additional information

Primary Reference Materials for contamination of fuel cell electrical vehicles.

All Primary Reference Materials (PRMs) presented in Table 1 were prepared gravimetrically from pure compounds (high purity nitrogen (>99.9999 % BIP+, Air Products), high purity carbon monoxide (> 99.998%, Air Products) or by dilution of NPL PRM (i.e., dilution of NPL PRM containing 10 µmol/mol of hydrogen sulphide in hydrogen) in high purity hydrogen (>99.9999 %, BIP+, Air Products). The reference materials were prepared according to ISO 6142-1 [13]. The cylinders used in this study were 10 litre aluminium cylinders with an internal SPECTRA-SEAL® passivation (BOC, UK). Depending on the mass of gas to be transferred, a direct transfer line was used for mass above 3 grams and a transfer vessel was used for mass below 3 grams. During each stage of the preparation, the amount of gas transferred was accurately weighed to determine final compositions using gravimetry. The balances used to perform weighing were either a balance with 0.1 mg uncertainty (Sartorius Research, UK) for masses below 3 grams or a balance with 20 mg uncertainty (model XPE26003LC, Mettler Toledo, UK) using an automated weighing facility (KRISS, SK) for masses above 3 grams.

Pure compounds with masses below 3 grams were added to a transfer loop *via* direct gas transfer. The transfer loop consisted of a piece of 1/8-inch external diameter tubing with Swagelok fittings on one end and a three-way valve on the other. The transfer loop and the valve were evacuated to a pressure of 1×10^{-6} mbar to ensure no contaminants or air were present in the system. The evacuated transfer loop and valve were then weighed on a balance (Sartorius Research, UK). Pure compound was then transferred directly into the transfer loop *via* the three-way valves of the transfer loop. The volume within the connection between the three-way valve and the pure compound cylinder was evacuated to a pressure of 1×10^{-6} mbar to remove contaminants and air. The pure compound was then transferred into the transfer loop. The transfer loop, filled with the pure compound, was then weighed again. An empty gas cylinder (10L aluminium with spectraseal passivation, BOC, UK), with an NPL-designed outlet diaphragm valve (Rotarex Ceodeux, Luxembourg) was evacuated below 5×10^{-7} mbar using a turbo molecular pump (Leybold Vacuum, UK) for at least 12 hours. The cylinder valve included an internal screw thread to minimise dead volume. The gas cylinder was connected to the transfer loop using a minimum dead volume connection. The volume within the connection between the transfer loop and the minimum dead volume fitting was evacuated to a pressure of 1×10^{-6} mbar to ensure no contaminants or air were present. The pure gas compound was then transferred from the transfer loop into the cylinder. After the transfer, the transfer loop was weighed again.

The addition of gas compounds above 3 grams into the cylinder was performed by direct transfer of a NPL PRM *via* a length of 1/16 inch stainless steel tubing (Swagelok, UK) that had undergone Silcosteel® passivation (Thames Restek, UK). The cylinder was weighed on a balance (XPE26003LC, Mettler Toledo, UK) after each transfer, and finally filled with 90 to 120 bar of hydrogen (purity > 99.9999%, BIP+, Air Products, UK). Upon completion of preparation, the mixtures were homogenised by rolling along the vertical axis for two hours.

Hydrogen quality at the hydrogen refuelling station

Table S1. Hydrogen fuel quality from the hydrogen refuelling station used to fill the FCEV. The analysis focussed only on the compounds that influenced the final composition (carbon monoxide, nitrogen, and sulphur). Additional compounds were measured (water, oxygen, and argon) to evaluate potential air contamination in the experimental setup.

