FUELLING CONFIDENCE

Adam Lomax, Joey Walker, and Jonathan Britain, EffecTech, consider the crucial role of reliable calibration gases in fiscal metering.

A medium-sized LNG terminal has the capacity to transfer up to 5 million tpy of LNG, which is approximately 7 billion m^3 of gas.[1] The measuring devices that determine the value of this gas should be set up to accurately report the total metered energy with a high degree of confidence to minimise fiscal risk during custody transfer. The critical importance of high-quality calibration gases with assigned low uncertainties in ensuring the highest level of confidence in total metered energy, is often overlooked. These reference materials are essential in reducing financial risks associated with fiscal flow metering.

The gas industry offers a wide variety of calibration gases with defined uncertainty levels that typically range from 0.1 – 5%. However, the impact on financial risk of the propagation of this uncertainty through the various calculations required for total energy determination, is not well understood. This article examines the effect of different quality calibration gases on fiscal risk, focusing on a hypothetical natural gas export meter transferring gas from an LNG terminal to a national transmission system.

The measurement of gas quality and volume are prerequisites for determining total metered energy.

A fiscal metering system consists of a flow element and a natural gas chromatograph (GC). Combining the measurements from both the flow and composition elements results in a total energy output described by the following equation:

$$E = \frac{HV\rho_L}{\rho_s}$$

Where:

- H is the gross volumetric calorific value at standard conditions (ISO 6976:2016).[2]
- ρ_s is the density at standard conditions (ISO 6976:2016).
- ρ_L is the density at line conditions (AGA 8).[3]
- V is the volume of gas at line conditions.

The first of the three inputs to the equation are determined from the gas composition, illustrating the importance of an accurate and reliable measurement from the GC.

Assessing the performance of gas chromatographs

The industry standard of assessing the performance of a GC is by carrying out an ISO 10723 performance evaluation.[4] This evaluation allows one to model the relationship between what the instrument thinks is correct and what is truly correct, allowing the errors in mismeasurement due to nonlinearity to be assessed. The model produced by the performance evaluation can be used to simulate the measurement of any gas composition within the standard's scope and output a measured composition with an associated uncertainty.

An ISO 10723 performance evaluation requires the measurement of a suite of reference gases which encompasses the expected measurement range of the instrument under test. First, the raw instrument response data is collected, then, using generalised least squared (GLS) regression (in accordance with ISO 6143[5]), a model of the instrument is generated. The model consists of:

- f, a function to calculate amount fraction from instrument response.
- g, a function to calculate instrument response from amount fraction.
- p, a function to calculate precision from amount fraction.

Assuming the instrument uses a typical single point through the origin calibration model, the measured amount fraction is given by:

$$x_{i,meas} = \frac{g(x_{i,true})}{g(x_{i,cal})} x_{i,cal}$$

The uncertainty on the measured composition is given by:

$$u(x_{i,meas}) = x_{i,meas}\sqrt{\left(\frac{u(x_{ical})}{x_{ical}}\right)^2 + \left(\frac{p\left(g(x_{i,true})\right)}{g(x_{i,true})}\right)^2 + \left(\frac{p\left(g(x_{i,cal})\right)}{g(x_{i,cal})}\right)^2}$$

The composition is then normalised in accordance with ISO 6974,[6] providing the inputs required for both ISO 6976 and AGA 8. The function (*f*) can be used to correct for nonlinearity within the GC, however that is beyond the scope of this paper.

The physical properties calculated in accordance with ISO 6976:2016 have well-defined analytical uncertainties included in the standard. The results of the simulation combined with the covariance calculated during normalisation gives the required uncertainties on the calorific value and the density at standard conditions.

However, the density at line conditions is calculated via an iterative root-finding approach that does not have an easily calculable analytical uncertainty, therefore necessitating the need for a Monte-Carlo approach. In this approach, the AGA 8 density is calculated for 10 000 sub-compositions; the uncertainty is then estimated from the standard deviation of the entire population of AGA 8 values.

Method for propagating calibration gas uncertainties

As this article is primarily concerned with propagation of the calibration gas uncertainty through the metering process, an uncertainty of 0.2% (k=2) relative for the metered volume will be used and the flow metering elements will be assumed to be fixed. Since the equation for the total energy is a simple product, the relative uncertainties of the variables can be added in quadrature to give the uncertainty in terms of energy.

