Quantity Conversions

Notes

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

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

Contents

1. Introduction

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

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.

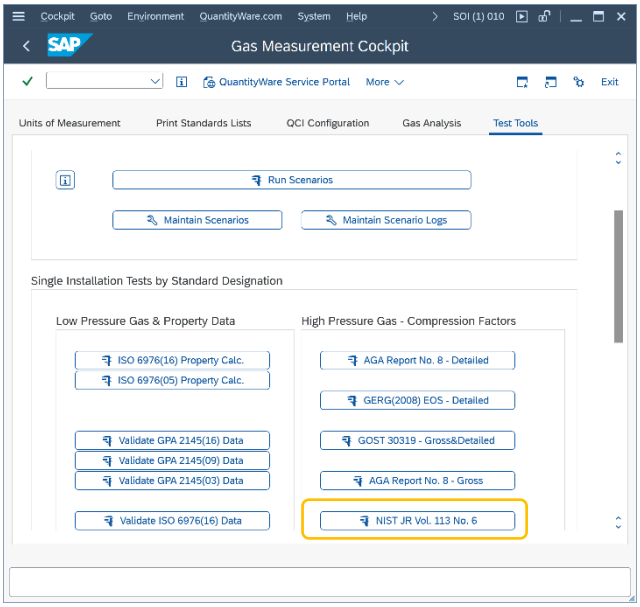
3. High Pressure Hydrogen – Measurement Standard

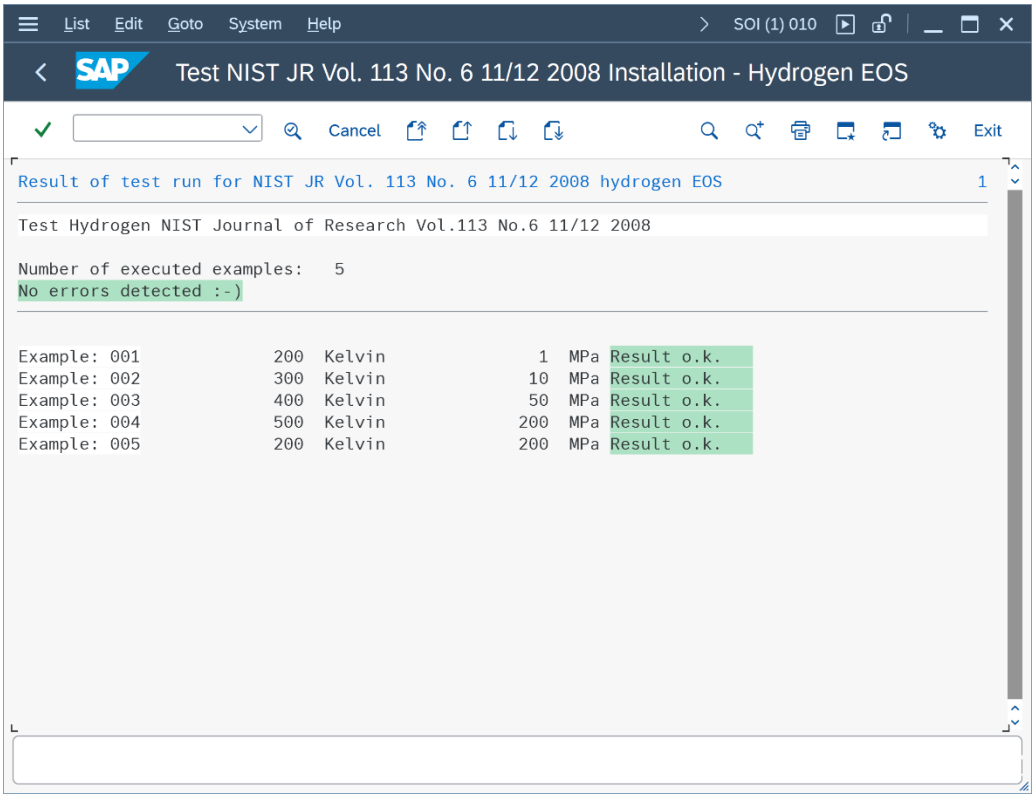
A complete and well defined measurement standard defining all required quantity conversions - including a precise implementation instruction – for high pressure H_2 calculations is not currently available. To provide a scientifically-based solution to meet the industries' needs, QuantityWare thus implemented 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_2 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	ρ(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

