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TECHNICAL REPORT

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Carbon dioxide capture, transportation, and geological storage — Cross Cutting Issues — CO_2 stream composition

Captage, transport et stockage géologique du dioxyde de carbone — Questions transversales— Composition du flux de CO_2

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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This document was prepared by Technical Committee ISO/TC 265, *Carbon dioxide capture, transportation, and geological storage.*

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Introduction

ISO Technical Committee (TC) 265 is developing standards and technical reports related to carbon dioxide (CO_2) capture, transportation and geological storage (CCS). This technology is a technically viable solution to reduce CO_2 emissions of large stationary point sources and therefore to limit future global temperature increases. A special report by the International Panel on Climate Change (IPCC, 2005) extensively described the fundamental technical, scientific, environmental, economic and societal dimensions of CCS and its potential role in the portfolio of climate change mitigation measures.

Depending among other things on the feedstock and the CO_2 generating and capture processes, CO_2 streams captured from industrial sources or power generation contain various impurities (that is, stream components other than CO_2). The impurities differ in their concentrations but also in their physical and chemical properties. Therefore, the composition of the originally captured CO_2 stream is a key starting point in ensuring the safety and reliability of the transport and geological storage of CO_2. Compositional information may assist operators in evaluating the need for treating a CO_2 stream, based on the intended transportation options (including mixing with other CO_2 streams), usage options (EOR or other), or dedicated storage in geologic formations.

Understanding CO_2 stream composition is also important for the commerciality of CCS activities because additional purification of the CO_2 stream increases CO_2 capture costs. In addition, CO_2 stream composition is an important input factor in quantifying the amount of CO_2 stored, for the purpose of greenhouse gas emissions reporting and crediting. Because capture and purification processes are continuously evolving, it is relevant to expose the range of impurities in CO_2 streams and their concentrations, including recent publications.

This document provides up-to-date consideration of CO_2 stream quality issues for operators, regulators and stakeholders based on research results and the experience of various pilot and industrial scale CCS projects. The first part of this report summarises existing information related to CO_2 stream composition that generally results from particular capture processes. Then this report describes possible impacts and effects of the various impurities that may occur in the CO_2 stream on various downstream elements of a CCS chain, including operational aspects, potential implications for health, safety and environmental issues, and quantification of greenhouse gas emissions.

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Carbon dioxide capture, transportation, and geological storage — Cross Cutting Issues — CO_2 stream composition

1 Scope

The primary aim of this document is to describe the main compositional characteristics of the CO_2 stream downstream of the capture unit, taking into account common purification options. Accordingly, this document will characterize the different types of impurities and present examples of concentrations determined in recent capture pilot projects as well as through literature review. It identifies ranges of concentrations, giving priority to in situ measurements when available.

The second aim of this document is to identify potential impacts of impurities on all components of the CCS chain, from surface installations (including transport) to the storage complex. For example, impurities can have a significant effect on the phase behaviour of CO_2 streams in relation to their concentration. Chemical effects also include the corrosion of metals. The composition of the CO_2 stream can also influence the injectivity and the storage capacity, due to physical effects (such as density or viscosity changes) and geochemical reactions in the reservoir. In case of a leakage, toxic and ecotoxic effects of impurities contained in the leaking CO_2 stream could also impact the environment surrounding the storage complex.

In order to ensure energy efficiency, proper operation of the whole CCS chain and not to affect its surrounding environment, operators usually limit the concentrations of some impurities, which can, in-turn, influence the design of the capture equipment and purification steps. Such limits are case specific and cannot be described in this report; however, some examples of CO_2 stream specifications discussed in the literature are presented in Annex A.

The required purity of the CO_2 stream delivered from the capture plant will to a large degree depend on the impurity levels that can be accepted and managed by the transport, injection and storage operations. The capture plant operators will therefore most probably need to purify the CO_2 stream to comply with the required transport, injection, storage specifications or with legal requirements.

