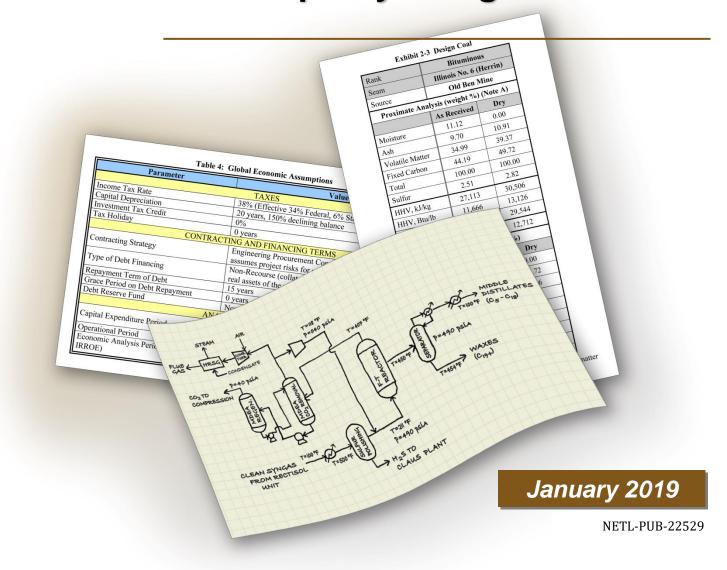




# QUALITY GUIDELINES FOR ENERGY SYSTEM STUDIES

# CO<sub>2</sub> Impurity Design Parameters





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# **CO<sub>2</sub> Impurity Design Parameters**

**Final Report** 

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# **Table of Contents**

1	Overview	11
2	Gas Stream Composition	12
	Venting	
	CCUS Technology-Specific Contaminants	
	Research Needs	
6	References	21
	FACHMENT A - QGESS Literature Search Spreadsheet	

# **Exhibits**

# **Acronyms and Abbreviations**

ACGIH	American Conference of	MEA	Monoethanolamine
	Governmental Industrial Hygienists	MESA	Mission Execution and Strategic
AEP	American Electric Power		Analysis
Ar	Argon	$mg/m^3$	Milligram per cubic meter
$C_2H_6$	Ethane	mol%	Mole percent
$C_3+$	Heavy hydrocarbons	MSDS	Material Safety Data Sheets
CCUS	Carbon capture, utilization, and	$N_2$	Nitrogen
	sequestration	NETL	National Energy Technology
$CH_4$	Methane		Laboratory
CO	Carbon monoxide	$NH_3$	Ammonia
$CO_2$	Carbon dioxide	NIOSH	National Institute for Occupational
COS	Carbonyl sulfide		Safety and Health
DOE	Department of Energy	NO	Nitric oxide
EOR	Enhanced oil recovery	$NO_2$	Nitrogen dioxide
EOS	Equations of State	$NO_x$	Oxides of nitrogen
FeCO <sub>3</sub>	Iron carbonate	$O_2$	Oxygen
FGD	Flue gas desulfurization	OSHA	Occupational Safety and Health Administration
$H_2$	Hydrogen	Dowt	
$H_2O$	Water	Part.	Particulates
$H_2S$	Hydrogen sulfide	$ppb_v$	Parts per billion (volume)
$H_2SO_4$	Sulfuric acid	ppm	Parts per million
HCl	Hydrochloric acid	$ppm_{v}$	Parts per million (volume)
HCN	Hydrogen cyanide	psig	Pounds per square inch gauge
HF	Hydrogen fluoride	QGESS	Quality Guidelines for Energy System Studies
Hg	Mercury	SAS	Saline aquifer sequestration
$HNO_2$	Nitrous acid	SCR	Selective catalytic reduction
IDLH	Immediately Dangerous to Life and Health	$SO_2$	Sulfur dioxide
IEA	International Energy Agency	$SO_x$	Sulfur dioxide
IGCC	Integrated gasification combined	TWA	Total Weighted Average
IGCC	cycle	TWA8	8-hour time weighted average
KSI	Kilopound per square inch	U.S.	United States
lbs/MMSCF	Pounds per million standard cubic	vol%	Volume percent
	feet		•

