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RESEARCH ARTICLE

New primary reference materials for gas composition for carbon capture, utilisation and storage and how they support industry and meet the technical specifications of European manufacturers

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Abstract

This work describes the development and validation of new Primary Reference Materials (PRMs) for trace impurities in carbon dioxide (CO_2), addressing a key metrological gap for carbon capture, utilisation, and storage (CCUS) applications. CO_2 streams captured from industrial sources inevitably contain impurities such as water, sulfur oxides, nitrogen oxides, hydrogen, and hydrocarbons. Accurate and traceable quantification of these species is essential to protect transport infrastructure, ensure compliance with project specifications, and enable safe long-term geological storage. International and project-specific guidelines, including ISO/TR 27913, Porthos, and Northern Lights, define stringent impurity limits, underscoring the need for reliable gas standards for calibration and validation of analytical instruments. Binary and multi-component PRMs were prepared by VSL, NPL, CMI, IPQ, and SINTEF ER using ISO 6142-1 gravimetric methods. The mixtures covered sulfur dioxide, hydrogen sulfide, nitrogen dioxide, nitrous oxide, water, dimethyl sulfide, ethanol, and non-condensable gases (N_2, Ar, H_2, O_2, CH_4, and CO) at amount fractions relevant to CCUS specifications. In parallel, dynamic preparation systems and a portable trace gas generator

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were validated as alternative approaches for producing low-level mixtures of reactive species such as ammonia. PRM stability was investigated over a two-year period. Sulfur dioxide, hydrogen sulfide, dimethyl sulfide, ethanol, and nitrous oxide demonstrated stability within their expanded uncertainties. In contrast, sulfur dioxide, nitrogen dioxide, and nitric oxide in multi-component mixtures exhibited significant degradation, indicating pronounced reactivity and wall effects. Dynamic dilution systems developed by VSL and NPL produced mixtures consistent with static PRMs within 1–5%, while the portable trace gas generator achieved ammonia generation in CO_2 with a relative uncertainty of approximately 2%. These results establish a robust metrological basis for impurity analysis in CO_2. The PRMs developed within MetCCUS provide traceable calibration capabilities aligned with European CO_2 quality specifications, supporting reliable monitoring and safe operation of CCUS infrastructure.

Plain language summary

Carbon capture, utilization, and storage (CCUS) is a way to reduce carbon dioxide (CO_2) emissions from industry. In this process, CO_2 is captured before it enters the atmosphere and then transported for reuse or stored deep underground. Before this can happen safely, the captured CO_2 must be checked for very small amount of other gasses, called impurities. These impurities can damage pipelines, affect storage sites, or create safety risks if they are not properly controlled.

This project focused on improving how these tiny impurities in CO_2 are measured. The researchers developed reference gas mixtures, which are used to check and calibrate measuring instruments. You can think of these reference materials as reliable “yardsticks” that help laboratories measure gases accurately and consistently.

The work was carried out by several national measurement institutes across Europe, including VSL (Netherlands), NPL (United Kingdom), CMI (Czech Republic), IPQ (Portugal), and SINTEF (Norway). Together, the team prepared and tested gas mixtures containing very small amounts of substances that are commonly found in captured CO_2. These included water, sulfur-containing gases, nitrogen-containing gases and hydrocarbons. In addition to bottled reference gas mixtures, the team tested portable systems that can produce very small and controlled amounts of certain gases on demand. These systems are especially useful for gases that are difficult to store for long periods, such as ammonia. The researchers checked whether these systems could reliably produce the right gas concentrations and compared the results with traditional bottled mixtures. The results showed that the portable systems worked well and produced accurate gas mixtures.

This work supports safer and more reliable CCUS projects across Europe. By improving how impurities in CO_2 are measured, it helps industry monitor CO_2 quality, protect infrastructure, and build trust in

large-scale carbon capture and storage as a tool to reduce climate change.