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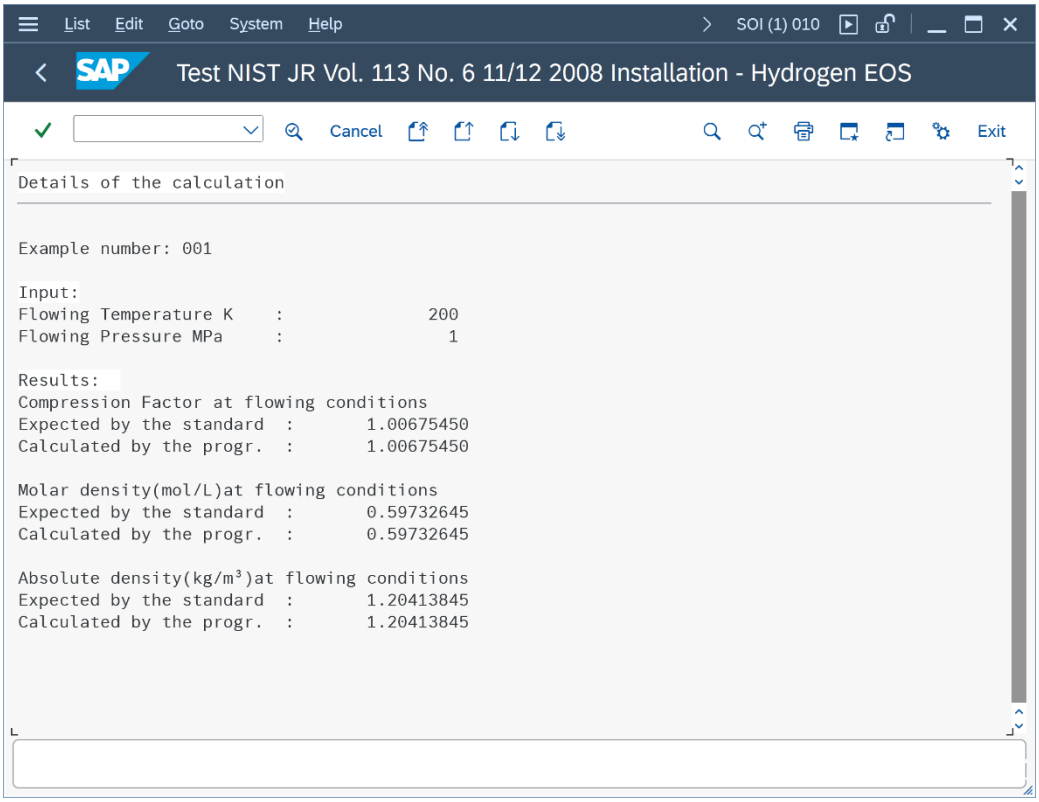
SOI (1) 010
Test NIST JR Vol. 113 No. 6 11/12 2008 Installation - Hydrogen EOS
Cancel
Exit
Result of test run for NIST JR Vol. 113 No. 6 11/12 2008 hydrogen EOS 1
Test Hydrogen NIST Journal of Research Vol.113 No.6 11/12 2008
Number of executed examples: 5
No errors detected :-)
Example: 001 200 Kelvin 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.


List Edit Goto System Help
SOI (1) 010
Test NIST JR Vol. 113 No. 6 11/12 2008 Installation - Hydrogen EOS
Cancel
Exit
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