Monitoring of the CO_2 stream composition plays an important role in the management of the entire CCS process. Methods of measuring the composition of the CO_2 stream and in particular the concentrations of impurities are described and other parameters relevant for monitoring at the various steps of the CCS chain are described.

The interplay between the set CO_2 stream specifications and the efficiency of the entire CCS process is also explained. Finally, the mixing of CO_2 streams coming from different sources before transport or storage is addressed, and the main benefits, risks and operational constraints are presented.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

3.1
CO_2 stream
stream consisting overwhelmingly of carbon dioxide

Note 1 to entry: The CO_2 stream typically includes impurities and may include substances added to the stream to improve performance of CCS and/or to enable CO_2 detection.

[SOURCE: ISO 27917:2017, 3.2.10]

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3.2
CO_2 stream composition
concentration (generally expressed in fraction by volume) of each component of the *CO2 stream* (3.1)

Note 1 to entry: The CO_2 stream composition is usually subject to regulatory discretion and approval. The CO_2 stream composition can also be reported as a mass concentration (e.g. mg/m^3).

3.3
CO_2 purity
percentage by volume of CO_2 as a component of the *CO2 stream* (3.1)

3.4
impurities
non-CO_2 substances present in the *CO2 stream* (3.1) as captured or derived from source materials or the capture process, or present as a result of mixing for transportation, or added, released, or formed in conjunction with sub-surface storage and/or leakage of CO_2

Note 1 to entry: As a subset of impurities, contaminants are non-CO_2 substances whose presence in the CO_2 stream is generally unwanted.

Note 2 to entry: As a subset of impurities, additives are substances added to the stream for the purposes of managing its physical or chemical behaviour (e.g., hydrate and corrosion inhibitors), for or from interaction with equipment (e.g., lubricants), or to track its distribution in the subsurface after injection (geochemical tracers).

[SOURCE: ISO 27917:2017, 3.2.18]

3.5
non-condensable substances
chemical substances that are partially in the vapour state at pipeline operating conditions.

Note 1 to entry: O_2, N_2, Ar, H_2 and CH_4 belong to this category

[SOURCE: ISO 27913:2016, 3.18]

4 Symbols and abbreviated terms

In this report volume fractions are expressed as % (10^{-2}) or ppm (10^{-6}), in order to be in line with the original publications and the usual technical exchanges within the CCS community.

Ar	Argon
As	Arsenic
BOS	Basic Oxygen Steelmaking
°C	Degree Celsius
CCS	Carbon Dioxide Capture and Storage
Cd	Cadmium
CH_4	Methane
CO	Carbon monoxide
CO_2	Carbon dioxide
COS	Carbonyl sulfide
EOR	Enhanced Oil Recovery

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EPA	Environmental Protection Agency
etc.	Et Cetera (Latin: And So Forth)
EU	European Union
GD	Guidance Document
GHG	Greenhouse Gas(es)
H_2	Hydrogen
Hg	Mercury
H_2O	Water
H_2S	Hydrogen sulfide
H_2SO_4	Sulfuric acid
i.e.	Id est (Latin: that is)
IEA	International Energy Agency
IEAGHG	International Energy Agency Greenhouse Gases R&D programme
IGCC	Integrated gasification combined cycle
IPCC	Intergovernmental Panel on Climate Change
K	Potassium
MDEA	Methyldiethanolamine
MEA	Monoethanolamine
Mn	Manganese
mg	Milligram
MPa	Mega Pascal
N_2	Nitrogen
NETL	National Energy Technology Laboratory
NH_3	Ammonia
Ni	Nickel
Nm^3	Normal cubic meter-being a cubic meter at 101,325 kPa absolute and 273 K
NO	Nitrogen monoxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxides
O_2	Oxygen
OPS	Office of Pipeline Safety

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Pb	Lead
PM	Particulate Matter
ppm (= ppmv)	Parts per million (= Parts per million by volume) = 10^{-6}
Psia	Pounds per square inch absolute
Se	Selenium
SO_2	Sulfur dioxide
SO_x	Sulfur oxides
SOP	Standard operating procedures
SRB	Sulphate Reducing Bacteria
TMEs	Trace Metal Elements
TOEs	Trace Organic Elements

5 Overview of chemical composition of CO_2 streams

5.1 Overview

In this clause available data on impurities present in CO_2 streams and the concentration ranges are described for different CO_2 sources and capture technologies. In situ measurements are emphasized.