Keywords
Carbon capture, utilisation and storage (CCUS), Primary reference materials (PRMs), Carbon dioxide impurities, Metrology, Gas standards

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Introduction

Carbon capture, utilization, and storage (CCUS) includes technologies that support global energy and climate objectives. Both carbon capture with permanent storage (CCS) and carbon utilization (CCU) are effective strategies for reducing carbon dioxide (CO_2) emissions, thereby contributing to the climate targets set by the European Commission. According to European green deal the production of CO_2 should be reduce of 55 % by 2030 and eliminated by 2055. To achieve these targets, large-scale deployment of CCUS is necessary. CO_2 can be captured from various industrial sources, including cement and steel production, biogas upgrading, fossil fuel combustion, and even directly from the air through direct air capture. Once captured, CO_2 is transported, typically via pipelines or ships, to designated storage sites, where it is injected into geological formations for long-term storage, or delivered to facilities for industrial utilization. The required quality of CO_2 depends on its source and the capture technology used, as this ensures proper process performance, protects system components, and safeguards health and safety. ISO/TR 27291:2020[1] outlines how impurities in the CO_2 stream can impact storage, with effects categorized as physical, chemical, microbiological, or toxicological. These impurities may alter the thermodynamic and transport properties of CO_2, influencing factors such as operating pressure, temperature, fluid density and safety risks.

A critical aspect of a safe and efficient CCUS chain is the accurate measurement of impurities in the captured CO_2 stream. These impurities such as CH_4, O_2, H_2, CO, H_2S, N_2, Ar, and SO_2 can significantly affect the physical and chemical properties of the gas[2,3]. They influence parameters such as the bubble point and energy required for liquefaction or compression. Moreover, reactive species like H_2O, H_2S, NO_x, and SO_x may form separate acidic phases, posing serious corrosion risks to transport infrastructure[3]. Reliable impurity quantification is therefore essential. It ensures compliance with specifications set by large-scale CCUS initiatives such as Porthos[4] and Northern Lights[5], protects the integrity of transport systems, and supports regulatory frameworks. Monitoring impurity levels at various stages, post-capture, during transport, and at the point of storage or utilization, can also inform operational decisions, such as whether further purification is required. To support this, robust analytical methods are essential for defining operational conditions and carrying out both online and offline measurements throughout the CO_2 capture, transport, and storage chain.

In order for these measurements to be accurate and comparable, reliable gas mixtures are needed to calibrate instruments used in monitoring impurity levels. These gas standards form the foundation of traceable measurements, enabling consistent and comparable data between monitoring systems and laboratories. However, a critical gap remains in the availability of primary reference standards (PRMs) for impurities in CO_2. Addressing this shortfall is essential to enable accurate impurity quantification and to ensure the long-term integrity and safety of transport and storage infrastructure. PRMs enable precise measurement of impurities with full metrological traceability. These materials are vital for validating analytical methods and calibrating the instruments used throughout the carbon capture and storage process.

This report paper covers the development of new PRMs for impurities in CO_2 and the systematic two-year stability study of these materials. The work includes the preparation of binary and multicomponent mixtures, validation of dynamic generation methods, and an assessment of suitable cylinder materials for long-term stability. In addition, the report outlines how the developed PRMs support industry by enabling traceable calibration of CO_2 impurity measurements and by meeting the technical requirements set by European manufacturers and CCUS projects. These materials allow operators to verify compliance with impurity thresholds and ensure safe and reliable CO_2 transport and storage.