Compounds	Amount fraction [µmol/mol]	Uncertainty [µmol/mol]
Carbon monoxide	< 0.010	n.a.
Total sulphur	< 0.001	n.a.
Water	0.92	0.12
Nitrogen	18.33	0.52
Oxygen	< 0.10	n.a.
Argon	1.119	0.028

Sampling system description

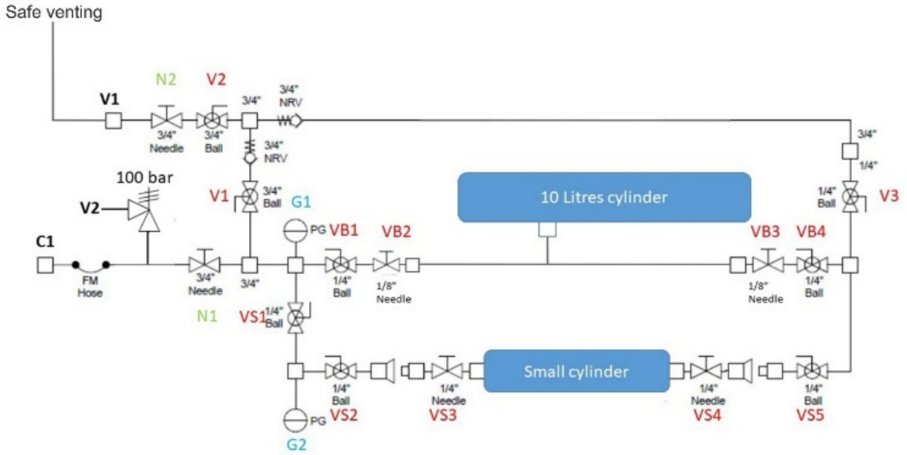

Figure S1. NPL sampling rig modified from Bacquart et al.[Error! Bookmark not defined.] including sulfinert passivated flow path from C1 to the cylinder.

hydrogen fuel added at the hydrogen refuelling station

Table S1. Evaluation of hydrogen mass in the FCEV based on pressure measurement from the venting tool and from the FCEV system including pressure and temperature sensors

	Mass of hydrogen refilled at HRS based on HRS metering [g]	Mass of hydrogen in the tank before contamination based on FCEV sensors (P & T) [g]
Contamination 1	1000 ± 50	1060 ± 50
Contamination 2	230 ± 12 1230 ± 52	1540 ± 80
Contamination 3	1000 ± 50	1080 ± 60
Contamination 4	1000 ± 50	1110 ± 60

hydrogen mass determination for the determination of the fuel composition in the FCEV tank

Table S2. Summary of the masses of hydrogen fuel inputs in the FCEV with the associated uncertainties. The masses were determined for each contamination experiments.

	Mass of hydrogen in the tank before contamination based on FCEV pressure and temperature readings [g]	Mass of hydrogen from contamination cylinder [g]	Mass of hydrogen from pure hydrogen cylinder [g]	Mass of hydrogen in the tank before contamination based on FCEV pressure and temperature readings [g]
Contamination 1	540 ± 27 g	8.4 ± 0.4	10 ± 2	1060 ± 50

Contamination 2	530 ± 27 g	8.65 ± 0.36	10 ± 2	1540 ± 80
Contamination 3	530 ± 27 g	12.95 ± 0.47	10 ± 2	1080 ± 60
Contamination 4	310 ± 16 g	19.3 ± 0.5	10 ± 2	1110 ± 60

Graphical representation of the results of contamination experiment 2

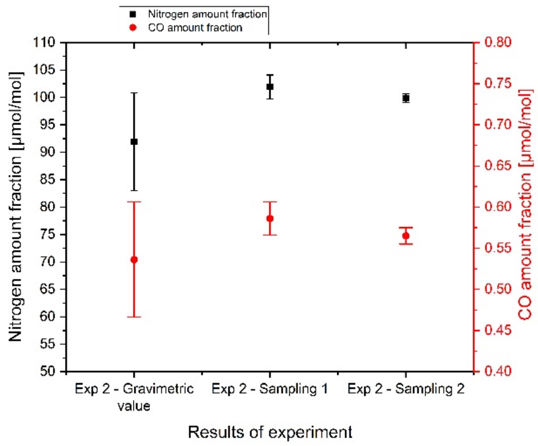

Figure S2. Results of 2nd synthetic hydrogen fuel made in the tank of the FCEV. The figure presents the gravimetric determination of CO and nitrogen in the hydrogen fuel in the FCEV tank compared to the results of analysis from the two samples taken from the FCEV. The expanded uncertainties are presented (*k*=2).