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## 1 Overview

This section of the Quality Guidelines for Energy System Studies (QGESS) provides recommended impurity limits for carbon dioxide (CO<sub>2</sub>) stream components for use in conceptual studies of CO<sub>2</sub> carbon capture, utilization, and storage systems. These limits were developed from information consolidated from numerous studies and are presented by component and application. Impurity levels are provided for carbon steel pipelines, sequestration through enhanced oil recovery (EOR), saline aquifer sequestration (SAS), and co-sequestration of CO<sub>2</sub> and hydrogen sulfide (H<sub>2</sub>S) in saline reservoirs. This QGESS is intended as a guideline only for conceptual studies under a generic scenario and should not be used for actual projects, which are likely to have requirements that differ from the generic scenario assumed herein.

Exhibit 2-1 provides the recommended limits for CO<sub>2</sub> stream impurities required by carbon steel transportation pipeline, EOR applications, and saline reservoirs. Each of the three design cases presents a design point and a range independent of the other design cases. For most impurities, the range indicates the maximum and minimum values found in the literature review and does not necessarily represent recommended limits; however, some represent an unofficial industry standard or the lack of information. In most cases, the design value matches the most restrictive constraint. Details for the design value and range for each impurity can be found in the subsections below Exhibit 2-1. Depending on the exact composition of the CO<sub>2</sub> stream, pipeline corrosion is of concern. Corrosion testing is difficult because of the multiple variables involved but is critical to determine standards for corrosion levels. (1) The impurity limits described in Section 2 are for isolated impurities and do not address the interactions between impurities.

The first set of data is for the compressed CO<sub>2</sub> transmission pipeline. Because it is assumed that the CO<sub>2</sub> stream to be sequestered remains at a constant 2,200 psig, the pipeline values are assumed to be independent of distance for EOR or SAS. However, it may be worthwhile in future efforts to characterize the effect of potential pressure losses on recommended ranges for certain components, as many components show different characteristics at different pressures.

EOR values are based on multiple EOR-recommended specifications and current EOR operations. Certain impurity limits will change depending on the oil quality and location. Also, certain health and safety hazards govern the design limitations. Refer to the notes for each contaminant listed in Section 2 for further detail.

SAS, like EOR, has multiple sources of information including the experience at American Electric Power's (AEP) Mountaineer plant—the first large-scale CCUS project.

Venting CO<sub>2</sub>, whether due to an upset condition in the plant or due to start-up of the CCUS system, can have detrimental effects, especially if certain impurities are present. The outermost column in Exhibit 2-1 indicates if the component could contribute to a hazardous or unlawful situation, depending on the quantity and the plant's emissions permit.

Attachment A is a list of 55 different CO<sub>2</sub> specifications found during the literature review. Pipeline design guides, pipe transportation specifications, and recommendations from multiple sources were used to evaluate and recommend limits based on the CO<sub>2</sub> source, such as plant type, air quality control systems, fuel used, gas transmission length, and other variables. This guideline does not attempt to tailor itself to every potential source variable, rather it is based on

the pipe and destination (whether a saline reservoir or oil reservoir) parameters necessary for  $CO_2$  to be handled safely, efficiently, and cost effectively.

# **2** Gas Stream Composition

Exhibit 2-1 below lists the recommended maximum (or minimum when noted) CO<sub>2</sub> impurities for EOR or saline reservoir CCUS.