CO_2 impurities specifications

Across the CCUS chain, from capture to transport and storage, different impurities may be present. The table S1 (Supplementary material) brings together impurity limits from a wide range of industrial, regulatory, and research sources. Some of these specifications are project-specific, while others are the result of international standardisation efforts or technical studies. For example, the Porthos and TAQA values[6] represent cluster-specific requirements for CO_2 transport and storage projects in the Netherlands, developed in close collaboration with industrial stakeholders. The Zero Emissions Platform (ZEP) specifications stem from a European technology platform that advises the European Commission on CCS deployment and provides guidance on common quality thresholds. Similarly, the DECARB project (Decarb WP 2.1.1) and other contributions come from the UK's National Physical Laboratory (NPL), whose ENV23 reports provide recommended impurity thresholds. In contrast, ISO/TR 27913[7] represents the international standard for pipeline transportation of CO_2, offering harmonised requirements that can be applied globally.

Key regulated impurities for pipeline CO_2 (as reflected in ISO/TR 27913 and industry guidelines) include water, H_2S/total sulfur, NO_x, SO_x, O_2, CO, hydrocarbons, non-condensable gases and particulates. Water (H_2O) is a dominant impurity of concern, with thresholds set between 20 and 50 ppm in most project specifications (ISO 27913, ECC, LBA), while some reservoir-based studies allow up to 300 ppm. Water is critical because even small amounts can combine with acid-forming species (SO_2, NO_x) to generate highly corrosive aqueous phases, and at higher levels can lead to hydrate formation in pipelines. Pipeline specs typically require ≤ 50 ppm (v/v) H_2O.

Hydrogen sulfide (H_2S) is one of the most toxic and corrosive impurities in CO_2 streams. Its presence can lead to accelerated metal corrosion. Across the specifications, limits are consistently set around ≤5 ppm, with slightly higher allowances (≤20 ppm). Sulfur oxides (SO_2, SO_x) and other sulfur compounds such as COS and mercaptans are also tightly controlled because of their capacity to form strong acids in the presence of water. Typical limits for SO_2 and total SO_x are ≤10 ppm, though transport-focused specifications sometimes allow up to 50 ppm. For other sulfur species, thresholds are often below

1 ppm, underlining the recognition that even traces are aggressive to materials.

Nitrogen oxides (NO_x) contribute to the formation of nitric acid when water is present, leading to rapid corrosion. Specifications vary from extremely strict (≤0.5 ppm in NPL studies) to more lenient (≤10 ppm in ISO/TR 27913). In practice, NO_x levels in captured CO_2 depend on the source (post-combustion flue gas can introduce 10–100 ppm NO/NO_3 unless scrubbed). Because NO_2 is particularly reactive/unstable (it can dimerize to N_2O_4 and adsorb or form HNO_2 in moist conditions). Ammonia (NH_3) is often restricted to ≤3–10 ppm (Porthos, ISO 27913), though up to 50 ppm is allowed in some storage specifications; amines are set at ≤1 ppm in Porthos, with other reports suggesting ≤10 ppm, glycols are restricted to trace levels (≤0.025–0.05 ppm). Hydrogen (H_2), although not corrosive by itself, poses risks for material integrity. Exposure to H_2 under high-pressure transport conditions can lead to hydrogen embrittlement in steels, weakening the pipeline structure. For this reason, specifications generally restrict H_2 to ≤0.75% (Porthos, TAQA, ISO 27913), with some studies suggesting even stricter values (≤0.3%). Oxygen (O_2) is often limited to low levels (as O_2 can induce oxidative corrosion and fuels side-reactions). For example, one CO_2 network set O_2 < 10 ppmv, whereas some specs allow O_2 in the order of 100 ppm.

An important objective is to map Primary Reference Materials (PRMs) against industrial specifications for CO_2 quality in transport and storage. Pipeline and storage operators define allowable impurity limits to ensure safe, non-corrosive operation and compliance with environmental rules. Notably, ISO 27913:2024 (for CO_2 pipeline transport) now stipulates that total impurities in the CO_2 stream should not exceed 5% (molar), with multiple requirements to safeguard pipeline integrity. This effectively requires ≥95% CO_2 purity, consistent with typical project specs ranging 93–98% CO_2 minimum. The balance (≤5%) can include N_2, O_2, Ar, H_2, CH_4 and other gases, but individual reactive impurities are constrained by stricter sub-limits. Therefore strict traceable gas composition measurements are required.

