QuantityWare

QuantityWare Working Paper

Butadiene: Vapor Space and CTL Comparison Calculations

Comparison of calculation results from different Butadiene measurement standards

Version History

Version	Date	Description
00	2019-05-19	Initial Version
01	2021-09-25	Modern QW document style applied
02	2023-11-01	Editorial revision and confirmation

Contents

1. Introduction & Management Summary

As described in great detail in our working paper LPG Vapor Space Calculations, LPG (Liquefied Petroleum Gas) products need to be stored in closed containers (closed shore tanks, LPG tankers, tank trucks, pipelines, cylinders, etc.), otherwise rapid and total evaporation loss of the product quantity in gaseous form to the atmosphere would occur. This is due to the high vapor pressure (compared to atmospheric pressure at ambient temperatures) of LPG products. In closed containers, the product is thus typically present with a liquid and gaseous (vapor) phase at equilibrium vapor pressure. This is also true for a wide range of other light petrochemical products, e.g., Butadiene.

In this working paper, we compare the ideal gas calculation results for the gaseous (vapor) mass and weight - defined e.g. in ISO 6578 for LPG products - with the alternative approach defined for Butadiene in ASTM D1550 and discuss the differences.

Stock control measurements as well as opening and closing tank dips in large tanks subsequently utilize such calculations, allowing a precise determination of product quantities (e.g., transferred mass and weight quantities of product out of a tank).

To complete our investigations in this paper on Butadiene, we also provide comparison calculations for liquid volume CTL (Correction for the effect of Temperature on Liquid) table values as defined in ASTM D1550 with the CTL calculations defined for Butadiene in DIN 51757 (Y Tables).

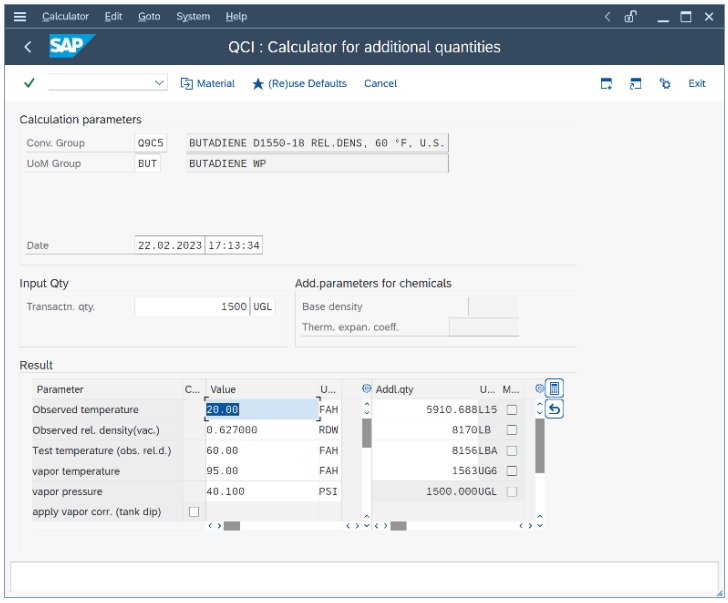
As demonstrated in this paper, different well-defined measurement-standard based calculations, applied to a single product, may lead to small, but noticeable differences of relevant product quantity values and properties. Thus, it is of utmost importance that business partners agree on a common measurement standard basis for their business transaction processes

Editorial Note:

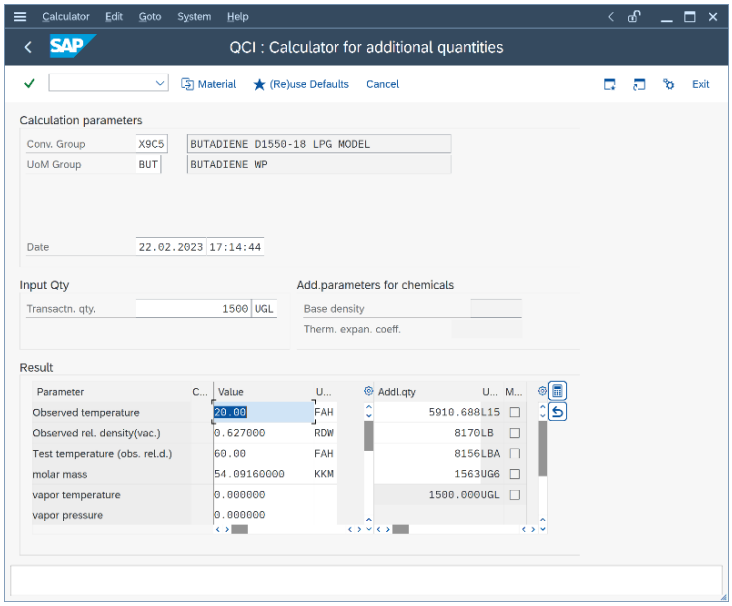
The decimal point and thousand separators for numbers and quantity values for this document are defined as follows: The decimal point is a dot '.', the thousand separator is a comma ','. Example: 123,456,789.987