For each simulation, a daily average volume flow of 20 million m^3 of gas was assumed, closely resembling that of a medium-sized LNG terminal. The calculated uncertainties for total metered energy were converted to a monetary uncertainty assuming a natural gas spot price of US$3/million Btu.[7]

This work utilised data from a real ISO 10723 performance evaluation of a GC that demonstrated an acceptable bias and uncertainty based on the UK's national transmission system benchmarks.

In this example, 10 000 gas compositions were produced using a bespoke software. The software ensures that 'real' gas compositions are produced by enforcing specific mixing rules based on a statistical analysis carried out on 10 000 real gas compositions measured within the UK transmission system.

The model of the GC requires a calibration gas composition and uncertainty input; therefore, it is possible to see how altering the uncertainty of the calibration gas affects the total metered energy uncertainty. A bespoke piece of software was developed to allow rapid iteration of gas compositions with a wide range of possible gases to be simulated. The data presented is based on a random data set of 10 000 gas compositions. For repeat simulations, the same seed was used to ensure reproducibility. This allows the effect of different calibration gas uncertainties to be assessed throughout the measurement process by fixing all other parameters.

For the AGA 8 calculation, an additional 10 000 sub-compositions were generated for each of original 10 000 gas compositions; allowing the uncertainty to be estimated from the standard deviation of the entire population of AGA 8 values.

Table 1 displays the simulated gas range which covers a broad range of gas compositions based on that expected for the UKs national transmission system (NTS).[8] The data is based on a single GC model and calibration gas composition, the only variable is the calibration gas uncertainty.

Table 2 shows the five sets of calibration gas uncertainties that will be trialled. The first two sets represent mixtures produced by an accredited calibration laboratory with rigorous uncertainty budgets. The uncertainties represent the calibration and measurement capability (CMC) for two classes of mixture; a primary reference gas mixture (PRGM) and calibration gas mixture (CGM). The other three gas mixtures (GM) A, B, and C represent lower quality mixtures, which have had blanket uncertainties applied to all components, an expanded uncertainty of 1%, 2%, and 5% was selected to cover the range of gas mixtures available on the market.

The method of how total metered energy uncertainty is decided is illustrated in Figure 1.

Table 1. Gas simulation range and calibration gas composition used in the Monte-Carlo assessment

Component	Units	Minimum	Maximum	X
Nitrogen	%mol.mol^{-1}	0	10.0000	4.4940
Carbon dioxide	%mol.mol^{-1}	0	7.0000	3.3135
Methane	%mol.mol^{-1}	78	100.000	80.378
Ethane	%mol.mol^{-1}	0	12.0000	7.0430
Propane	%mol.mol^{-1}	0	7.0000	3.3290
Iso-butane	%mol.mol^{-1}	0	1.00000	0.49990
N-butane	%mol.mol^{-1}	0	1.00000	0.50160
Neo-pentane	%mol.mol^{-1}	0	0.1500	0.10957
Iso-pentane	%mol.mol^{-1}	0	0.3500	0.11031
n-pentane	%mol.mol^{-1}	0	0.3500	0.10964
n-hexane	%mol.mol^{-1}	0	0.3500	0.11060

Results and discussion

Figure 2 shows the risk profiles for each calibration gas, and this is represented by the uncertainty on the total metered energy cost at a confidence interval of 95%. Each point represents a composition and its associated risk. For example, the point (90.256, 11 000) represents a composition with 90.256% methane and an uncertainty of US$11 000, so the total metered energy would have a value of US$2 721 000 ± US$11 000, this means that with 95% confidence the true value of the metered energy will be US$2 710 000 – US$2 732 000. The lower the uncertainty the tighter this band will be, and hence the lower the risk.