In the MetCCUS project, European National Metrology Institutes (NMIs) have prepared a suite of PRMs, i.e. high-accuracy calibration gas mixtures, to support traceable measurement of key impurities in high-purity CO_2 streams. These PRMs target the low-level contaminants expected in captured CO_2 prior to transport and storage. Table 1 summarizes the PRMs developed by various NMIs, including the impurity species and amount-of-substance fractions (concentrations) achieved.

Stability data

Table 1 summarises the impurities and mixtures prepared the participants. VSL prepared mixtures of H_2O (10 ppm), NO_2 (10 ppm and 1 ppm) and SO_2 (20 ppm), while IPQ focused on H_2S (10 ppm) and SO_2 (20 ppm). CMI selected NO_2 (100 ppm) and N_2O (10 ppm) at higher concentration levels, and SINTEF ER prepared SO_2 (20 ppm) and H_2O mixtures (50 ppm). NPL contributed ethanol (≤20 ppm) and dimethyl sulfide (≤1 ppm). MetCCUS included O_2 in multi-component reference mixtures, see Table 2 (e.g. NPL and IPQ prepared mixtures of CO_2 containing O_2 along with CO, SO_2 or H_2S). Methane (CH_4) was included in certain multi-component mixtures (IPQ prepared an H_2S+CO+CH_4+O_2 in CO_2 mixture).

The binary PRMs developed in this project were evaluated over periods of up to two years to assess their long-term stability and suitability as traceable calibration materials for impurity analysis in CO_2. The stability study applied repeated verification measurements following ISO 6143 procedures[8], with the detailed measurement results, analytical datasets, and uncertainty evaluations provided in section S2 of Supplementary material. Overall, the stability behaviour of the binary mixtures was strongly impurity-dependent, with several species demonstrating excellent long-term stability while others exhibited clear compositional degradation driven by adsorption, chemical transformation, or interactions with cylinder surfaces.

Among the stable species, sulfur dioxide (SO_2) mixtures prepared by both VSL, IPQ[9] and SINTEF showed highly consistent performance. The VSL mixtures displayed a small decrease of approximately one percent within the first six months after preparation, followed by stable behaviour for the remainder of the 600–750 day monitoring period (Figure S1, supplementary material). IPQ mixtures similarly showed no statistically significant deviation from the gravimetric values, as indicated by normalized error values consistently within $|En| \leq 1$. The

Table 1. Overview of selected impurities, amount fractions, and cylinder types for mixtures prepared by participants.

	Mixture 1			Mixture 2			Mixture 3
Participants	Impurity	Amount fraction	Cylinder type	Impurity	Amount fraction	Cylinder type	Impurity
VSL	H_2O	10 ppm	Aculife IV	NO_2	10 & 1 ppm	Alphatech	SO_2, ≤20 ppm
NPL	C_2H_5OH	≤20 ppm	-	DMS	≤1 ppm	-	-
CMI	NO_2	≤ 100 ppm	AL/ Aculife	N_2O	≤ 10 ppm	AL/ Aculife	-
IPQ	H_2S	10 ppm	Aculife III/ IV	SO_2	≤20 ppm	Aculife III/ IV	-
SINTEF ER	SO_2	≤40 ppm	Aculife III/ IV	-	-	-	-

Table 2. Overview of selected impurities, for multi-component mixtures prepared by participants.