5.1.1 Types of impurities

A number of gases could be present as impurities in the flue gas or process gas (before capture), and therefore are potentially present at the exit of the capture process. Their concentrations vary greatly from one capture technology (or process) to another, due to the various reaction pathways and to the various design options for capture and purification.

Some gases (also called "non-condensable substances") such as Ar, O_2, and N_2 can reach several percent of the CO_2 stream at the immediate exit from the capture process, before purification and compression (IEAGHG, 2011)[40]. The content of H_2O (condensable) can also reach several percent there. Other gases (NO_x, SO_x, H_2S, CO, and others), although present at lower concentrations, could still influence CO_2 stream behaviour.

Impurities other than gases have been reported in low concentration, (IEA-GHG, 2011)[40], and in the case of a post-combustion capture process, solvents used in the process (e.g. amines or NH_3) and their degradation products could be present in the captured CO_2 stream. Further impurities could include particulate matter, trace metal elements (TMEs) and trace organic elements (TOEs), depending on the fuel or feedstock used. Intrinsic toxicity levels of TMEs and TOEs is often high, but concentration levels are usually very low.

When comparing data from different sites, an important difference between an industrial site and a capture pilot plant is that the latter might not include a drying-compression phase before transport. Therefore, differences in impurity concentrations could occur. When CO_2 is compressed, gases tend to dissolve in condensed water at each compression stage and are therefore removed from the CO_2 stream before transport. See also standard ISO 27913:2016[48] on pipeline transportation systems.

5.1.2 Measurements and estimates

It is necessary to distinguish i) data that are estimates resulting from modelling from ii) measurements on the captured CO_2 stream. Published data, both measured and modelled, typically emphasize

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concentrations of main impurities. Here, we focus on measurements and quote modelling estimates only where measurements are not available. However, modelling studies are also of value, because process models enable, among other things, the representation of various combinations of impurity concentrations. Other models allow predicting possible effects in other parts of the CCS chain, as will be illustrated in Clause 6, e.g. for fluid density or chemical reactions.

5.1.3 Data sources

CO_2 stream composition data was compiled from existing literature by the expert group appointed by ISO/TC 265 from "WG5-Cross-cutting issues", based on existing review reports (e.g., from international organisations or research consortia) and on results from pilot, demonstration, or commercial projects in Europe, North America, Australia, and Japan.

Note Examples of regulatory requirements, in relation with these projects, are given in Annex B.

The bulk of this document's data compilation was drawn from several review publications and reports:

a) Anheden, et al. (2004)[7]: summarises impurities by capture process (before condensation or purification steps),

b) IEAGHG (2004, 2011)[39][40] review reports,

c) Farret, et al., 2012[32]: review report of the French ClubCO_2,

d) Porter, et al., 2015[81]: complete review of concentrations of impurities in power plants and in the industry.

The present document draws heavily upon the above publications because they contain a significant amount of data and because they generally identify the origins of these data. Of course, other publications are also considered, as well as other ISO works, such as Table A.1 from ISO/TC 265 standard 27913:2016[48] on pipeline transportation systems (see Annex B). References to publications lacking data source are avoided. For pre-combustion IGCC processes and for trace metals, many data encountered are unsourced.

Capture and purification processes are evolving and generally purity levels have increased. Several regulatory regimes require the CO_2 stream to consist "overwhelmingly" of CO_2. This is often approximated as a purity of at least 95 % (cf. ISO 27913:2016 on pipeline transportation systems).

Data on CO_2 stream composition are not readily at hand. The literature is not rich and is especially sparse on results from recent plants or pilot plants. Therefore, Technical Committee ISO/TC 265 addressed a data call to its member countries and to operators. Some technology suppliers could not answer the questionnaire for proprietary reasons. Original data from five capture pilots and demonstrators on power plants and one on a hydrogen production plant were collected, most of them are compared below to existing literature.