Exhibit 2-1 CO<sub>2</sub> stream compositions recommended limits

Component	Unit (Max unless otherwise noted)		on Steel eline	Enhanced C	Oil Recovery	Saline Re Sequest		Saline R CO <sub>2</sub> & I seques		Venting Concerns (See Section 3)
		Conceptual Design	Range in Literature	Conceptual Design	Range in Literature	Conceptual Design	Range in Literature	Conceptual Design	Range in Literature	ve.
CO <sub>2</sub>	vol% (Min)	95	90–99.8	95	90–99.8	95	90- 99.8	95	20–99.8	Yes-IDLH 40,000 ppm <sub>v</sub>
H₂O	ppmv	500	20–650	500	20–650	500	20– 650	500	20–650	
N <sub>2</sub>	vol%	4	- 7	1	0.01 - 2	4	- 7	4	0.01–7	
O <sub>2</sub>	vol%	0.001	0.001-4	0.001	0.001-1.3	0.001 0.001-		0.001 0.001–4		
Ar	vol%	4	0.01-4	1	0.01–1	4	0.01–4	4	0.01–4	
CH₄	vol%	4	0.01–4	1	0.01–2	4	0.01-4	4	0.01–4	Yes- Asphyxiate, Explosive
H <sub>2</sub>	vol%	4	- 4	1	- 1	4	- 4	4	- 4	Yes- Asphyxiate, Explosive
со	ppm₀	35	10-5000	35	10–5000	35	10- 5000	35	10– 5000	Yes-IDLH 1,200 ppm <sub>v</sub>
H₂S	vol%	0.01	0.002- 1.3	0.01	0.002-1.3	0.01	0.002- 1.3	75	10-77	Yes-IDLH 100 ppm <sub>v</sub>
SO <sub>2</sub>	ppm₀	100	10– 50000	100	10-50000	100	10– 50000	50	10–100	Yes-IDLH 100 ppm <sub>v</sub>
NOx	ppm₀	100	20–2500	100	20–2500	100	20– 2500	100	20– 2500	Yes-IDLH NO- 100 ppm <sub>v</sub> , NO <sub>2</sub> -200 ppm <sub>v</sub>
NH₃	ppm√	50	0–50	50	0–50	50	0–50	50	0–50	Yes-IDLH 300 ppm <sub>v</sub>
COS	$ppm_v$	trace	trace	5	0–5	trace	trace	trace	trace	Lethal @ High Concentrations (>1,000 ppm <sub>v</sub> )

Component	Unit (Max unless otherwise noted)		n Steel eline	Enhanced C	Dil Recovery	Saline Re Sequest		Saline R CO <sub>2</sub> & F sequesi		Venting Concerns (See Section 3)
	(Max unle	Conceptual Design	Range in Literature	Conceptual Design	Range in Literature	Conceptual Design	Range in Literature	Conceptual Design	Range in Literature	Venti (See
C <sub>2</sub> H <sub>6</sub>	vol%	1	0–1	1	0–1	1	0–1	1	0–1	Yes- Asphyxiant, Explosive
C <sub>3</sub> +	vol%	<1	0-1	<1	0-1	<1	0-1	<1	0–1	
Part.	ppm <sub>v</sub>	1	0–1	1	0-1	1	0–1	1	0–1	
HCI	ppm₀	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	Yes-IDLH 50 ppm <sub>v</sub>
HF	ppmv	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	Yes-IDLH 30 ppm <sub>v</sub>
HCN	ppm <sub>v</sub>	trace	trace	trace	trace	trace	trace	trace	trace	Yes-IDLH 50 ppm <sub>v</sub>
Hg	ppm₀	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	Yes-IDLH 2 mg/m³ (organo)
Glycol	ppb√	46	0–174	46	0–174	46	0–174	46	0–174	
MEA	ppm√	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	MSDS Exp. Limits 3 ppm <sub>v</sub> , 6 mg/m <sup>3</sup>
Selexol	ppm <sub>v</sub>	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	N.I.*	

<sup>\*</sup>Not enough information is available to determine the maximum allowable amount

Several of the contaminant design limits were developed to address specific potential issues common to several contaminants. Examples of these include the following:

- Nitrogen (N<sub>2</sub>), Methane (CH<sub>4</sub>), and Hydrogen (H<sub>2</sub>) all have a lower critical temperature that would require increased pipe strength to minimize ductile fracture potential. (2)
- Non-condensables (N<sub>2</sub>, Oxygen (O<sub>2</sub>), Argon (Ar), CH<sub>4</sub>, H<sub>2</sub>) should be limited to reduce the amount of compression work; total non-condensables should be limited to less than 4 percent by volume. (3) In addition, non-condensables not only replace CO<sub>2</sub> in storage but reduce the density of the mixture causing total storage capacity to drop. (4) In addition, these non-condensables can affect the required well depth and injection pressure, as well as the injection lifetime of the well. It is estimated that for a flue gas of 80 mol% CO<sub>2</sub> and 20 mol% N<sub>2</sub> the pipeline capital cost and operational costs of the injection system would increase 10–25 percent. Additionally, the depth requirements increase 10–20 percent, and the flue gas would take up 2–4 times more pore space than a pure CO<sub>2</sub> stream. (5)