Participant	Multicomponent mixture	Amount of fraction (µmol/mol)	
		Mixture 1	**Mixture 2**
NPL	H_2	2500	2500
	O_2	50	95
	CO	50	100
	CH_4	15000	10000
	N_2	10000	20000
	Ar	10000	7500
	NO	10	5
	SO_2	5	10
CMI		**Mixture 1 (Aluminium)**	**Mixture 2 (Aculife IV)**
	N_2O	9.5	9.4
	SO_2	9.00	8.7
	NO_2	23	27.2
	H_2	6986.4	7070.2
	CH_4	35140.9	22552.8
	N_2	20611.9	19618.4
IPQ		**Mixture 1**	**Mixture 2**
	CO	666.1	669.5
	O_2	0.594	0.586
	CH_4	-	1.9685
	SO_2	14.26	-
	H_2S	-	9.83

expanded uncertainties associated with these verifications, typically between one and one-and-a-half percent (k = 2), fully encompassed the observed variations (Table S3, supplementary material). The stability evaluation of the SO_2 cylinder of SINTEF shows that both mixtures remain stable more than one year after preparation. Across three verification measurements performed in 2025, the observed amount fractions for both cylinders remained constant within their expanded uncertainties ($k=2$) (Table S4, supplementary material). Hydrogen sulfide (H_2S) exhibited comparable stability characteristics: across all IPQ measurements over 12–18 months, the observed differences between verification points remained within the combined uncertainty, confirming that H_2S can be maintained as a static PRM in CO_2 when stored in appropriately treated cylinders (Table S6, supplementary material).

Nitrous oxide (N_2O) was found to be one of the most stable impurity species in this study. Mixtures prepared at CMI in both Aculife-treated and polished aluminium cylinders showed negligible drift over 24 months, with all measurement points remaining within approximately 0.4 µmol mol^{-1} of the gravimetric value. The expanded uncertainties associated with N_2O measurements, typically around one to one-and-a-half percent, were sufficient to account for all observed variability (Table S9, supplementary material). Volatile organic impurities such as dimethyl sulfide (DMS) and ethanol (EtOH) produced by NPL (Table S5,S10 supplementary material) also demonstrated very good stability. DMS mixtures showed no measurable degradation over 25 months, with analytical values consistent with gravimetric preparation within the four-percent uncertainty envelope. Ethanol behaved similarly, with verification results

over a 23-month period revealing no systematic drift and combined relative uncertainties consistently below three percent (See Figure S6, supplementary material).

In contrast, the stability of water (H_2O) in CO_2 proved more challenging. VSL's binary water PRMs showed an initial loss of approximately five to ten percent shortly after preparation, attributable to adsorption processes on cylinder walls or internal treatments. After this initial decline, the mixtures stabilised and subsequent verification results remained consistent within the four-percent measurement uncertainty. Nevertheless, the variability observed between different cylinders suggests that surface interactions and storage conditions have a significant influence on water stability, and regular re-verification is recommended to ensure continued traceability. (See Figure S3, supplementary material)

Nitrogen dioxide (NO_2) exhibited the most pronounced instability among all binary mixtures. For 10 µmol mol^{-1} mixtures, a modest decline of around two percent was observed over 600 days; however, the behaviour at lower levels was more severe, with decreases of up to ten percent for 1 µmol mol^{-1} mixtures (See Figure S4 and table S7, supplementary material). The studies conducted by CMI highlighted an even more dramatic dependence on cylinder material. In Aculife IV-treated aluminium cylinders, NO_2 showed ongoing degradation but remained detectable over the 24-month period. In polished aluminium cylinders, however, NO_2 concentrations dropped to near-zero within 12 months, followed by partial re-desorption at the 24-month point. Additional analysis confirmed the formation of secondary species including N_2O_4 and HNO_3[10], indicating that NO_2 undergoes chemical transformation rather than simple physical adsorption (Table S8, supplementary material)

The uncertainty evaluation across all binary mixtures reflects two dominant contributions. The first arises from the initial gravimetric preparation according to ISO 6142-1[11], which typically contributes between 0.1 and two percent to the overall uncertainty depending on impurity purity, weighing precision, and gas molar masses. The second source relates to stability, measured through repeat verifications over time. For stable species such as SO_2, H_2S, N_2O, DMS and ethanol, the stability component remains small and generally negligible compared to analytical uncertainty. For water and especially NO_2, stability contributes significantly to the expanded uncertainty and must be explicitly included to avoid underestimation of the total uncertainty when these mixtures are used as calibration materials.