5.2 Ranges of impurity concentrations for coal fired power plants

5.2.1 Gaseous components

The composition of the CO_2 stream and thus the concentrations of the impurities varies from one capture technology to another. The flue gas from oxy-combustion is enriched in CO_2, SO_x and other minor components as a result of elimination of nitrogen from the air, and such products are then removed or captured downstream in the CO_2 purification unit. Oxy-combustion contributes to significant amounts of nitrogen, argon, and oxygen as well as oxidizing forms of sulfur and nitrogen (i.e. NO_x, SO_x) in the CO_2 stream. Post-combustion capture technologies usually produce CO_2 streams of high purity also containing oxidizing impurities such as O_2, SO_x, and NO_x. In contrast, pre-combustion capture results in impurities with reducing properties such as H_2, H_2S, or CO. However, even within a single capture technology the variability of impurity concentrations is high (up to two or three orders of magnitude; Figure 1), depending on the process itself and on the final purification steps (e.g., desulfurization equipment). Porter, et al. (2015)[81] present a summary of ranges for impurities from

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commonly considered CO_2 capture technologies for coal fired power plants. This publication references most of the previous publications, including individual results from specific plants. In Table 1 below, only data referring to the final CO_2 stream (after pre-compression and purification in the case of oxy-combustion) are reported, for common capture technologies.

Note Here, post-combustion capture technologies refer essentially to chemical absorption technologies based on amine solvent. Other post-combustion technologies exist such as membrane-based CO_2 separation process. The description of capture technologies is out of scope of this document. For more detailed information see ISO/TR 27912 (2015) Carbon dioxide capture systems, technologies, equipment and processes for power and industry[52].

Table 1 — Ranges from common CO_2 capture technologies for coal fired power plants (data from Porter, et al. 2015[81])

Impurities *(ppm, unless specified differently)*	Oxy-combustion with purification				Precombustion		Postcombustion	
	Double flashing		Distillation					
	Min	max	min	max	min	max	Min	max
Ar *% vol*	0,4	0,61	Trace	0,1	0,000 1	0,15	0,001 1	0,021
As					0,006 65	0,006 65	0,08	0,08
Benzene					0,014	0,014	0,019	0,019
CH_3OH					20	200		
CH_4					0	112		
Cl					17,5	17,5	0,56	0,56
CO			10	50	0	2 000	1,2	10
H_2					20	30 000		
H_2O	0	0	0	100	0,1	600	100	640
H_2S/COS					0,2	34 000		
Hg					0,000 584	0,000 584	0,024 9	0,024 9
N_2 *% vol*	1,6	2,03	0,01	0,2	0,019 5	1	0,045	0,29
Naphthalene					0,000 8	0,000 8	0,001 2	0,001 2
NH_3					38	38		
Ni					0,009	0,009	0,002	0,002
NO					400	400		
NOx	0	150	5	100	400	400	20 (1,5 NO_2)	38,8
O_2 *% vol*	1,05	1,2	0,001	0,4	0	0	0,003 5	0,015
Pb					0,004 5	0,004 5	0,001	0,001
Se					0,013 5	0,013 5	0,31	0,31
SO_2	0	4 500	0,1	50	25	25	1	67,1

NOTE "0" values are reported as such in Porter, et al. (2015); empty box indicates no available data as stated in Porter, et al. (2015).

For oxy-combustion, Porter, et al. (2015)[81] integrated many references from previous industrial and research projects, including measurements from the industrial capture pilot at Schwarze Pumpe (Anheden, et al., 2011[7]; White, et al., 2013[111]). For oxy-combustion, Porter, et al.[81] also considered raw/dehumidified CO_2 (those data are not reported in Figure 1). For oxy-combustion a pre-compression stage (15 bar to 30 bar) is usually performed before or during purification.