- Some of the component limits are based on the toxicity of the component (i.e., carbon monoxide (CO), H<sub>2</sub>S), which becomes a concern because of the potential for inadvertent releases. Toxic components with Immediately Dangerous to Life and Health (IDLH) concentration set by the National Institute for Occupational Safety and Health (NIOSH) (6) are listed in Exhibit 2-1. The IDLH concentration is not a short-term exposure limit to be encountered under normal working conditions, but a concentration from which escape may be made in 30 minutes without injury or irreversible health effects, and without deleterious/severe impediment to escape.
- EOR has specific limitations on O<sub>2</sub> concentration due to potential unwanted exothermic reactions with the hydrocarbons and limitations on H<sub>2</sub>S and sulfur dioxide (SO<sub>2</sub>), as they can be reproduced at the pumping well when the CO<sub>2</sub> front breaks through.

Additional information on specific contaminants is provided below.

#### 2.1 CO<sub>2</sub>

Once all impurities in the gas stream are identified and measured, the  $CO_2$  component is arrived at by difference. The range was determined from multiple sources and can be affected by cosequestration and levels of impurities. The highest concentration listed as a design parameter in the literature search that didn't include food-grade specifications is 99.8 percent. (7) The IDLH for  $CO_2$  is 40,000 ppm. (6)

#### 2.2 Water (H<sub>2</sub>O)

Moisture content requirements vary widely and depend mostly on the amount of sulfur and other impurities in the gas stream. The lower range is typically for higher sulfur content and the higher range is for lower sulfur content. Sulfur and H<sub>2</sub>O can combine to form sulfuric acid (H<sub>2</sub>SO<sub>4</sub>), which corrodes standard piping. Many moisture content specifications in the literature were derived from instrument air standards producing an unnecessarily stringent requirement. Multiple design parameters mention a maximum of 30 lbs/MMSCF (650 ppm<sub>v</sub>). 500 ppm<sub>v</sub> was chosen as a compromise among the multiple sources ranging from 20 ppm (8) to 30 lbs/MMSCF (650 ppm<sub>v</sub>) with many in the higher range. (2) Moisture content, however, is very site-specific depending on the other impurities such as oxides of nitrogen (NO<sub>x</sub>) and sulfur dioxide (SO<sub>x</sub>), which can form acids in the presence of H<sub>2</sub>O. (4) H<sub>2</sub>O in the presence of CO<sub>2</sub>, NO<sub>x</sub>, and SO<sub>x</sub> can form equipment damaging hydrates, depending on the pressure and temperature. Therefore, dehydration may be required at frequent intervals, particularly compression stages. (9) In carbon steel pipelines, "rigorously dry CO<sub>2</sub>" does not cause corrosion. However, the introduction of H<sub>2</sub>O has compounding effects on other impurities, such as O<sub>2</sub> and SO<sub>2</sub>. (10)

## $2.3 N_2$

The design point for  $N_2$  was taken from multiple sources with the range being set by pipeline specification. (2) (7)  $N_2$  is a non-condensable species requiring additional compression work and has a concentration limit of typically less than 4 percent by volume (11) for most applications; however, it should also be noted that  $N_2$  compression concentration could be as high as 7 percent by volume when coming from an oxycombustion system, but it is not recommended. (8) As mentioned earlier, the presence of  $N_2$  can also require increased transport pipe strength due to ductility issues. For EOR applications,  $N_2$  increases the miscibility pressure, making it more difficult to recover oil, which requires the design limit to be reduced to 1 percent by volume. (3)