2. Butadiene: Vapor Space Comparison Calculations

For the comparison calculations, two conversion groups are used, that are derived from our BCS template. Conversion group Q9C5 is the reference template conversion group based on ASTM D1550-2018:



Conversion group X9C5 is a copy of Q9C5, where we simply replace the ASTM D1550 vapor space calculation model function with the generic LPG ideal gas vapor space calculation model function and define the molar mass of Butadiene in the reading group.



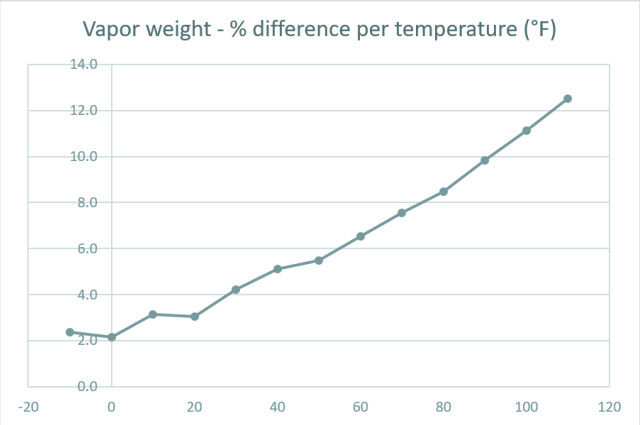
For the comparison calculations of the vapor space quantities, we define a tank capacity of 10,000 gallons in the reading group and utilize a liquid transaction volume quantity of 1,500 gallons. Then we vary the observed liquid volume temperature between -10 °F and 110 °F in 10 °F increments, with an identical vapor temperature variation. The vapor pressure (gauge value) is determined by ASTM D1550 through the vapor temperature (Table 3 in ASTM D1550-18). This gauge pressure value is easily converted to an absolute value, which is required for the LPG ideal gas vapor calculation model as an input value.

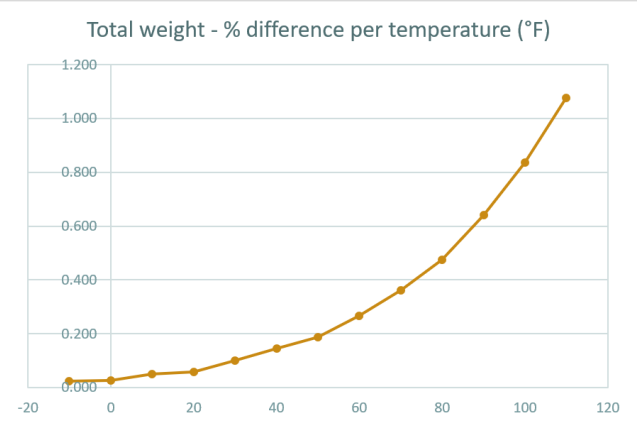
The following table lists the calculation results of both conversion groups for comparison - note that by design, both conversion groups calculate identical liquid weight and mass values if vapor space calculations are turned off.

Temp / °F	ASTM D1550 - total weight (lb)	LPG model - total weight (lb)	Liquid weight (lb)	ASTM D1550 vapor weight (lb)	LPG Ideal gas - vapor weight (lb)	Vapor weight – Difference (abs) (lb)	Vapor weight - % deviation	Total weight - % deviation
-10	8,477	8,475	8,391	86	84	2	2.4	0.023
0	8,421	8,418	8,313	108	106	2	2.2	0.027
10	8,369	8,365	8,234	134	130	4	3.1	0.049
20	8,322	8,317	8,156	166	161	5	3.0	0.059
30	8,281	8,273	8,078	203	195	8	4.2	0.099
40	8,238	8,226	7,992	247	235	12	5.1	0.146
50	8,209	8,194	7,913	296	280	15	5.5	0.188
60	8,180	8,158	7,827	353	331	22	6.5	0.265
70	8,160	8,131	7,741	419	390	29	7.6	0.362
80	8,148	8,110	7,655	493	454	39	8.5	0.475
90	8,139	8,087	7,561	578	526	52	9.8	0.640
100	8,148	8,081	7,475	673	606	67	11.1	0.835
110	8,161	8,075	7,381	780	693	87	12.5	1.075