Further, Porter, et al.[81] compiled detailed data on CO_2 stream composition at different steps of the capture process for the oxy-combustion pilot plant at Schwarze Pumpe: Before purification, CO_2 purity is 87 % and O_2 content is 4 %, whereas after purification by rectification CO_2 purity is 99,9 % and O_2 content is <0,001 %;. SO_x concentrations decreased from <30 ppm before purification to <1 ppm after. Similarly, NO_x concentration is <350 ppm before purification and <10 ppm after purification.

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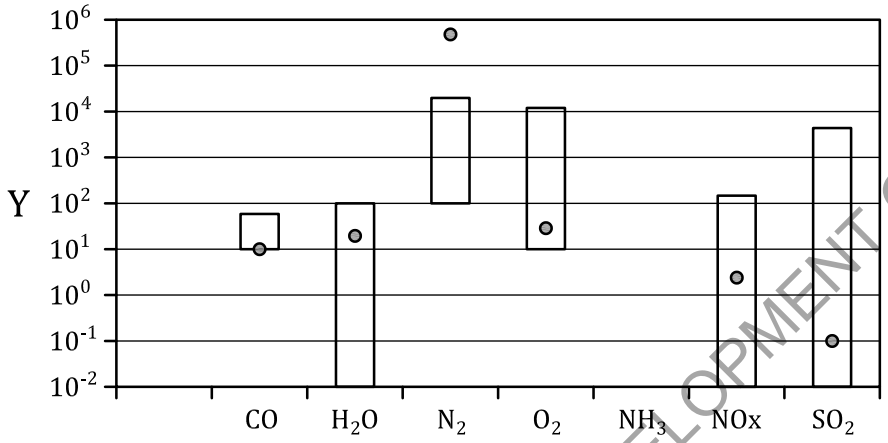
Figure 1 shows the ranges of impurity concentrations for oxy-combustion that are given in Table 3 of Porter, et al. (2015)[81] after purification by double-flashing or distillation phase separation. They are compared to recent values collected by ISO/TC 265 in 2017 on the Callide demonstrator plant.

Note Also considering Spero, C. Callide Oxyfuel Project — Final Results. Global CCS Institute, April 2018. http://decarboni.se/sites/default/files/publications/202090/cop-finalresults-publicreport-march2018.pdf



Keys

Y impurity content, ppm

□ range (Porter 2015)
New data ISO/TC 265, 2017

● Callide (Spero, 2018)

Figure 1 — Streams from oxy-combustion technology from Porter, et al., 2015[81] (bars) and recent values collected within ISO/TC 265 (symbols)

NOTE As concerns the Callide demonstrator plant, data for CO, NO_2 and SO_2 represent maximum values since measurements are below the detection limits for that specific project[15].

For post-combustion capture, Figure 2 below compares the concentration ranges according to Table 6 in Porter, et al. (2015)[81] to values recently collected within ISO/TC 265.

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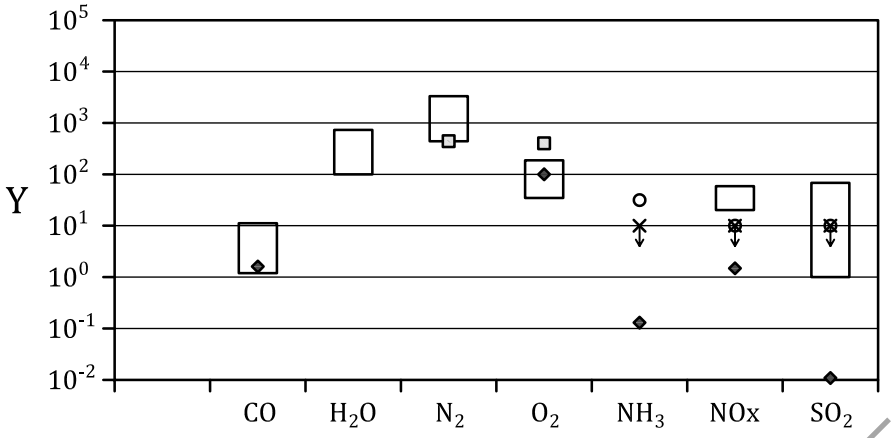