The risk profile has contributions from the flow and composition/property uncertainties, similarly the composition/property uncertainties have several sources; the precision of the instrument, the uncertainties on constants used during the calculation of properties and the calibration gas uncertainties. All sources other than

Table 2. Calibration gas categories used in the Monte-Carlo assessment

			Calibration gas type									
			PRGM (CMC)		*CGM (CMC)*		*GM-A (1% U)*		*GM-B (2% U)*		*GM-C (5% U)*	
Component	**Units**	**x**	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*
Nitrogen	%mol.mol^{-1}	4.4940	0.0057	0.13%	0.0117	0.26%	0.0449	1.00%	0.0899	2.00%	0.2247	5.00%
Carbon dioxide	%mol.mol^{-1}	3.3135	0.0034	0.10%	0.0061	0.18%	0.0331	1.00%	0.0663	2.00%	0.1657	5.00%
Methane	%mol.mol^{-1}	80.378	0.015	0.02%	0.030	0.04%	0.804	1.00%	1.608	2.00%	4.019	5.00%
Ethane	%mol.mol^{-1}	7.0430	0.0087	0.12%	0.0176	0.25%	0.0704	1.00%	0.1409	2.00%	0.3522	5.00%
Propane	%mol.mol^{-1}	3.3290	0.0050	0.15%	0.100	0.30%	0.0333	1.00%	0.0666	2.00%	0.1665	5.00%
Iso-butane	%mol.mol^{-1}	0.49990	0.00090	0.18%	0.00150	0.30%	0.00500	1.00%	0.01000	2.00%	0.02500	5.00%
n-butane	%mol.mol^{-1}	0.50160	0.00090	0.18%	0.00150	0.30%	0.00500	1.00%	0.01000	1.99%	0.02510	5.00%
Neo-pentane	%mol.mol^{-1}	0.10957	0.00040	0.37%	0.00090	0.82%	0.00110	1.00%	0.00220	2.01%	0.00550	5.00%
Iso-pentane	%mol.mol^{-1}	0.11031	0.00030	0.27%	0.00070	0.63%	0.00110	1.00%	0.00220	1.99%	0.00550	5.00%
n-pentane	%mol.mol^{-1}	0.10964	0.00030	0.27%	0.00060	0.55%	0.00110	1.00%	0.00220	2.01%	0.00550	5.00%
n-hexane	%mol.mol^{-1}	0.11060	0.00060	0.54%	0.00120	1.08%	0.00110	1.00%	0.00220	1.99%	0.00550	5.00%

the calibration gas uncertainty were kept constant for all risk profiles so any differences are caused by the calibration gas alone.

There is significant overlap between the PRGM and CGM – this indicates that the contribution from the calibration gas is small, and the other sources of uncertainty dominate the final risk profile. For GM-A, the calibration gas uncertainty is a significant contributor to the risk profile and for GM-B and GM-C, the calibration gas uncertainty is discernibly the dominant source of uncertainty for the risk profile.

Table 3 represents a single gas composition taken as a snapshot from Figure 2 (marked as example composition on Figures 2a and 2b) when measured with each of the calibration gas uncertainties from Table 1. The table includes the uncertainties on both the composition and physical properties. The properties marked with a † are dependent on flow; the remaining properties are independent of flow.

For the physical properties calculated from composition, both PRGM and CGM uncertainties have low contributions to the overall measured uncertainties. The dominant uncertainty contribution here is the precision of the instrument. However, for GM-A, the contribution from the calibration gas uncertainties starts to become a major contributor to the measured uncertainties. Subsequently, for the GM-B and GM-C calibration gases, the dominant contributions to the measurement uncertainties are the calibration gas uncertainties.

For both PRGM and CGM calibration gases, the flow-dependent properties, energy and price, exhibit measurement uncertainties that are overwhelmingly dominated by the flow uncertainty. Looking at columns *PRGM %U(x)* and *CRM %U(x)* in Table 3, the flow uncertainty accounts for 0.2% of the total uncertainty budget, while the compositional uncertainties contribute a negligible 0.01%. Consequently, the impact on total energy metering uncertainty is negligible for these two calibration gas categories. In contrast, GM-A shows a significant contribution of 0.07% from compositional uncertainties to the overall uncertainty budget for total energy and price. For GM-B, the compositional uncertainties slightly outweigh those from flow, contributing 0.2% to the final uncertainty budget. For GM-C, the compositional uncertainties are the primary contributors to the total uncertainty, with a 0.69% contribution, significantly exceeding the flow uncertainty.