(All pound(lb) values are rounded to 0 decimals; other values are rounded to the number of decimals displayed)

To illustrate these results, we print the vapor weight and total weight % deviations as a function of product temperature:



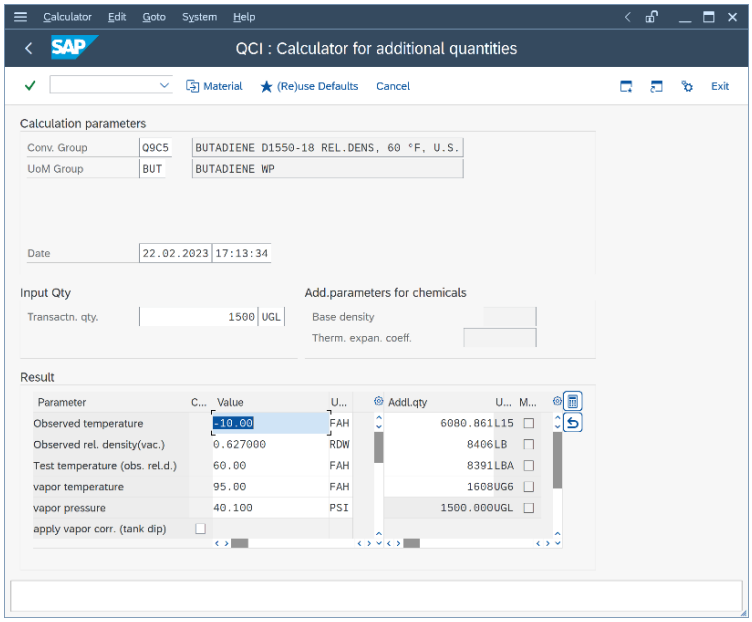


While the total weight deviations are considerably small for temperatures below 60 °F and only exceed the 1 % threshold for temperatures above 100 °F, the vapor weight differences display an almost linear increase from 2 % at low temperatures to 12 % at high temperatures.

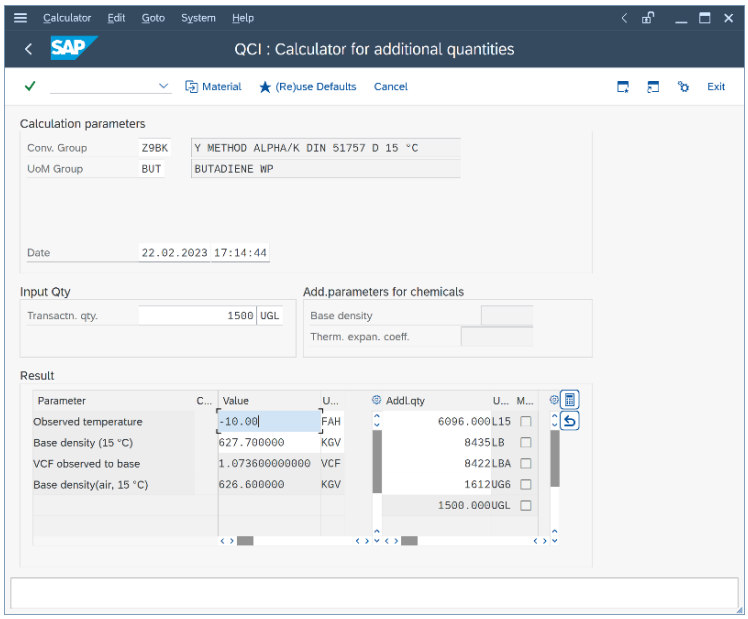
Apparently, the LPG ideal gas calculation model shows an increasing deviation (as expected) for higher temperatures, when compared with the (assumed) more realistic ASTM D1550 Butadiene specific "real gas" vapor data values.

3. Butadiene: CTL Comparison Calculations

For the CTL comparison calculations, we also utilize two conversion groups derived from our BCS template. Again, conversion group Q9C5 is the reference template conversion group based on ASTM D1550-2018.