Keys

Y impurity content, ppm

□ range (Porter 2015)
New data ISO/TC 265, 2017

▫ SECARB

◆ Germany

○ CSIRO Loy Yang

× CSIRO Tarong

Figure 2 — Impurity concentrations for CO_2 streams from post-combustion capture from Porter, et al., 2015[81] (bars) and recent values collected within ISO/TC 265 (symbols)

NOTE Arrows on the Figure 2 represent measurements that are below the detection limits for that specific project.

These data show high variability of impurity concentrations, depending on the capture technology as well as site-specific process configurations. This variability is further discussed in 5.4.1.

5.2.2 Trace elements

Metallic elements in the CO_2 stream originate in the feedstock or fuel (e.g., coal). Their concentration is very low, hence they also called trace metallic elements or TMEs. IEAGHG (2011)[40] states that mercury (Hg) can be expected to be present with pre- and post-combustion processes. Apps (2007)[9] states that only Hg and Se are expected in high concentrations in gas phase, according to modelling results. Main values for metal concentrations are presented in Table 2 below.

For mercury, only estimated values were found in the literature (IEAGHG, 2004[39]; EC, 2011[27]; Apps, 2007[9]; Shah, et al., 2010[99]). The values are very low (sometimes below the detection limits) and show high variability (see examples in Figure 3 below). Given the toxicity of mercury, it is suggested that operators consider these reported concentrations with care and confirm by insitu measurements. Mercury removal from the CO_2 stream is likely during the downstream compression/drying stages, but uncertainties remain as it might be present both in the gas phase (because it is highly volatile) and in the particulate phase, adsorbed on aerosols (EC, 2011[27]).

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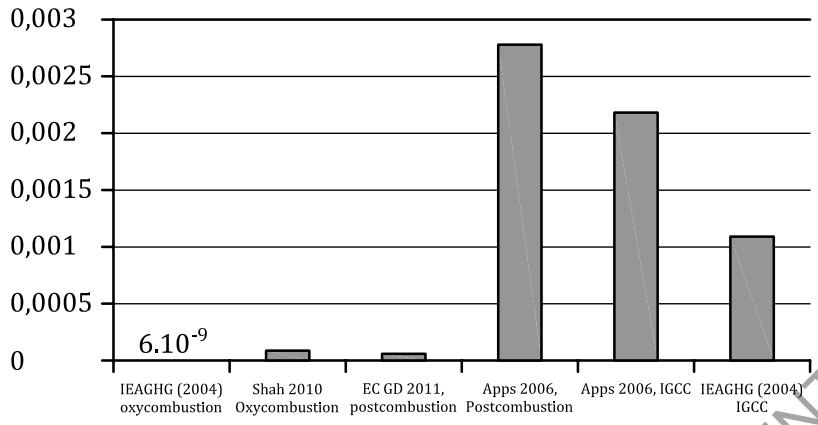

Figure 3 — Hg concentrations (ppm) in the CO_2 streams captured from coal power plants by different capture technologies estimated values, from Farret, et al. (2012)[33]

In contrast to metals, organics generally present no direct relationship between the elemental composition of the starting material and the subsequent concentration of organics in the CO_2 stream. The concentration of organics is usually very low and depends strongly on reaction conditions during industrial processes (CO_2 generation and capture) including gaseous species, temperature, pressure, and residence time. Examples for benzene and naphthalene concentrations are given in Table 2 below.