In summary, the binary stability study confirms that several impurities critical for CCUS, most notably SO_2, H_2S, N_2O, DMS and ethanol, can be realised as long-term stable PRMs in CO_2, with performance fully compatible with industrial calibration needs. Conversely, H_2O and particularly NO_2 exhibit impurity-specific instabilities that require careful consideration of cylinder materials, regular re-verification, or the use of dynamic and generator-based reference methods. The complete datasets supporting these conclusions are available in section 2 of Supplementary materials.

Alongside the stability studies, dynamic methods were established to enable the generation of mixtures across a range of amount of fractions summarized in section 3 of supplementary material. Dynamic gas mixture preparation systems developed at VSL and NPL were validated as complementary methods for generating traceable low-level impurity mixtures in CO_2. Verification by NPL against static PRMs demonstrated that dynamically prepared mixtures agreed with gravimetric reference values typically within 1–5 %, with relative expanded uncertainties ranging from 0.04 % for major components to ~6 % for trace species. For permanent gases by VSL, such as N_2, CH_4, O_2, Ar and H_2, dilution factors were reproduced reliably, and biases remained below 4 %. The VTT trace gas generator produced NH_3 at 10–20 µmol mol^{-1} with a relative expanded uncertainty of ~1.9 %. Overall, the results confirm that dynamic dilution offers a robust and traceable route for producing reference mixtures when static PRMs are impractical or when extremely low amount fractions are required.

Use of PRMs by CCUS industry and compliance with specifications

The reference materials developed within the MetCCUS project address a critical need across the CCUS value chain, where accurate quantification of impurities in captured, transported and injected CO_2 is essential for process control, safety, and regulatory compliance. Industrial stakeholders, including capture plant operators, pipeline network owners, storage site operators and suppliers of online gas analyzers, rely on traceable calibration materials to verify the performance of sensors and analytical systems that monitor impurities such as SO_2, H_2S, H_2O, NO_x, VOCs and oxygen. These impurities influence corrosion behaviour, compressor efficiency, pipeline integrity, geochemical interactions in storage reservoirs and compliance with pipeline specifications.

The binary PRMs produced in this project provide industry with high-quality calibration materials that enable traceability to the SI and support harmonised monitoring strategies across Europe. They can be used to calibrate or verify online analyzers (e.g., TDLAS, CRDS, NDIR, UV-Vis, electrochemical sensors), to perform laboratory-based validation using GC-SCD, GC-MS, FTIR or other reference techniques, and to support comparability assessments across different industrial sites or monitoring campaigns. For pipeline operators and transport network developers, PRMs directly support the qualification and acceptance testing of measurement instrumentation required to demonstrate compliance with maximum impurity thresholds. Similarly, for storage-site operators, these materials help ensure that CO_2 streams entering injection wells meet the impurity limits necessary to avoid operational problems such as scale formation or unintended reservoir reactions.

With respect to compliance, the developed PRMs were evaluated against the typical impurity ranges defined in industrial specifications for CO_2 transport and storage. The concentration levels realised in this project generally fall within or near the ranges required for calibration of industrial instruments. For SO_2, H_2S, N_2O, ethanol and dimethyl sulfide, the prepared

mixtures match the expected impurity levels found in post-combustion and industrial capture streams, and the demonstrated long-term stability ensures that these PRMs can serve as reliable reference points for industrial calibration routines.