#### $2.4 O_2$

O<sub>2</sub> is another non-condensable species requiring additional compression work and a concentration limit of less than 4 percent by volume (11) for most applications. The German Federal Institute for Materials Research and Testing in Berlin conducted testing on pipe material with O<sub>2</sub> concentrations up to 6,600 ppm (0.66 percent by volume) and found no negative pipeline effects when SO<sub>2</sub> concentration was kept to a minimum. (12) However, O<sub>2</sub> in the presence of H<sub>2</sub>O can increase cathodic reactions causing thinning in the CO<sub>2</sub> pipeline. (13) Because of this, the typical standard found for pipeline designs is 0.01 percent by volume; however, operating pipelines tend to be even more conservative in the 0.001 to 0.004 percent by volume range. (8) The maximum O<sub>2</sub> content was set by specification (2), which is also used by the AEP Mountaineer project. (14) Preliminary conclusions from an ongoing National Energy Technology Laboratory (NETL) study indicate that the cost of a CO<sub>2</sub> purification system used to lower O<sub>2</sub> content doesn't vary significantly based on final O<sub>2</sub> concentration (10,100 or 1,000 ppm<sub>v</sub>).

The introduction of  $O_2$  can inhibit the formation of iron carbonate (FeCO<sub>3</sub>), which is a protective layer that works to prevent corrosion.  $O_2$  also provides cathodic reaction paths that lead to corrosion of carbon steel pipes. (10)

 $O_2$  can also cause the injection points for EOR to overheat due to exothermic reactions with the hydrocarbons in the oil well. (15) In addition, high  $O_2$  content can cause aerobic bacteria to grow in the reservoir and at the injection points. (16)

In sequestration applications, O<sub>2</sub> can react with SO<sub>2</sub> forming H<sub>2</sub>SO<sub>4</sub>, and nitric oxide (NO) forming nitrogen dioxide (NO<sub>2</sub>), which in H<sub>2</sub>O, could form nitrous acid (HNO<sub>2</sub>). Dissolved O<sub>2</sub> can also react with the caprock if it contains iron, manganese, and other metals. If dissolved ferrous ions are present in H<sub>2</sub>O within the formation, ferric oxide-hydrate, or ferric hydroxide, could form potentially plugging pore space as well. (4)

#### 2.5 Ar

Ar is another non-condensable species requiring additional compression work and a typical limit of less than 4 percent by volume. (11) For EOR applications, Ar also increases the miscibility pressure, reducing its EOR limit to 1 percent by volume. (3)

#### 2.6 CH<sub>4</sub>

CH<sub>4</sub> is another non-condensable species with a lower critical temperature requiring increased pipe strength due to ductility issues (2), and typically limited to concentrations of less than 4 percent by volume (3) as outlined earlier. The design point is taken from multiple sources. The CH<sub>4</sub> range was set by pipeline specification. (7) (2) CH<sub>4</sub> also increases the miscibility pressure, making it more difficult to recover oil, so the EOR limit is reduced to 1 percent by volume. (3)

#### $2.7 H_2$

H<sub>2</sub> is another non-condensable species with a lower critical temperature requiring increased pipe strength due to ductility issues (2) and is typically limited to concentrations of less than 4 percent by volume (3) as outlined earlier. The design point was taken from multiple sources. The range was set by pipeline specification. (17) (8) H<sub>2</sub> also increases the miscibility pressure, making it more difficult to recover oil, so the EOR limit is reduced to 1 percent by volume. (3)

#### 2.8 CO

CO is toxic and is thus controlled more stringently due to fears of unintended release into the atmosphere. The Total Weighted Average (TWA) concentration limit, set by NIOSH, is 35 ppm<sub>v</sub>. The TWA is the maximum allowable average concentration of a chemical in air for a normal 8-hour working day and 40-hour work week. (7) The range is set by the previous NETL Systems Analysis Guidelines as the minimum and the maximum was derived from Vattenfall. (7) Other specifications not addressing health hazards allow for concentrations in the 1000–5000 ppm<sub>v</sub> range. (18) (8) This toxic gas can also be a concern for EOR as it can be released at the pumping well when the CO<sub>2</sub> front breaks through. The IDLH concentration for CO is 1,200 ppm<sub>v</sub>. (6)