Table 2 — $C0_2$ impurities (trace elements) from pulverized coal with post-combustion (from Porter, et al., 2015[81])

	MEA postcombustion plant Source EC 2011[27] (estimated data)	Average values of relevant sources, including Anheden, et al., 2004[7], Apps, 2007[9], Oosterkamp & Ramsen, 2008[8], Farret, et al. 2012[33]
CO_2 % v/v	99,7	—
Hg ppm	0,000 69	0,002 8
As ppm	0,005 5	0,002 2
Se ppm	0,017	0,012 2
Mn ppm		0,03
Ni ppm		0,002
Pb ppm		0,001 1
Benzene ppm		0,019
Naphthalene ppm		0,001 2

5.2.3 Particulate matter

Particulate matter in solid or liquid form is a matter of concern in common industrial applications not specific to CCS, e.g. turbo machinery or jet engines. Particles in gas streams could considerably increase wear, e.g. in pipes or turbo machinery used for compression of gas streams for or during transport (booster stations), especially if high pressures and high fluid velocities are achieved. Particulate matter in the form of dust/particles or droplets can be present in captured CO_2 streams. For example, particulate matter might result from combustion processes or capture processes that are based on chemical looping. Post combustion capture applying amine solutions could introduce droplets into gas streams. Further downstream, corrosion products could potentially be transported within the CO_2 stream.

Note Chemical looping consists of using a metal oxide as a bed material providing the oxygen for combustion.

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5.3 Ranges of impurity concentrations from industrial emitters

Various industrial facilities emit considerable amounts of CO_2. In principle two different cases can be distinguished:

1) Energy-intensive industries, i.e. facilities requiring heat and/or other forms of energy for processing of their materials, such as pulp and paper mills, or recycling glass fabrication. For these facilities, application of post combustion or oxy-combustion capture technologies is comparable to their application to power plants and the final CO_2 stream composition depends on the fuel, the capture and cleaning processes.

2) Industry with process-related emissions, i.e. facilities processing raw materials, that emit CO_2 streams of variable compositions, e.g., H_2 production, cement and lime kilns, integrated iron and steel works, and bio-gas works.

For both cases, various options for CO_2 capture exist that can be retrofitted or integrated into production processes. Some raw materials contain carbon and other elements that are released during the processing leading to a further diversification of the resulting CO_2 streams. The application of CCS in industry sectors could represent half of the emissions reductions achieved through CCS by 2050 as mentioned in IEA (2013)[38] and GCCSI (2016)[36].

As compared to power plants described in 4.2, fewer data are available on CO_2 stream compositions from industrial facilities. One reason is that only very recently have the first pilot plants been set up for capturing CO_2 from industrial facilities that do not remove CO_2 from the product stream as part of their overall production process.

5.3.1 Cement industry

The cement industry is globally one of the major CO_2 emitting industries. Cement production takes place on all inhabited continents in large scale plants. Cement production consists of two major steps:

1) calcination, traditionally in shaft furnaces, nowadays mostly in multi-stage cyclone preheaters followed by pre-calciners (e.g., CEMCAP, 2017[18]);

2) clinker burning, mostly in long rotary kilns (ZEP, 2015[114]).

The calcination process yields about 60 % of the plant's total CO_2 emissions, and energy production accounts for the remainder. The clinker burning process is typically fuelled by coal and/or refuse-derived products (animal meal, sewage sludge, etc.).

CO_2 capture strategies on a cement plant include capturing the nearly pure CO_2 stream from the calcination process, using oxy-combustion in the rotary kiln, and applying post-combustion capture processes to the mixed gas streams from the calcination process and rotary kiln. Another envisaged option is calcium looping, in which the plant's first semi-product, the burnt lime, is used as an absorbent.

CO_2 concentration in cement plant flue gas is about 15 %–30 % (e.g., CEMCAP, 2017[18]), which is higher than in flue gases from fossil fuel power plants. The CO_2 stream composition after capture depends on where and how the CO_2 is captured as well as on the type of fuel burnt and its composition.

The cement industry is presently testing CO_2 capture in pilot plants in several countries including Norway, Belgium, the U.S., and China (e.g. LEILAC, 2016[60], Jordal, et al., 2017[56]). So far, measured composition data on CO_2 streams captured from these pilot plants have not been published. For reference, estimated/modelled values for CO_2 stream composition from post-combustion capture (amine scrubbing) at a cement plant are given in Table 3.

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