Support for industry

The suite of PRMs developed in the MetCCUS project is designed to help industrial users meet the CO_2 purity requirements set by international standards and major CCS projects. Technical specifications such as ISO/TR 27913 and project-specific guidelines (e.g. Porthos and Northern Lights) demand that captured CO_2 be overwhelmingly pure CO_2 (typically ≥95% by volume) with tightly limited impurities to protect pipeline and storage integrity. For example, the Porthos specification requires $CO_2 \geq 95\%$ and caps critical contaminants at low levels ($H_2O \leq 70$ ppm, $O_2 \leq 40$ ppm, total NOx ≤ 5 ppm, etc.) to prevent corrosion and safety hazards. The updated Northern Lights CO_2 quality criteria likewise define strict maximum concentrations for a broad range of impurities, reflecting the latest industry insights on material compatibility and cross-reactions. By aligning with these benchmarks, the reference materials from MetCCUS directly support industry in demonstrating compliance with required CO_2 purity and impurity limits.

The PRMs cover many of the impurities that feature in CO_2 quality specifications at relevant amount fractions. In practice, this means traceable calibration gas mixtures have been prepared for key components and contaminants across the expected concentration ranges. This includes PRMs for permanent gas impurities like N_2, Ar, H_2, O_2, and CH_4 in CO_2 at percent or sub-percent levels, as allowed in transport specifications. Likewise, reactive impurities have been addressed by low-level reference mixtures: for instance, CO in CO_2 around the 1000 ppm scale, and sulfur- or nitrogen-containing species (H_2S, SO_2/SOx, NO/NOx) at ppm concentrations matching the limits in standards. These PRMs enable calibration of analyzers to detect impurities at the threshold values mandated by ISO/TR 27913 and projects like Porthos, thus ensuring that on-line monitors and laboratory analyses can reliably verify CO_2 stream quality against the specifications. In short, the available PRMs encompass most of the critical impurity types at the amount fractions relevant for carbon capture and storage operations, giving industry the necessary tools to quantify those impurities with metrological traceability.

However, the full scope of impurities listed in emerging CO_2 purity standards is broad, and not every minor compound or extreme condition is yet covered by available PRMs. Specifications such as Porthos include potential contaminants, ranging from VOCs (e.g. methanol, acetaldehyde) to amines, glycols, mercury, or particulate matter, many of which are present only in trace quantities or are challenging to stabilize in a cylinder. While the MetCCUS project's reference materials address the major categories of gaseous impurities, there remain gaps for certain species and very low concentration levels.

To help close the remaining gaps, the project has explored dynamic methods of generating reference gas mixtures on demand. The project demonstrated the use of dynamic generation systems, which offer an alternative route for achieving traceable mixtures when static PRMs are impractical. Dynamic dilution systems at VSL and NPL successfully generated low-level mixtures of permanent gases with relative expanded uncertainties ranging from approximately 0.04 % (major permanent gases at high levels) to ~6 % (trace components), with bias typically below 4 %. These results confirm that the dynamic systems are capable of producing mixtures with metrological equivalence to static PRMs for many impurity classes.

Furthermore, the portable trace gas generator evaluated within the project (VTT) demonstrated that dynamic generation can be extended to impurities that exhibit even stronger surface interactions, such as ammonia. Achieving agreement within ~3 % of the expected concentration indicates that this approach can meet industrial calibration requirements for a subset of highly reactive species. As industrial specifications continue to evolve, particularly with expected growth in amine-based capture and the associated impurities, such dynamic systems will be essential for delivering reference mixtures at μmol mol^{-1} and nmol mol^{-1} levels.

In summary, the PRMs developed in MetCCUS provide robust support for industrial compliance with CO_2 quality requirements, enabling accurate quantification of most regulated impurities through traceable, stable calibration materials. Where static mixtures are limited by chemical stability or incomplete analyte coverage, dynamic dilution and generator-based systems offer a viable and validated pathway to extend metrological traceability to all impurity classes critical for safe and efficient CO_2 transport and storage across Europe.