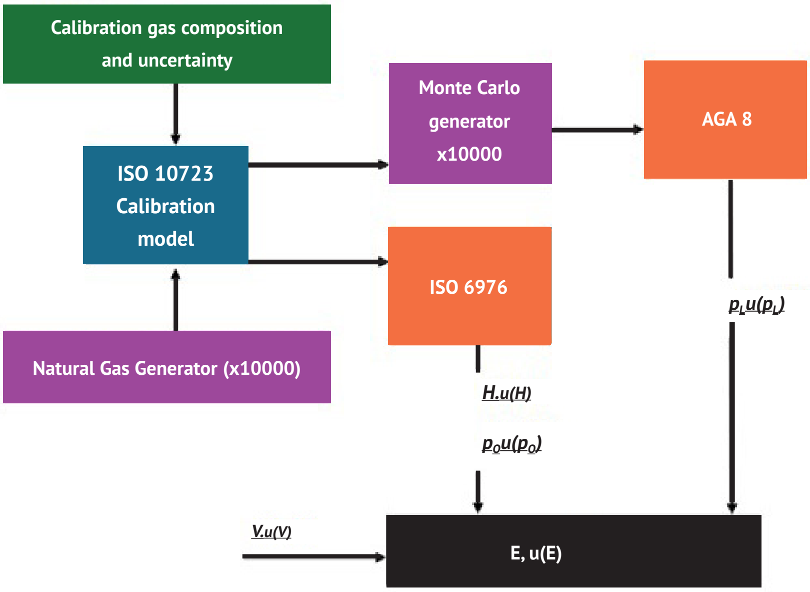

Figure 1. Inputs required to model the total metered energy uncertainty.

Conclusion

This article has demonstrated that calibration gas uncertainties play a significant role in reducing overall measurement uncertainty for total metered energy. By simulating different categories of calibration gases with real data, it was possible to show the impact of how those calibration gas uncertainties propagate through to

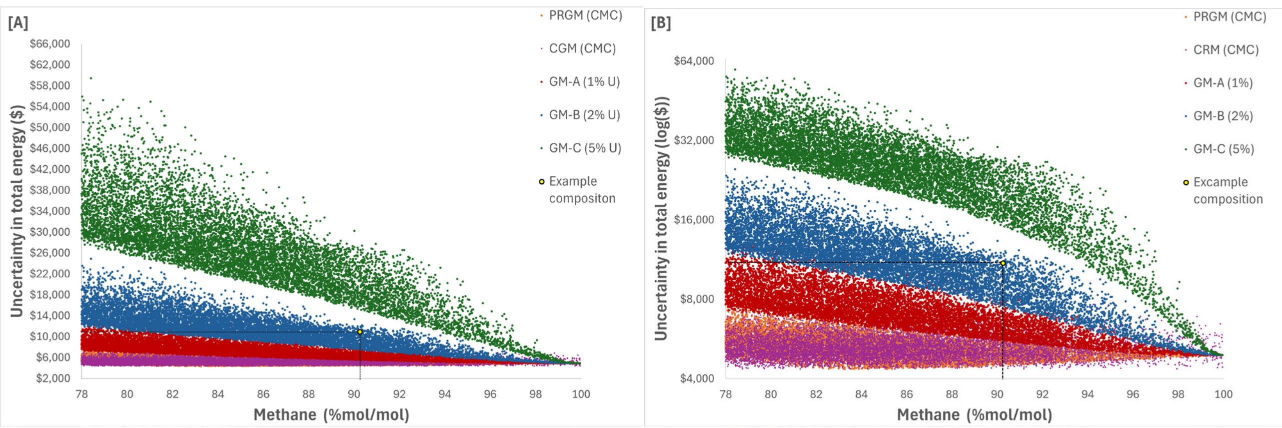

Figure 2. (a) monetary uncertainty (US$) for total metered energy with different quality calibration gases for 20 million m³ gas daily exported to NTS. (b) log plot of monetary uncertainty (US$).

physical properties and finally to total metered energy. The main conclusions that can be drawn from this work are:

- PRGMs have no real benefit to fiscal risk.
- GM-A, -B, and -C mixtures contribute significantly to fiscal risk with higher uncertainties leading to a substantial increase in risk.
- CGM mixtures reduce fiscal risk; the cost difference between a CGM and lower quality gas is less than the amount of risk introduced by using a lower quality gas.

