

Article

Credible Uncertainties for Natural Gas Properties Calculated from Normalised Natural Gas Composition Data

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Abstract: The evaluation of measurement uncertainty of natural gas properties calculated from composition data are an essential aspect of fiscal metering in the trade of natural gas. For conformity assessment, and in gas allocation, it is essential to have a reliable value for the uncertainty. This need is also reflected in, e.g., ISO 6976, the standard for computing natural gas properties, which follows the requirements of the “Guide to the expression of uncertainty in measurement” much more closely. Normalised compositions and their associated standard uncertainties do not suffice for this purpose. A novel algorithm is provided to recover these correlations from the normalised fractions and associated standard uncertainties, enabling the industry work with the data already stored in their repositories. The standard uncertainties are reproduced within 2%, which is acceptable for uncertainty calculations. The correlation coefficients obtained from the recovery algorithm agree with the ones obtained by normalisation.

Keywords: natural gas; ISO 6974; ISO 6976; calorific value; composition; correlation; measurement uncertainty; fiscal metering; custody transfer

1. Introduction

The calculation of natural gas properties is fundamental to the trade in natural gas. Many contracts in this area are energy-based, which means that the energy content (calorific value) of the gas transmitted plays as important a role as the volume or mass of natural gas [1–3]. The current edition of ISO 6976 [4], i.e., ISO 6976:2016, the documentary standard for calculating natural gas properties, takes on a more rigorous approach to the calculation of the measurement uncertainty of natural gas properties than its predecessor (ISO 6976:1995) [5]. ISO 6976:2016 takes the uncertainties associated with the pure substance enthalpies of combustion, the molar masses, and the compressibility factors of the components in natural gas at given reference pressure and temperature into account. Also, the propagation of the standard uncertainties and correlations of the natural gas are taken into account, as required by the Guide to the expression of Uncertainty in Measurement (GUM) [6,7].

Furthermore, credible values for natural gas properties such as the calorific value play an important role in studies into the effects of the blending of hydrogen with natural gas [8–10], obtaining an appropriate calorific value in engine combustion studies [11,12]. The need for normalised compositions with a complete uncertainty structure is not limited to the calorific value; however, obtaining a compressibility factor or density for the volume conversion in flow metering [1–3] is equally important. Equations of state used for this purpose, such as the GERG-2008 [13,14] and AGA-8 [15,16], also take a normalised composition as one of their inputs, and for evaluating the measurement uncertainty of the



Academic Editor: Patrick Da Costa

Received: 3 November 2024

Revised: 8 December 2024

Accepted: 17 December 2024

Published: 25 December 2024

Citation: Van der Veen, A.M.H. Credible Uncertainties for Natural Gas Properties Calculated from Normalised Natural Gas Composition Data. *Methane* **2025**, *4*, 1. <https://doi.org/10.3390/methane4010001>

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parameters calculated from these models, it is essential to propagate the uncertainty from the composition as well [14,17], including its full uncertainty structure [6,18].

Fundamental to the calculation of natural gas properties is the availability of the natural gas composition. In these calculations, the composition of natural gas is defined as a series of (normalised) amount fractions of all components. Normalised amount fractions are always correlated [19,20], but the uncertainty structure can be different. For instance, the composition calculated from gravimetric gas mixture preparation, ISO 6142 [21,22], has a different uncertainty structure than the composition measured using gas chromatography in accordance with ISO 6974 [23,24] after normalisation.

The transmission and distribution system operators responsible for the transport, trade, and distribution of natural gas generally record the normalised composition of the natural gas measured at gas metering stations [1]. These data alone do not suffice to duly evaluate the measurement uncertainty when calculating natural gas properties such as the calorific value or compressibility factor. Often, the standard uncertainties of the normalised amount fractions are known, for example, from the performance evaluation of the natural gas analyser in such metering stations [25]. Reverting to the raw (non-normalised) composition as obtained by the gas chromatograph [23,24] is impractical and, from the view point of data logistics, complicated. It would also require substantial extra data storage capacity. Where it is recommended to provide measurement results with an uncertainty, and where relevant, also with covariances (or, equivalently, correlation coefficients) [6,18,26], the practice is different. Yet, it can be readily shown that, in the case of natural gas properties, ignoring the correlations between the amount fractions of the components has a serious impact (see Section 3).