#### $2.9 H_2S$

H<sub>2</sub>S is toxic and concentrations for non-sequestration applications are set at 0.01 percent by volume based on the IDLH concentration from NIOSH. (6) As discussed earlier, the IDLH concentration is not a short-term exposure limit to be encountered under normal working conditions, but a concentration from which escape may be made in 30 minutes without injury or irreversible health effects and without deleterious/severe impediment to escape. The targeted value of 0.01 percent by volume falls between the TWA recommendation from NIOSH of 10 ppm, which would be extremely costly to obtain, and the 200-ppm recommendation in *DYNAMIS* CO<sub>2</sub> quality recommendations. (11) The 200-ppm recommended limit was established based on health and safety effects by applying a safety factor of 5 on the known maximum exposure limit of 1000 ppm. (11) The maximum range limit of 1.3 percent by volume is from Vattenfall, one of the few references to specify a limit. (7) The H<sub>2</sub>S co-sequestration limit is based on NETL's Carbon Sequestration Systems Analysis Technical Note 10 (19) with the highest concentration, 77 percent, taken from the literature review. (20) It should be noted, however, that large quantities of H<sub>2</sub>S co-sequestered with CO<sub>2</sub> is done with the absence of O<sub>2</sub>. With the presence of SO<sub>2</sub>, elemental sulfur could be deposited in the rock formation's pores, especially if a catalyst is present in the rock formation, such as alumina or silica. The loss of sequestration space can be significant. (4) Because of its toxicity, H<sub>2</sub>S can be a concern for EOR, as it can be emitted at the pumping well when the CO<sub>2</sub> front breaks through.

#### 2.10 SO<sub>2</sub>

The literature review indicates that a design level of 100 ppm<sub>v</sub> for SO<sub>2</sub> is easily achievable with current air quality control systems. (2) (11) Additionally, SO<sub>2</sub> is being investigated for cosequestration with CO<sub>2</sub>. Preliminary reports predict that 5 percent by volume (50,000 ppm<sub>v</sub>) could be captured and have a negligible effect on the critical point of CO<sub>2</sub>. (21) The Global CCS Institute study on the effects of impurities on geological storage of CO<sub>2</sub> found that SO<sub>x</sub> can increase dissolution of the caprock, as it can form H<sub>2</sub>SO<sub>4</sub>; however, concentrations at 200 ppm or lower should have an insignificant impact. (4) The IDLH for SO<sub>2</sub> is 100 ppm<sub>v</sub> (6); therefore, this potentially toxic concentration can be a concern for EOR, as it can be reproduced at the pumping well when the CO<sub>2</sub> front breaks through. Vattenfall is one of a few entities to set this limit, so their value is used as the design target for SO<sub>2</sub> and the range's maximum amount. (7) Cosequestration of H<sub>2</sub>S and CO<sub>2</sub> has a reduced maximum SO<sub>2</sub> than the other scenarios. This is because injection of H<sub>2</sub>S in conjunction with SO<sub>2</sub> can result in the deposition of elemental sulfur causing severe pore blocking. (4) In the absence of H<sub>2</sub>O, SO<sub>2</sub> will not corrode carbon steel pipes. (10)

#### $2.11 \text{ NO}_{x}$

The literature review indicates that a design level of 100 ppm for NO<sub>x</sub> is easily achievable with current air quality control systems. (17) (11) The NO<sub>x</sub> range was determined from a reference study that included the minimum and maximum values. (7) The Global CCS Institute study on the effects of impurities on geological storage of CO<sub>2</sub> found that NO<sub>x</sub> can increase dissolution of the caprock, as it can form NO; however, concentrations at 200 ppm<sub>v</sub> or lower should have an insignificant impact. (4) This toxic gas at higher concentrations can be a concern for EOR, as it can be reproduced at the pumping well when the CO<sub>2</sub> front breaks through. The IDLH limits for NO and NO<sub>2</sub> are 100 ppm<sub>v</sub> and 200 ppm<sub>v</sub>, respectively. (6)

#### 2.12 Ammonia (NH<sub>3</sub>)

The allowed concentration at the AEP Mountaineer CCUS project is 50 ppm<sub>v</sub>. It is one of the few physical plants outlining an NH<sub>3</sub> concentration. Because of this, it was set as the design point and maximum amount. The IDLH for NH<sub>3</sub> is 300 ppm<sub>v</sub>. (6)

#### 2.13 Carbonyl Sulfide (COS)

This toxin can be a concern for EOR, as it can be reproduced at the pumping well when the  $CO_2$  front breaks through. Vattenfall is one of few entities to set this limit, so their value is used as the design target for COS and the range's maximum amount. (7) Although an IDLH has not been established for COS, it is known to be lethal at high concentrations (>1000 ppm<sub>v</sub>).