These findings underscore the importance of selecting high-quality calibration gases to minimise fiscal risk and improve the reliability of energy metering, ultimately improving confidence in custody transactions. **LNG**

References

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Table 3. Uncertainty propagation through physical properties for a typical LNG gas composition for different category calibration gases

			Calibration gas type									
			PRGM (CMC)		*CGM (CMC)*		*GM-A (1% U)*		*GM-B (2% U)*		*GM-C (5% U)*	
Component	**Units**	**x**	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*	*U(x)*	*%U(x)*
Nitrogen	%mol.mol^{-1}	0.8821	0.0042	0.47%	0.0046	0.53%	0.0125	1.42%	0.0240	2.72%	0.0019	1.84%
Carbon dioxide	%mol.mol^{-1}	0.0000	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%
Methane	%mol.mol^{-1}	90.256	0.029	0.03%	0.032	0.04%	0.108	0.12%	0.211	0.23%	0.016	0.02%
Ethane	%mol.mol^{-1}	6.003	0.025	0.41%	0.027	0.46%	0.082	1.36%	0.158	2.64%	0.014	0.48%
Propane	%mol.mol^{-1}	1.4980	0.0046	0.31%	0.0060	0.40%	0.0204	1.36%	0.0403	2.69%	0.0031	0.45%
Iso-butane	%mol.mol^{-1}	0.6006	0.0022	0.37%	0.0027	0.45%	0.0083	1.38%	0.0163	2.71%	0.0007	1.44%
n-butane	%mol.mol^{-1}	0.5997	0.0022	0.37%	0.0027	0.45%	0.0083	1.38%	0.0162	2.71%	0.0010	2.03%
Neo-pentane	%mol.mol^{-1}	0.0000	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%
Iso-pentane	%mol.mol^{-1}	0.0804	0.0011	1.43%	0.0012	1.52%	0.0016	1.94%	0.0024	3.04%	0.0006	5.85%
n-pentane	%mol.mol^{-1}	0.0803	0.0014	1.77%	0.0015	1.84%	0.0018	2.21%	0.0026	3.21%	0.0011	10.49%
n-hexane	%mol.mol^{-1}	0.0000	0.000	0.00%	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%	0.0000	0.00%
Property	**Units**	***P***	*U(p)*	*%U(p)*	*U(p)*	*%U(p)*	*U(p)*	*%U(p)*	*U(p)*	*%U(p)*	*U(p)*	*%U(p)*
Gross CV	MJ.m^{-3}	41.208	0.018	0.04%	0.019	0.05%	0.040	0.10%	0.075	0.18%	0.182	0.44$
Net CV	MJ.m^{-3}	37.224	0.018	0.05%	0.018	0.05%	0.038	0.10%	0.070	0.19%	0.170	0.46%
Density standard	kg.m^{-3}	0.76343	0.00024	0.03%	0.00025	0.03%	0.00088	0.11%	0.00171	0.22%	0.00424	0.56%
Relative density		0.62295	0.00019	0.03%	0.00021	0.03%	0.00072	0.11%	0.00139	0.22%	0.00346	0.56%
Gross Wobbe	MJ.m^{-3}	52.210	0.020	0.04%	0.020	0.04%	0.027	0.05%	0.041	0.08%	0.092	0.18%
Molar mass	g.mol^{-1}	18.0055	0.0053	0.03%	0.0057	0.03%	0.0205	0.11%	0.0400	0.22%	0.0994	0.55%
Density line	kg.m^{-3}	52.947	0.016	0.03%	0.018	0.03%	0.054	0.10%	0.105	0.20%	0.261	0.49%
Energy †	TJ/total E	956.6	2.0	0.21%	2.0	0.21%	2.6	0.27%	3.9	0.40%	8.5	0.89%
Price †	M$/total E	2.721	0.006	0.21%	0.006	0.21%	0.007	0.27%	0.011	0.40%	0.024	0.89%