Conversion group Z9BK is a copy of BCP template conversion group Q9BK with DIN 51757 calculation parameters defined for Butadiene:



For the comparison calculations of the CTL factor related quantities, we vary the observed liquid volume temperature between -10 °F and 110 °F in 10 °F increments and turn the vapor space calculations off. The following table summarizes the comparison calculation results for the quantity values of UoM LBA (lb, pound in air) and UG6 (gallon, ugl @ 60 °F):

Temp / °F	DIN 51757 lb	ASTM D1550 lb	Ratio lb in %	DIN 51757 ugl @ 60 °F	ASTM D1550 ugl @ 60 °F	Ratio ugl in %
-10	8,411	8,391	0.24	1,612	1,608	0.25
0	8,331	8,313	0.22	1,597	1,593	0.25
10	8,247	8,234	0.16	1,581	1,578	0.19
20	8,164	8,156	0.10	1,565	1,563	0.13
30	8,080	8,078	0.02	1,549	1,548	0.06
40	7,998	7,992	0.08	1,533	1,532	0.07
50	7,912	7,913	-0.01	1,516	1,517	-0.07
60	7,826	7,827	-0.01	1,500	1,500	0.00
70	7,740	7,741	-0.01	1,483	1,484	-0.07
80	7,654	7,655	-0.01	1,467	1,467	0.00
90	7,566	7,561	0.07	1,450	1,449	0.07
100	7,478	7,475	0.04	1,433	1,433	0.00
110	7,390	7,381	0.12	1,416	1,415	0.07

(All pound(lb) and gallon(ugl) values are rounded to 0 decimals; other values are rounded to the number of decimals displayed)

For both the pound (lb) values and the gallon @ 60 °F values, the differences between the two calculation models are rather small (0.25 % and lower), with largest deviations for very low temperatures. This suggests that the ASTM D1550 CTL table values have been derived with a model function which is like that defined in DIN 51757.

Since the DIN 51757 Butadiene conversion group calculates a CTL from observed to 15 °C, and the ASTM D1550 Butadiene conversion group calculates a CTL from observed to 60 °F, these two CTL cannot be directly compared.

However, if one considers that the DIN 51757 CTL from 60 °F to 15 °C is utilized to perform a second conversion from 15 °C to 60 °F by division, one can compile the following CTL comparison table, which explains the differences listed as % ratios in the table above.

Temp / °F	DIN 51757 CTL - observed to 15 °C	ASTM D1550 CTL - observed to 60 °F	DIN 51757 Combined CTL - observed to 60 °F	DIN 51757 CTL 60 °F to 15 °C
-10	1.0736	1.0720	1.07478	**0.99890**
0	1.0633	1.0620	1.06447	
10	1.0527	1.0520	1.05386	
20	1.0421	1.0420	1.04325	
30	1.0314	1.0320	1.03254	
40	1.0207	1.0210	1.02182	
50	1.0098	1.0110	1.01091	
60	0.9989	1.0000	1.00000	
70	0.9879	0.9890	0.98899	
80	0.9769	0.9780	0.97798	
90	0.9658	0.9660	0.96686	
100	0.9545	0.9550	0.95555	
110	0.9433	0.9430	0.94434	

(DIN 51757 CTL are calculated and rounded to 4 decimals; ASTM D1550 CTL are given as table values with 3 decimal accuracy - the combined DIN 51757 CTL is displayed with 5 decimals; the calculations utilize full floating-point accuracy)

In general, such differences are noticeable in business transactions by business users. Thus - as already stated in the introduction of this working paper - contractual agreements (or binding legal requirements), that define the measurement standard to be chosen for each product, are essential for business process calculations.

4. Conclusion

With QuantityWare BCS, vapor space and CTL calculations for Butadiene and LPG products can be easily integrated into your SAP Oil & Gas logistics transactions. The comparison calculations that we described briefly in this working paper are all reproduceable with QuantityWare BCS being installed in your system in your reference template client.

As shown by these comparison calculations, the question concerning such calculations is not how accurately the results of different measurement standard implementations match, but that business partners need to agree as to which measurement standards are to be utilized in which country for each of their bulk products.

Vapor space calculations update mass and energy values (in any UoM), but **not the volume quantities**, which always represents the liquid part of the product (ISO 6578 definition, business practice) - thus for your Butadiene and LPG products, you must use a **mass**, **weight** or **energy** UoM in the SAP material master if vapor space calculations are relevant, if valuation calculations within SAP ERP processes consider the total product quantity.

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