#### 2.14 Hydrogen Cyanide (HCN)

These design parameters are established by Vattenfall. (7) Further research is needed as no other references were found other than ones that allowed trace amounts. This is a toxic compound with an IDLH of 50 ppm. (6)

# 2.15 Ethane (C<sub>2</sub>H<sub>6</sub>)

These design parameters are based on Dixon Consulting EOR, Dakota Gasification specification, and Strawman Composite. (18) Although this is not a toxic compound, it is potentially explosive and might cause asphyxiation at high concentrations.

# 2.16 Heavy Hydrocarbons (C<sub>3</sub>+)

These design parameters are based on Dixon Consulting EOR, Dakota Gasification specification, and Strawman Composite. (18)

#### 2.17 Particulate

These design parameters are based on Dixon Consulting EOR, Dakota Gasification specification, and Strawman Composite. (18)

# 2.18 Hydrochloric Acid (HCl)

Not enough information is available to determine the maximum allowable amount. Future research is needed. HCL is a toxic compound with an IDLH of 50 ppm<sub>y</sub>. (6)

## 2.19 Hydrogen Fluoride (HF)

Not enough information is available to determine the maximum allowable amount. Future research is needed. HF is a toxic compound with an IDLH of 30 ppm<sub>v</sub>. (6)

#### 2.20 Mercury (Hg)

Not enough information is available to determine the maximum allowable amount. Future research is needed. Hg is a toxic compound with an IDLH of 10 mg/m<sup>3</sup> for compounds and 2 mg/m<sup>3</sup> for organomercury.

## 2.21 Glycol

Pipe specification limits were used because excess glycol carry-over can cause damage to seals and other components. (2) The range here is a value of zero to the maximum value of 174 ppb<sub>v</sub>, which is listed in the International Energy Agency (IEA) presentation referenced as an "Industrial Working Group Prelim Spec 2005." (18)

#### 2.22 Monoethanolamine (MEA)

Not enough information is available to determine the maximum allowable amount. Future research is needed. Although MEA is not an acute toxin and does not have an IDLH, Material Safety Data Sheets (MSDS) 8-hour time weighted average (TWA8) exposure limits are 3 ppm (TWA8 American Conference of Governmental Industrial Hygienists (ACGIH)) and 6 mg/m<sup>3</sup> (TWA8 Occupational Safety and Health Administration (OSHA)).

#### 2.23 Selexol

Not enough information is available to determine the maximum allowable amount. Future research is needed.

# 3 Venting

Venting of CO<sub>2</sub> will occur during start-up of the CCUS system as well as during upset conditions of the plant. Standards for venting are complex and extremely area specific. Exhibit 2-1 outlines specific contaminants that could cause a hazard to the populace, such as the hydrocarbons and sulfur components. Toxic contaminant IDLH levels are presented in Exhibit 2-1. In addition, M.W. Kellogg considered other items (22):

- Local, national, and international regulations
- Contaminants in the stream—particularly NH<sub>3</sub> (ammonia slip), H<sub>2</sub>S, other sulfur components, and hydrocarbons—and how they affect the plant's emissions permit
- Duration and frequency of venting
- Dispersion scenarios including a range of atmospheric conditions and proximity to population centers

M.W. Kellogg also indicated that atmospheric dispersion is the largest safety concern. If the dispersion does not occur rapidly enough, a dense CO<sub>2</sub> plume could drop to grade level and might cause asphyxiation. In that event, the recommendation is to flare the gas by adding natural gas to disperse the dense mixture before igniting it.

# 4 CCUS Technology-Specific Contaminants

Some contaminants are specific to the CO<sub>2</sub> capture technology employed. Below is a list of specific concerns and major contaminants associated with pre-combustion, post-combustion, and oxycombustion technologies.