In many uncertainty calculations in metrology, it is impossible to recover covariances without having a detailed insight in the underlying measurement models and uncertainty calculations. In the case of natural gas composition data, it is fortunate that there is an agreed method to normalise the data (described in ISO 6974 [23,24]). Under the assumption that the normalisation method of ISO 6974 has been used, it is possible to recover the covariances from the normalised compositions and their associated standard uncertainties alone. The algorithm is presented in Section 2.

2. Normalisation of Composition

2.1. Normalised and Non-Normalised Amount Fractions

For use in calculations, the natural gas composition should meet the requirement of any composition, namely that the sum of all fractions forming it is exactly equal to a constant [19]. This condition can be expressed as

$$\sum_{j=1}^n x_j = \kappa, \quad (1)$$

where x_j denote the normalised amount fractions of the components j , and n the number of components. κ is the normalisation constant. When expressing amount fractions in mol mol^{-1} , $\kappa = 1 \text{ mol mol}^{-1}$, whereas when expressing these in cmol mol^{-1} , $\kappa = 100 \text{ cmol mol}^{-1}$, and so on [19].

A composition calculated from a (gravimetric) gas mixture preparation [21,27] always meets the normalisation constraint (Equation (1)), as it is inherent to the measurement equation used. Not all measurement procedures provide an amount fractions that sum exactly to the normalisation constant. When using compositional data from, e.g., a gas chromatographic determination, the constraint must be enforced by normalising the amount fractions. Amount fractions that do not meet the mathematical constraint of a composi-

tion are sometimes called “raw” amount fractions, to distinguish them from (normalised) amount fractions that satisfy the condition.

Ensuring that a composition expressed in amount fraction satisfies this condition can be achieved by using, e.g., the normalisation procedure from ISO 6974 [23,24], also known as closure of a composition [19]. The normalisation procedure is described in ISO 6974-1 [23], and the uncertainty calculation is given in ISO 6974-2 [24]. This procedure is the industry standard, but there are alternatives for carrying out normalisation [28]. Considering that the set of amount fractions forming a composition can be expressed as a vector, a convenient way to express the associated uncertainty information is in the form of a covariance matrix [18].

According to ISO 6974, the normalised amount fraction x_i is related to the raw amount fraction \tilde{x}_i as follows [23,24]:

$$x_i = \frac{\kappa \tilde{x}_i}{\sum_{j=1}^n \tilde{x}_j}. \quad (2)$$

The covariance matrix associated with the vector of the normalised amount fractions \mathbf{x} , \mathbf{U}_x , can be calculated from the covariance matrix $\mathbf{U}_{\tilde{x}}$ associated with the raw amount fractions as follows [18]:

$$\mathbf{U}_x = \mathbf{C} \mathbf{U}_{\tilde{x}} \mathbf{C}^T, \quad (3)$$

where the elements of the sensitivity matrix \mathbf{C} are given by [23,24]

$$C_{ii} = \frac{\kappa}{\Xi} - \frac{\kappa \tilde{x}_i}{\Xi^2}, \quad (4)$$

$$C_{ij} = -\frac{\kappa \tilde{x}_i}{\Xi^2} \quad (i \neq j), \quad (5)$$

and $\Xi = \sum_{j=1}^n \tilde{x}_j$. This calculation in matrix form is identical to the calculation given in ISO 6974 [23,24].

The covariance matrix of a normalised composition has some special features. In each row (and column), the elements of \mathbf{U}_x add to zero, which is a property of the uncertainty of a composition [19]. Considering that κ in Equation (1) is a constant without uncertainty, the uncertainty of the sum of all normalised amount fractions should also be zero. Equation (6) is a convenient way to verify whether the covariance matrix of a composition is valid for use in uncertainty calculations [19]. The right-hand side of Equation (6) calculates the variance of the sum of the normalised amount fraction. In matrix form, this check can be performed by verifying whether

$$\mathbf{1}^T \mathbf{U}_x \mathbf{1} = 0, \quad (6)$$

where $\mathbf{1}$ denotes a column vector of length n , whose elements are all 1. This vector $\mathbf{1}$ is holding the sensitivity coefficients in the summation of the normalised amount fractions (see Equation (1)).