Conclusion

This work demonstrates the successful development, validation and long-term assessment of Primary Reference Materials (PRMs) for a broad range of impurities relevant to the CO_2 value chain. Binary and multicomponent mixtures were prepared in accordance with ISO 6142-1 and verified through repeated measurements over a period of up to two years. The stability studies show that several key impurities, most notably SO_2, H_2S, N_2O, ethanol and dimethyl sulfide, remain stable within their expanded uncertainties, confirming their suitability as long-term calibration materials for industry. In contrast, strongly reactive species such as NO_2, NO and, to a lesser extent, H_2O exhibit significant instability and cylinder-surface interactions, highlighting the need for careful selection of cylinder treatments, regular re-verification, or alternative dynamic preparation methods.

The comparison of dynamic dilution systems developed by VSL and NPL with static gravimetric PRMs demonstrates that dynamic generation can provide traceable mixtures within 1–5 % agreement, offering a robust route for impurities that cannot be stabilised in cylinders. The validation of a portable trace gas generator further expands metrological capabilities to highly reactive compounds such as NH_3, which are increasingly relevant for amine-based capture technologies.

Overall, the PRMs developed within MetCCUS provide a solid metrological foundation for impurity measurements in CO_2 streams and directly support industrial compliance with European CO_2 quality specifications. While the work successfully addresses most major impurity classes, gaps remain for certain highly reactive species, underscoring the need for continued research, improve measurement technologies and further development of dynamic reference methods.

Ethics and consent

Ethical approval and consent were not required.

Data and software availability

The dataset for this study are available in the following repository: https://doi.org/10.5281/zenodo.17948575[12]

This projects contains the following underlying data:

- Extended data:
  - supplementary_materials.docx: This document contains stability data of PRMs, multi-component mixtures and dynamic dilutions

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http://www.doi.org/10.5281/zenodo.17948575

Open Peer Review

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The manuscript addresses a topic related to the development of Primary Reference Materials (PRMs) for impurity measurements in CO_2 streams within CCUS systems. The study has strong industrial relevance and provides valuable long-term stability data for several key impurities. Overall, the manuscript is technically sound and potentially useful for both academia and industry. However, several aspects still require improvement to strengthen the scientific contribution, clarity, and overall impact of the work. The following points should be addressed before the manuscript can be considered for indexing :

- Please, clarify the novelty and scientific contribution of the work, particularly in comparison with previous studies on calibration gas mixtures and CCUS impurity monitoring.
- The methodology section should be expanded with more detailed descriptions of preparation procedures, analytical instruments, verification protocols, uncertainty calculations, cylinder treatments, and statistical approaches used for stability assessment.
- The discussion should be strengthened with deeper scientific interpretation, particularly regarding adsorption/desorption mechanisms, chemical instability pathways, effects of cylinder materials, and implications for industrial-scale CCUS deployment.
- Several sections are repetitive, particularly those related to industrial applications and specification compliance. Please restructure the manuscript to improve coherence, clarity, and overall flow while reducing redundancy.
- The English language requires further polishing. Several grammatical errors, awkward sentence structures, and typographical inconsistencies are found, for example:
- “According to European green deal the production of CO_2 should be reduce of 55 % by 2030…” It is recommended to revise as follows: “According to the European Green Deal, CO_2 emissions should be reduced by 55% by 2030…”
- “This report paper covers the development…” (redundant wording); “report paper” should be simplified to either “report” or “paper”
- “Table 1 summarises the impurities and mixtures prepared the participants.” (missing preposition); should be “prepared by the participants.”, etc.
- The conclusion section should be strengthened by emphasizing the broader scientific

significance, practical implications, limitations of the current work, and future research directions.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
No

If applicable, is the statistical analysis and its interpretation appropriate?
I cannot comment. A qualified statistician is required.

Are all the source data underlying the results available to ensure full reproducibility?
Partly

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: CO_2 capture, energy

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.