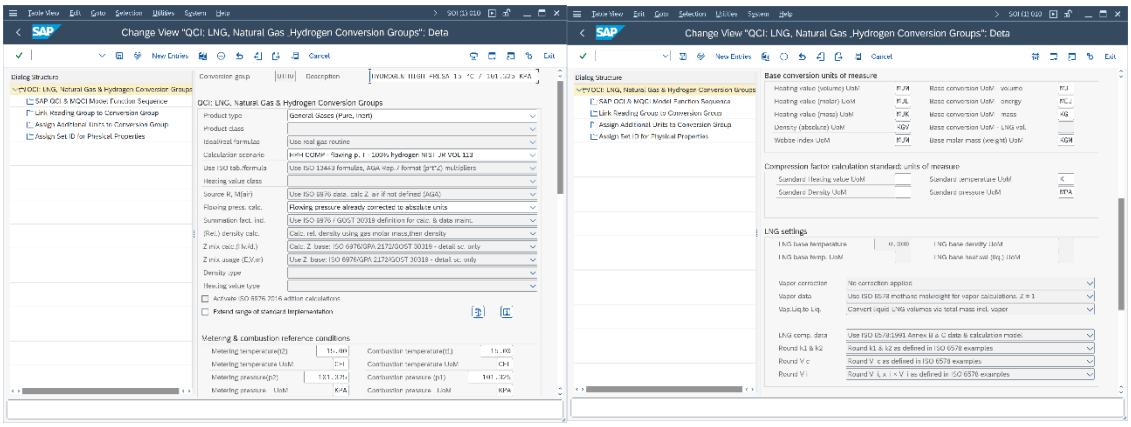
4. Configuration Details

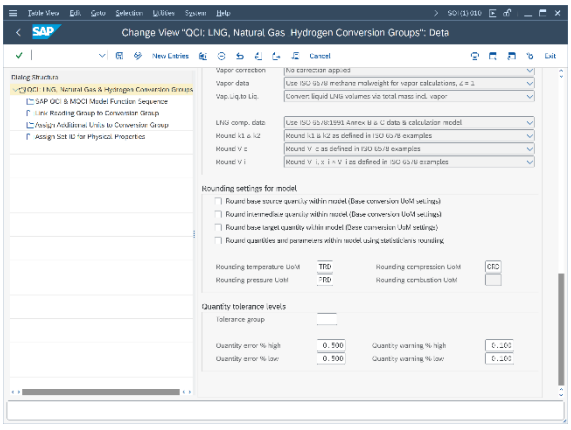
- For hydrogen, the existing SAP QCI product type:

  B General Gases (Pure, Inert)

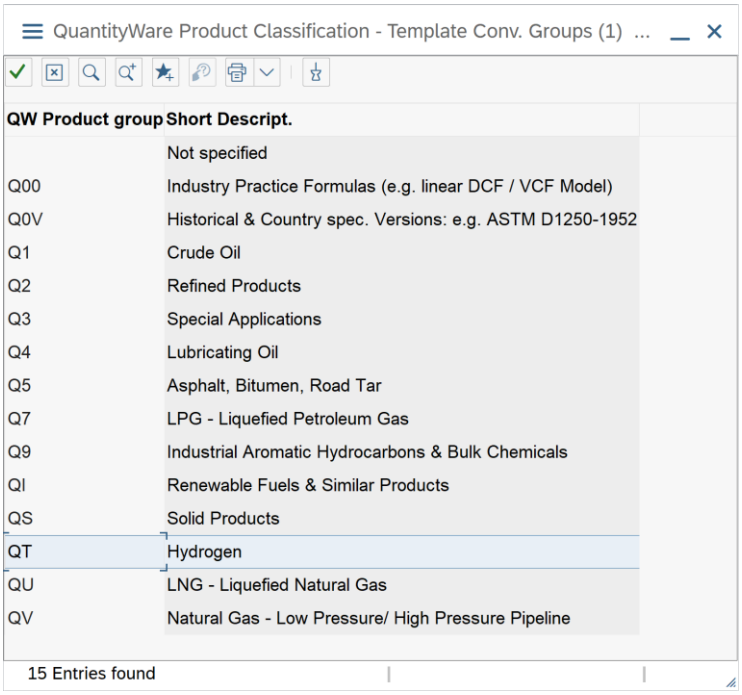
is utilized. This required extension of the natural gas/LNG conversion groups customizing transaction allows selection of this product types' conversion groups for maintenance and exclusion from the crude oil & products conversion group maintenance.

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





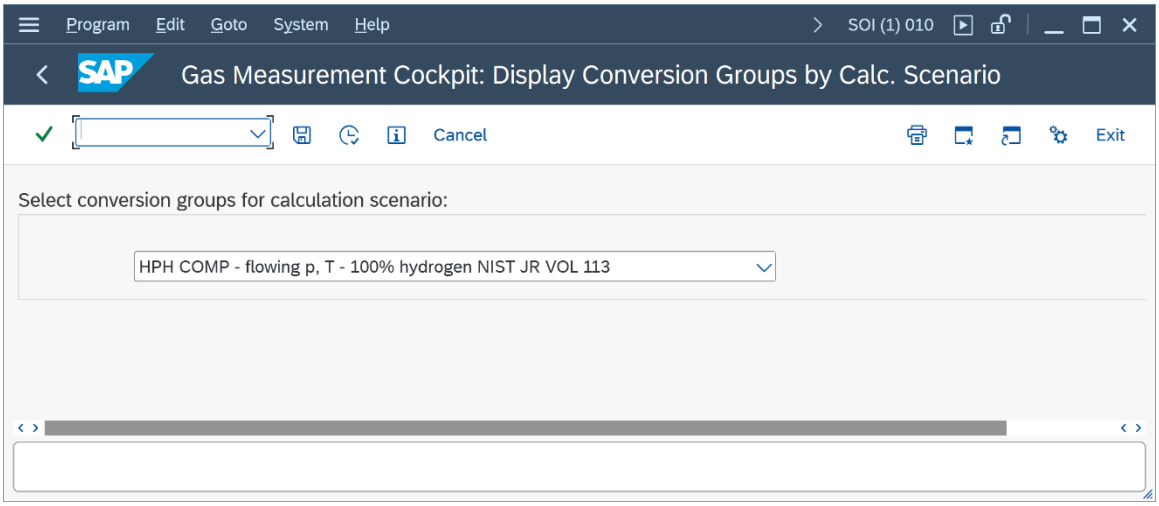
1. A new QuantityWare Product Group – QT - Hydrogen & Similar Products – has been defined:

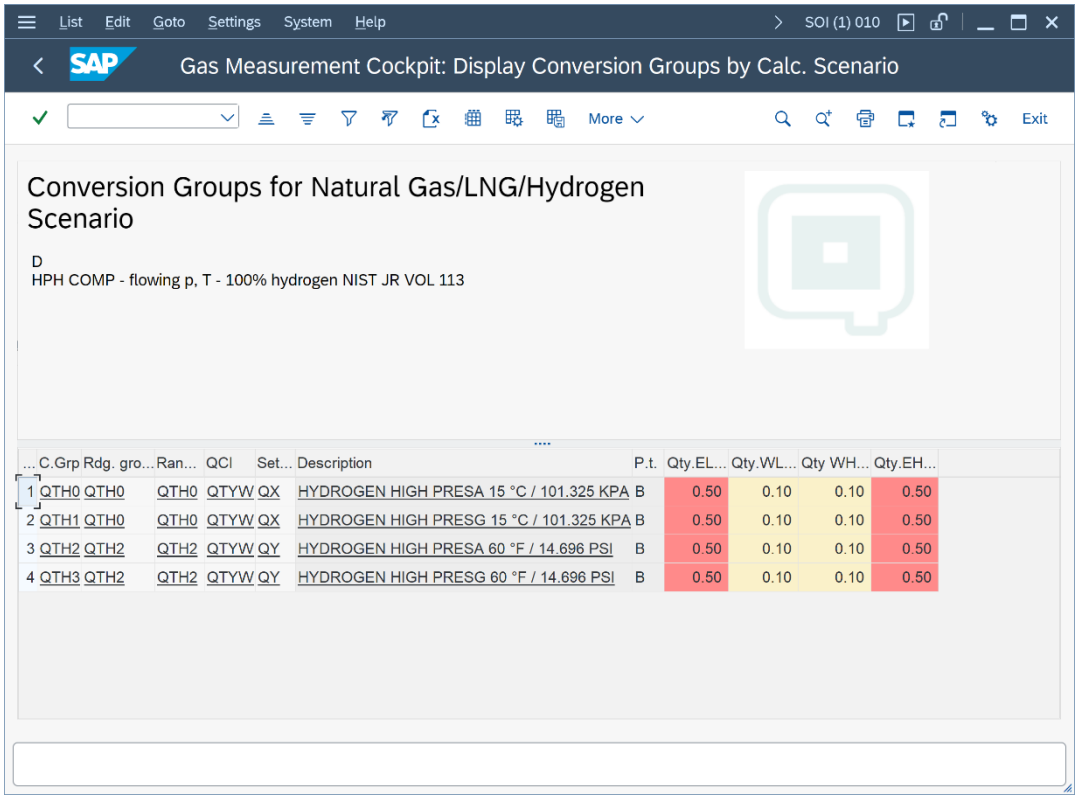


   - The new template conversion groups for hydrogen will start with **QT**

2. A new hydrogen calculation model has been developed.

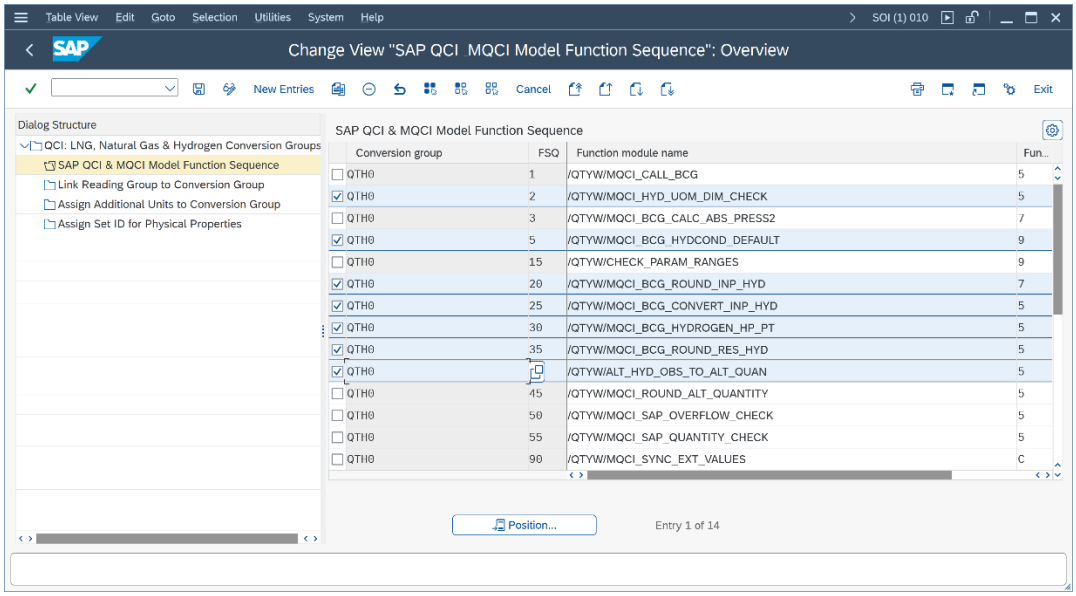
3. A new calculation scenario has been defined, which requires a new scenario function (/QTYW/MQCI_BCG_HYDROGEN_HP_PT) that implements all physical property parameter calculations and correction factor calculations:

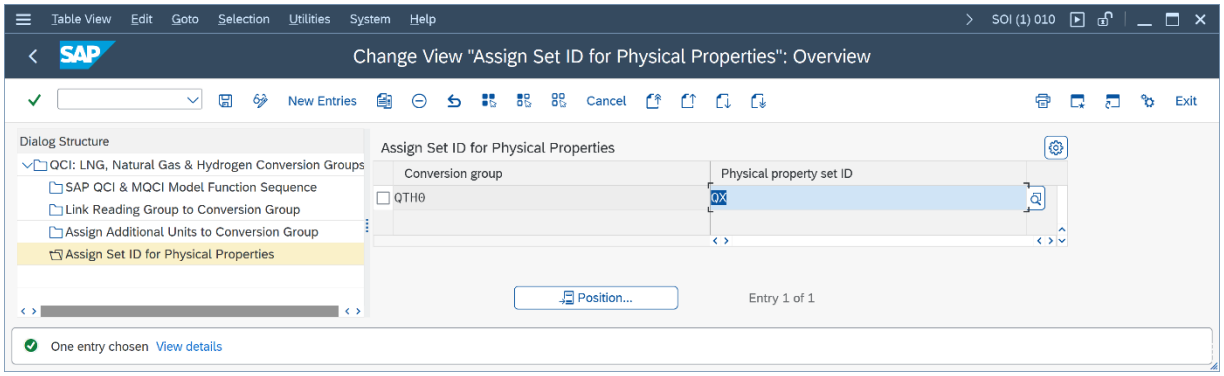




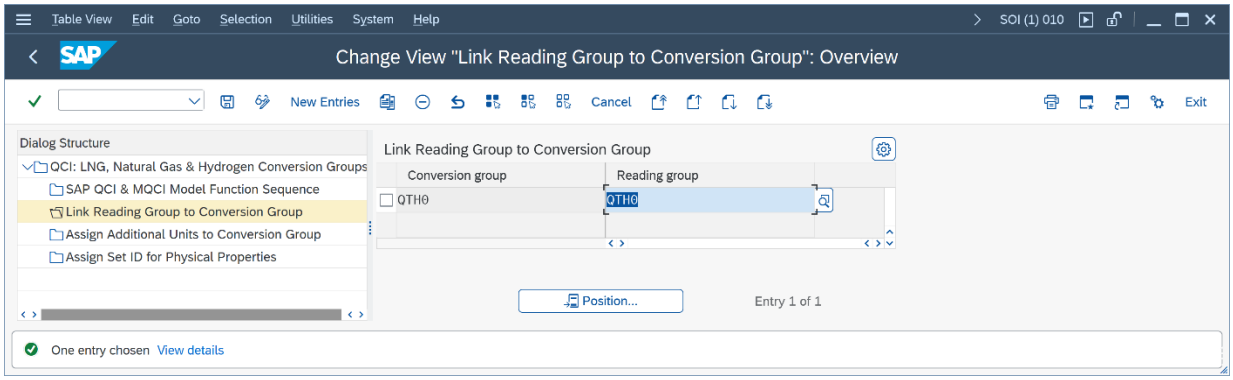
Four new template conversion groups are defined (and are delivered with the BCS 3.0 CSP in Q4 2023); two for the ISO base conditions (either absolute or gauge pressure input) and two for the U.S. customary base conditions (either absolute or gauge pressure input).