2.2. Recovery Algorithm for the Covariances in a Normalised Composition

The calculations in the previous section demonstrate that there are, at least a priori, cogent reasons for taking the correlations between the amount fractions in a normalised composition into account. Current industry practice is, however, that the normalised natural gas compositions are recorded and transmitted, and that the standard uncertainties associated with the fractions of the components are known from, e.g., validation of the analysis methods or the performance evaluation of the online natural gas analysers (see also ISO 10723 [25]). Usually, it is impossible to retrieve the full uncertainty structure of a set of variables from their values and standard uncertainties only.

In the case of a normalised composition, however, it is possible to reconstruct the covariance matrix to a degree that it is suitable for the uncertainty calculations in ISO 6976 [4],

provided that the normalisation was carried out as described in ISO 6974 [23,24]. In this work, this conventional normalisation ([23], Definition 3.19) is chosen, as it is among the commonest methods applied in industry. The algorithm outlined shortly involves some matrix algebra, as a set of linear equations needs to be solved. As the emphasis of the modelling is on putting calculations into software systems, this is not considered a practical obstacle for its use.

The reconstruction of the covariance matrix is based on the considerations discussed in Section 2. The expressions for the sensitivity coefficients (see Equations (4) and (5)) require the raw sum Ξ and the raw amount fractions \tilde{x}_i . These are, however, unknown when only normalised fractions are at hand, but they can be approximated by $\Xi \approx \kappa$ and $\tilde{x}_i \approx x_i$ for all components i . These approximations are sufficient for the uncertainty calculation, but obviously not to provide values for the raw amount fractions. Only when the raw sum Ξ were known, these raw fractions can be reconstructed as well, and there would be no need to approximate the sensitivity matrix C using Equations (8) and (9).

The first step in the recovery algorithm is to calculate the variances (squared standard uncertainties) associated with the raw amount fractions. These are related to the variances of the normalised ones through Equation (3). For $u^2(x_k)$, this relationship reads as

$$u^2(x_k) = \sum_{j=1}^n C_{kj}^2 u^2(\tilde{x}_j), \quad k = 1, \dots, n. \quad (7)$$

The sensitivity coefficients can be approximated by

$$C'_{ii} \approx 1 - \frac{x_i}{\kappa}, \quad (8)$$

$$C'_{ij} \approx -\frac{x_i}{\kappa}, \quad (i \neq j), \quad (9)$$

which follows from Equations (4) and (5) by considering that $x_i \approx \tilde{x}_i$ for all i and $\Xi \approx \kappa$. Substituting Equations (8) and (9) into the n Equations (7) leads to a set of n linear equations where the $u^2(\tilde{x}_j)$ are the unknowns. This set can be represented as

$$A v_{\tilde{x}} = v_x, \quad (10)$$

where $v_x = (u^2(x_1), \dots, u^2(x_n))^T$, and $v_{\tilde{x}} = (u^2(\tilde{x}_1), \dots, u^2(\tilde{x}_n))^T$. The elements of the matrix A are $A_{ij} = C'_{ij}{}^2$, where C' is given by Equations (8) and (9).

The solution of Equation (10) is given by $v_{\tilde{x}} = A^{-1}v_x$, but directly inverting the matrix A is not the best way of solving a set of linear equations. The set can better be solved using a stable numerical method, such as QR-factorisation or singular value decomposition [29]. Using QR-factorisation for example, compute first the factorisation

$$A = QR$$

where Q is an orthogonal matrix and R an upper triangular matrix. Then, compute

$$v'_x = Q^T v_x$$

and then solving

$$R v_{\tilde{x}} = v'_x \quad (11)$$

by back substitution ([30], Section 2.4). In R [31], the solution of the set of linear Equation (10) can be obtained by a call to the function `qr.solve()` with the matrix A and vector v_x as arguments (see Appendix A).

Once the vector $v_{\tilde{x}}$ is obtained, it can be converted to (an approximation of) the diagonal covariance matrix $U_{\tilde{x}}$ and used in Equation (3) to obtain the full covariance matrix U_x .

3. Results

The recovery algorithm for the covariance matrix of the composition (see Section 2.2) has been implemented in R [31]. The default solver for a set of linear equations is using the QR-factorisation. Consider the simple raw composition in Table 1. The standard uncertainties in this example are not intended to represent typical performance, let alone state-of-the-art natural gas measurement results. The increase in the relative standard uncertainties from methane (CH₄) to propane (C₃H₈), as well as those for nitrogen and carbon dioxide, represent a typical uncertainty structure for a composition measurement of natural gas. The sum of the amount fractions is $\Xi = 99.034 \text{ cmol mol}^{-1}$.

