atmosphere

MDPI

Supplementary Materials:

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Table S1. Masses and volumes used for the correlation experiment between NIST 3133 (20 ºC), pipetted from the 1.044 ng g^{-1} standard, and the gas standard (10 ºC).

Mass of Hg (pg) from NIST 3133	Mass of NIST 3133 solution (mg)	Gas standard volume (µL)
27.8	26.6	5
55.5	53.3	10
111	106.5	20
166.6	159.8	30
222.1	213	40
277.6	265.6	50

Note: the signal for the NIST 3133 used for the correlation was the one corresponding to the corrected mass of Hg in the standard that matches the one of the gas standard.

Equations S2 and S3 are the general models used for the uncertainty propagation in the case of water analysis by using NIST 3133 and the gas standard for calibration, respectively. Equations S4 and S5 are the models for air analysis, using the same standards for calibration. The first two terms are common as the mass of mercury is calculated based on the ratio between the signals given by the sample and the standard, multiplied by the mass of mercury that is in the standard. As we calculate the concentrations of mercury present in water samples and air samples in different units (ng L^{-1} for water samples and ng m^{-3} for air samples), the remaining parts of the models tackle the uncertainties regarding these variables. In the case of the water samples, as we analyze approximately 50 g, we calculated the respective masses contained in one litter of sample. For the uncertainty of the density, the contribution of the mass and the volume of the samples to the uncertainty have been calculated as type B uncertainties. In the case of air samples, as we sampled 20 L of air, we calculated the mass of mercury in one cubic meter for each sample. Since all these terms carry uncertainties, the source of uncertainty from each component has been taken into account.

The uncertainty components are almost the same as in the case of the mercury determination in the gas standard. In the case of mercury analysis in water, the volume of the sample is replaced by mass as each sample was weighed. Due to the units of the results which are in ng L^{-1}, we considered also the uncertainty coming from the density of the sample. In equations 4 and 5, m(std) is used when the calibration is done with NIST 3133, and when the calibration is done with the gas standard, we replace the m(std) with V(std).

$$c(S) = \frac{A'(S)}{A'(std)} \times \frac{m_{Hg}(std)}{m(S)} \times \frac{1}{\rho} \quad \text{(S2)}$$

$$c(S) = \frac{A'(S)}{A'(std)} \times \frac{\gamma_{Hg}(std)}{m(S)} \times \frac{1}{\rho} \quad \text{(S3)}$$

$$c(S) = \frac{A'(S)}{A'(std)} \times \frac{m_{Hg}(std)}{V(S)} \quad \text{(S4)}$$

$$c(S) = \frac{A'(S)}{A'(std)} \times \frac{\gamma_{Hg}(std)}{V(S)} \quad \text{(S5)}$$

Table S2. The main components of uncertainty, contributors to uncertainty, and the types of uncertainty for the determination of Hg in the gas standard.

Main uncertainty components	Contributors to uncertainty	Type of uncertainty
A′(S)	Repeatability	A
	Blank subtraction	A
A′(std)	Repeatability	A
	Blank subtraction	A
m(std)	Certificate uncertainty	A
	Dilutions	B
	Laboratory temperature	B
V(S)	Syringe resolution	B
	Syringe calibration	N/A
	Thermometer resolution	B
	Equation uncertainty	N/A

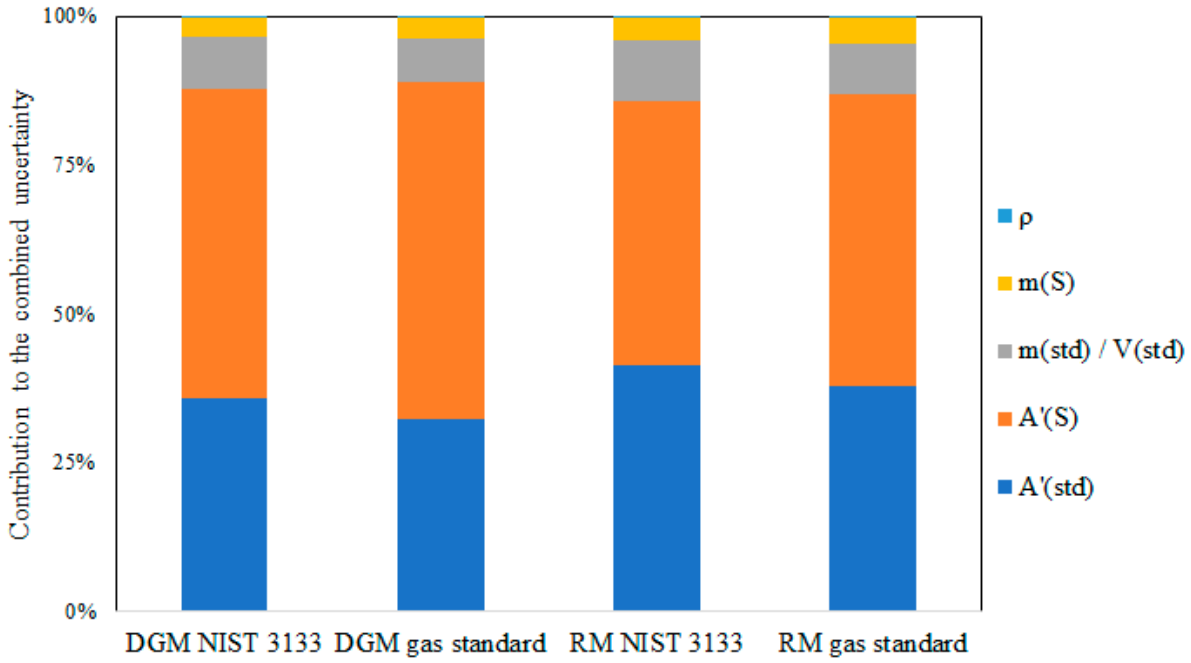

Figure S1 The contribution index for the determination of DGM and RM at station 2, by using both NIST 3133 and gas standard; m(std) is used when quantifying the uncertainty due to NIST 3133 mass, while V(std) is used when quantifying the uncertainty due to the volume of the gas standard.