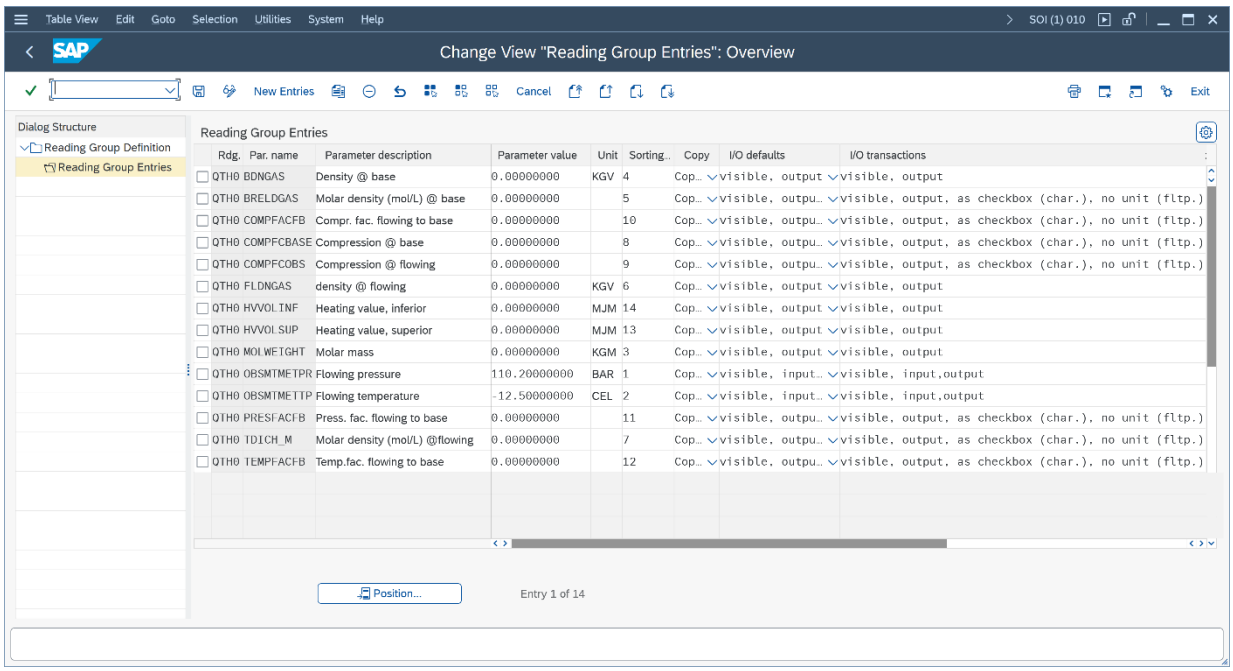
Configuration Example: 7 new hydrogen MQCI model functions have been developed:





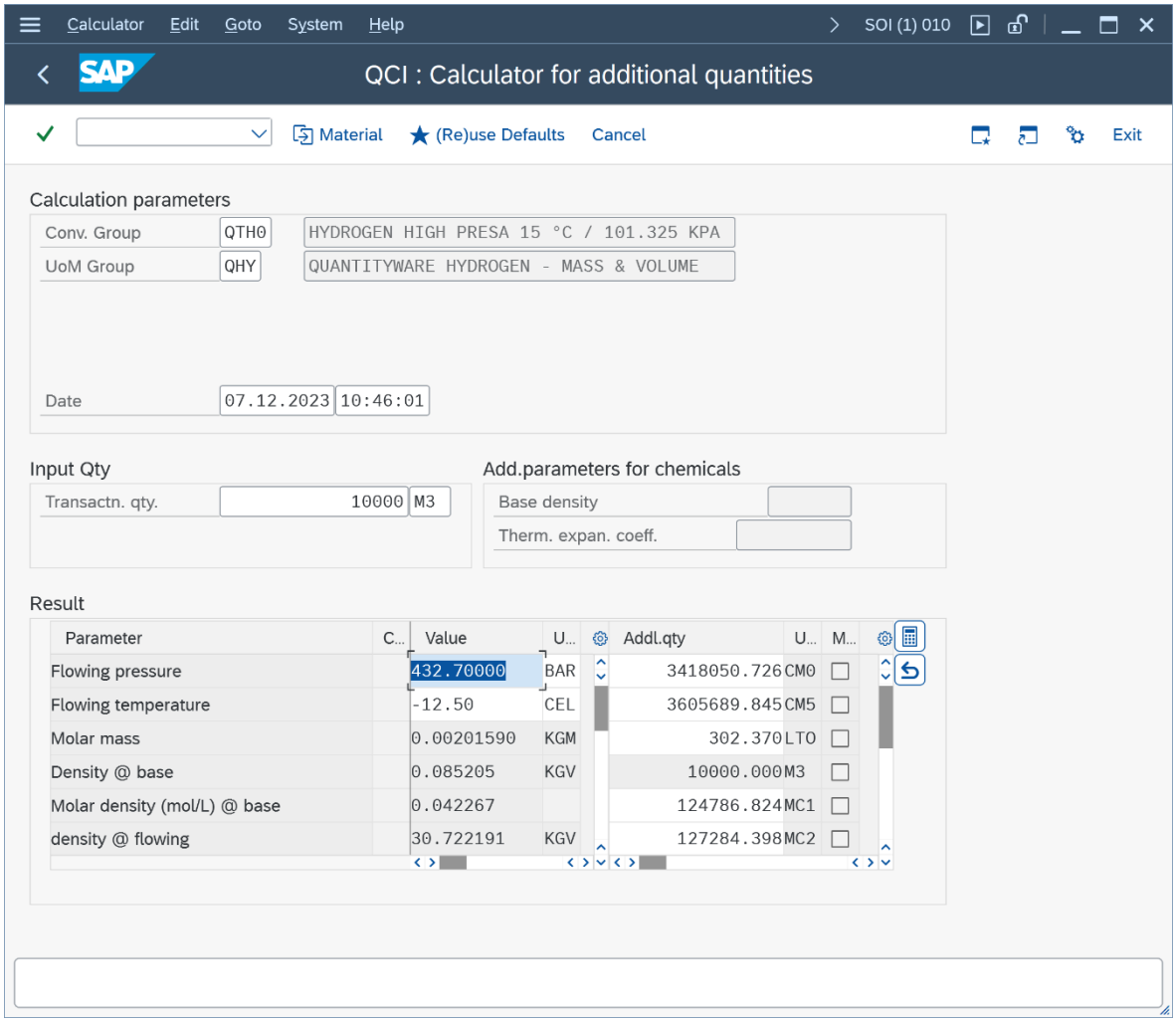
Note: The Physical property set contains hydrogen data only – e.g. from GPA 2145-16 (or other sources, depending on customer requirements)