Table 1. Non-normalised composition of a natural gas containing 5 components, expressed in amount fractions (cmol mol^{-1}).

Component	\tilde{x} cmol mol^{-1}	$u(\tilde{x})$ cmol mol^{-1}	$u_{\text{rel}}(\tilde{x})$
Nitrogen	3.248	0.021	0.65 %
Carbon dioxide	2.398	0.018	0.75 %
Methane	83.520	0.209	0.25 %
Ethane	6.523	0.044	0.67 %
Propane	3.345	0.113	3.38 %

To illustrate the recovery algorithm, the normalised composition computed from the data in Table 1 is used, i.e.,

$$\begin{aligned} x^{\text{T}} &= (3.280, 2.421, 84.335, 6.587, 3.378), \\ v_x^{\text{T}} &= (0.022^2, 0.019^2, 0.111^2, 0.044^2, 0.110^2). \end{aligned}$$

Solving the set of linear equations yields

$$v_{\tilde{x}}^{\text{T}} = (0.021^2, 0.018^2, 0.209^2, 0.044^2, 0.113^2),$$

which are the recovered standard uncertainties associated with the raw amount fractions. The relative difference between the standard uncertainties associated with the raw amount fractions thus recovered and the original ones (see Table 1) is -0.97% , which is acceptable for an uncertainty calculation. The covariance matrix U_x computed with the recovered values for the standard uncertainties differs negligibly from that computed directly from the data in Table 1. The performance of this recovery algorithm depends on the value of the raw sum Ξ . In most practical cases, the raw sum is $98 \text{ cmol mol}^{-1} \leq \Xi \leq 102 \text{ cmol mol}^{-1}$, which is close enough to $100 \text{ cmol mol}^{-1}$ for using this recovery algorithm. An R-script reproducing these calculations is shown in Appendix A.

The correlation matrices after normalisation and from recovery are shown in Table 2. The values of the correlation coefficients are identical up to four digits, which is more than sufficient for accepting the outcome of the recovery algorithm for an uncertainty evaluation [26,32].

Table 2. Correlation matrices of the normalised composition (upper triangle) and from recovery (lower triangle).

Component	N ₂	CO ₂	CH ₄	C ₂ H ₆	C ₃ H ₈
N ₂	1	0.0635	-0.0703	0.0367	-0.1543
CO ₂	0.0635	1	-0.0605	0.0320	-0.1341
CH ₄	-0.0703	-0.0605	1	-0.2531	-0.8782
C ₂ H ₆	0.0367	0.0320	-0.2531	1	-0.1609
C ₃ H ₈	-0.1543	-0.1341	-0.8782	-0.1609	1

In Table 3, a comparison is shown for selected natural gas properties calculated from ISO 6976, i.e., the molar calorific value, molar mass, the compressibility factors, and the calorific values on a mass and volume (real gas) basis for the three cases: (1) with the covariance matrix from normalisation according to ISO 6974, (2) with the reconstituted covariance matrix, and (3) without covariances. The composition of the natural gas is given in Table 1. The metering and combustion temperatures are both 15 °C, and the reference pressure is 101.325 kPa.

Table 3. Calculation of natural gas properties with correlations, using the recovered correlation matrix, and without correlations. Shown are the molar superior calorific value (H , kJ mol⁻¹), molar mass (\bar{M} , g mol⁻¹), compressibility factor (Z), superior calorific value on a mass basis (H_m , MJ kg⁻¹), and on volume basis for a real gas (\tilde{H} , MJ m⁻³).

	With Correlations		Recovery		Without Correlations	
	x	$u(x)$	x	$u(x)$	x	$u(x)$
H	929.8	1.5	929.8	1.5	929.8	2.7
\bar{M}	18.984	0.030	18.984	0.030	18.984	0.055
Z	0.997448	0.000045	0.997448	0.000045	0.997448	0.000048
H_m	48.977	0.030	48.977	0.030	48.977	0.20
\tilde{H}	39.423	0.065	39.423	0.065	39.423	0.117

The calculated values are identical in all three scenarios. The calculated standard uncertainties with and without correlations are mostly vastly different. The only exception is the compressibility factor Z , for which the standard uncertainties in both scenarios are quite similar. Considering the correlations between the amount fractions leads generally to a reduction in the standard uncertainty. The use of the recovered correlation matrix (“Recovery” in Table 3) provides identical values for the standard uncertainties for the statistically meaningful digits.