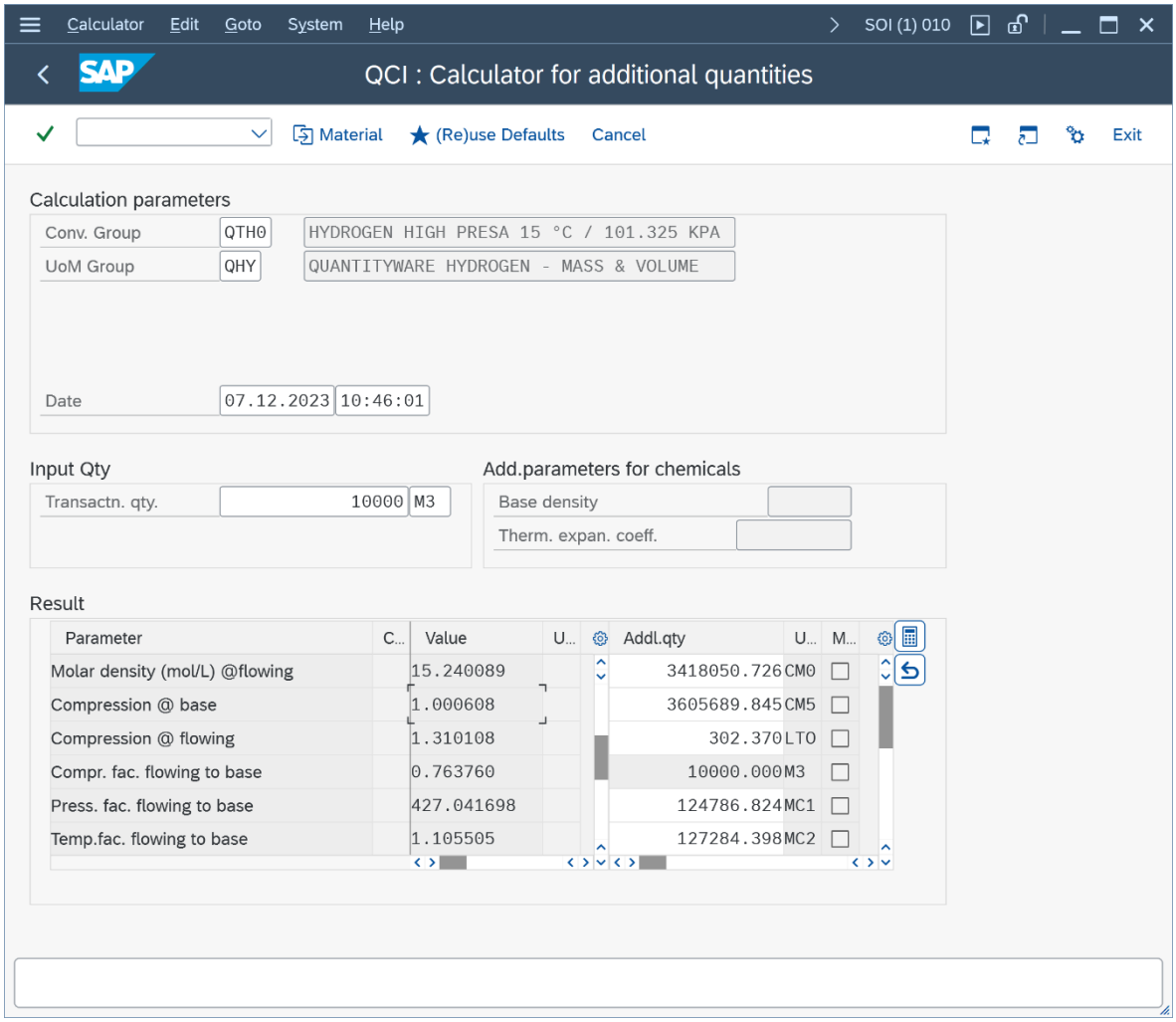




5. Calculation Scenario HPH 1 - Details

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:




Calculator Edit Goto System Help
SOI (1) 010
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...
Addl.qty
U...
M...
Molar density (mol/L) @flowing
15.240089
3418050.726
CM0
Compression @ base
1.000608
3605689.845
CM5
Compression @ flowing
1.310108
302.370
LTO
Compr. fac. flowing to base
0.763760
10000.000
M3
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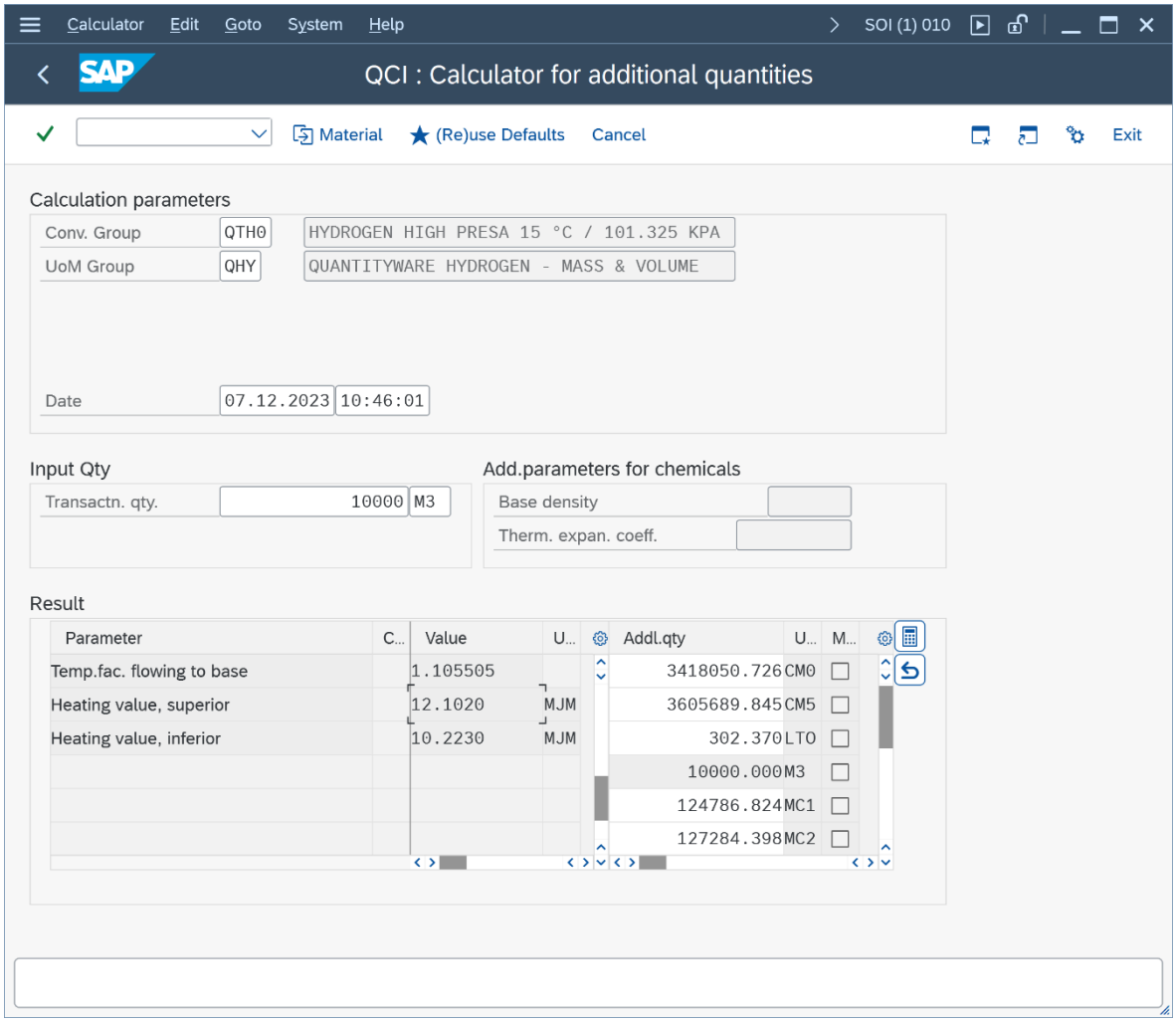
124786.824
MC1
Temp.fac. flowing to base
1.105505
127284.398
MC2



a. Calculation of molar densities and compression factors is achieved via the NIST function described above.

b. 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).

c. 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.

d. 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.

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