4. Conclusions

Using a normalised natural gas composition and a full covariance matrix are key to obtaining acceptable results with credible values for the uncertainties. While the assumption that the raw composition are mutually uncorrelated can be disputed, the approach for recovering the correlation matrix is a useful tool for processing measurement data in the natural gas industry, where often only the normalised composition of the metered natural gas is transmitted and the associated uncertainties of the amount fractions known, or approximately so.

The assumption that for measurement results from ISO 6974 the corresponding normalisation procedure had been used is reasonable. The sum of the raw amount fractions should lie between 98 cmol mol⁻¹ and 102 cmol mol⁻¹, so that assuming that it does not deviate too much from 100 cmol mol⁻¹ is fit for purpose for obtaining an acceptable approximation of the sensitivity matrix used in the recovery algorithm.

Finally, ISO 6976 should not entertain the idea of performing an uncertainty evaluation of natural gas properties while ignoring the correlations between the amount fractions of the natural gas composition. Not only does this idea contradict the guidance in the GUM [6,18], it also leads to a substantial overrating of the standard uncertainties for most parameters.

Funding: This research was funded by the Ministry of Economic Affairs of The Netherlands. The APC was funded by MDPI.

Data Availability Statement: Data are contained within the article.

Conflicts of Interest: The author declares no conflicts of interest.

Appendix A

The following R [31] code reproduces the calculation as shown in Section 3:

```
# -----  
# Non-normalised composition  
  
xdata.val = c(3.248,2.398,83.520,6.523,3.345) # (in cmol/mol)  
xdata.unc = c(0.021,0.018,0.209,0.044,0.113) # (in cmol/mol)  
  
normalise = function (x,kappa = 1.0) {  
  x*kappa/sum(x)  
}  
  
# -----  
# normalised composition  
xnorm.val = normalise(xdata.val,kappa = 100)  
# 3.279682  2.421391  84.334673  6.586627  3.377628  
  
# -----  
# uncertainty of normalised composition  
  
norm.sensmat = function(x,kappa = 1.0) {  
  num = length(x)  
  sum.x = sum(x)  
  cvmat = matrix(nrow = num,ncol = num)  
  for (i in 1:num) {  
    for (j in 1:num) {  
      cvmat[i,j] = -kappa * x[i]/sum.x^2  
      if (i == j) cvmat[i,j] = cvmat[i,j] + kappa/sum.x  
    }  
  }  
  cvmat  
}  
  
# sensitivity matrix normalisation  
xnorm.sens = norm.sensmat(xdata.val,kappa = 100)  
  
# covariance matrix of the non-normalised composition  
xnorm.cvm = diag(xdata.unc^2)  
  
# calculation of the covariance matrix of the normalised composition  
xnorm.cvm = xnorm.sens %>% xnorm.cvm %>% t(xnorm.sens)  
  
# from covariance matrix to standard uncertainties ...  
xnorm.unc = sqrt(diag(xnorm.cvm))  
  
# [1] 0.02202324 0.01870065 0.11095691 0.04444736 0.11049269  
  
# -----  
# reconstruction algorithm
```

```

norm.recon = function(y,uy,kappa = 1.0) {
  b = uy^2
  num = length(y)
  A = matrix(nrow = num,ncol = num)
  sol = numeric(num)
  for (i in 1:num) {
    for (j in 1:num) {
      if (i==j) {A[i,j] = 1.0-y[i]/kappa} else {A[i,j] = -y[i]/kappa}
      A[i,j] = A[i,j]^2
    }
  }
  sol = qr.solve(A,b)
  sqrt(sol)          # return standard uncertainties u(x[i])
}

# reconstructed standard uncertainties non-normalised composition
xdata.unc1 = norm.recon(xnorm.val,xnorm.unc,kappa = 100.0)
0.02120484 0.01817558 0.21103863 0.04442919 0.11410223

```

The function `norm.recon` implements the recovery algorithm, taking as arguments the normalised composition (y), the standard uncertainties of the normalised composition (uy), and the normalisation constant ($kappa$). It returns the standard uncertainties of the non-normalised composition. The numerical results shown are those obtained with data from Table 1.

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