#### 4.1 Pre-Combustion

For the purposes of this guideline, pre-combustion capture from an integrated gasification combined cycle (IGCC) unit is assumed. Pre-combustion produces a fairly clean CO<sub>2</sub> stream. Organic impurities can still be present, as complete combustion that may remove them does not take place prior to CO<sub>2</sub> separation. These include CH<sub>4</sub>, HCN, COS, and other sulfur compounds. These compounds can cause corrosion and formation of hydrates during CCUS. Some of these impurities are also toxic to humans. (7)

Depending on how the physical process works, the Selexol or other acid gas removal solvents might be found in the gas stream; however, it is unknown what amount of Selexol will cause damage to the CCUS system or the reservoir itself. (7)

#### 4.2 Post-Combustion

For the purpose of this guideline, a post-combustion MEA absorption system is assumed. CO<sub>2</sub> from a post-combustion process generally contains fewer numbers of different impurities than the other two technologies, as some may be consumed during combustion, as mentioned above. Still, the obvious NO<sub>x</sub>, SO<sub>x</sub>, and particulate can be a problem if the system does not have a properly functioning flue gas desulfurization (FGD), selective catalytic reduction (SCR), and/or baghouse. (23)

In addition, O<sub>2</sub> in the flue gas can lead to induced oxidative degradations of the MEA that can end up in the CO<sub>2</sub> product and cause corrosion. (24)

# 4.3 Oxycombustion

The  $CO_2$  stream from an oxycombustion process contains the excess  $O_2$  from the boiler. If no steps are taken to reduce  $O_2$  content, it can exceed 3 percent by volume. Boiler air in-leakage increases the impurity concentrations by introducing non-condensables such as Ar and  $N_2$  along with the  $O_2$  that can become part of the  $CO_2$  product. (25)

#### 5 Research Needs

Several areas of research have been identified to better understand the impact of contaminants in supercritical CO<sub>2</sub>, and their effect on transport and underground sequestration systems.

Although there is a significant amount of information available on pure supercritical CO<sub>2</sub>, there is very limited data on mixtures with contaminants and H<sub>2</sub>O. Information/data needs have been identified in the following areas:

- Supercritical CO<sub>2</sub> Equations of State (EOS) for supercritical mixtures including speed of sound, entropy, enthalpy, viscosity, dew point
- Simpler/faster algorithms or lookup tables for supercritical CO<sub>2</sub> mixtures

- CO<sub>2</sub> data at 10–15 kilopound per square inch (KSI) (1kilopound=1,000 lb/in²) at 400–700 K
- CO<sub>2</sub> corrosion and compressibility data with contaminants and H<sub>2</sub>O
- A better understanding of the supercritical CO<sub>2</sub> gas phase dynamics and contaminant impacts on phase diagrams at critical points
- A better understanding of CO<sub>2</sub> dehydration in order to reduce corrosion and hydrate formation

Additional areas of research have also been identified to determine the impact of impurities on the underground sequestration of CO<sub>2</sub> including the following:

- Impact on plume dispersion
- The effect on the physical properties of storage formation, including the density and wettability of the rock; and the potential for contaminants to react in the formation, which may impact the functioning of the sequestration system
- The effect on potential anaerobes at injection depths and their potential for creating plugging and contamination issues
- Data on supercritical CO<sub>2</sub>-mixture storage in coal seams, including the effect on coal mechanical properties, swelling, CO<sub>2</sub> sorption, and CO<sub>2</sub> permeation
- Solubility data of SO<sub>2</sub> and H<sub>2</sub>S in brine for saline reservoir storage

Information needs have also been identified to better understand the impact of supercritical CO<sub>2</sub> contaminants on the transport pipeline. These include the following:

- Impact of pipeline pressure drops and temperature excursions
- Potential of additives to passivate corrosion
- Data on the response of elastomers (seals and gaskets) to supercritical CO<sub>2</sub> mixtures
- Design/methods to mitigate potential of boiling liquid expanding vapor explosion risks

Additional information also needs to be developed concerning the potential carryover of capture system components (NH<sub>3</sub>, amines) into the supercritical CO<sub>2</sub> stream.

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# **ATTACHMENT A - QGESS Literature Search Spreadsheet**

Туре	2		NETL DESIGN BASIS	8		NON-NETL DESIGN BASIS									
Application	ccs	EOR	EOR	ccs	ccs	ccs	ccs	ccs	ccs	Generic	Generic	Generic	Generic	Generic	Generic
Misc				Remote destin.							- Control of	MEA	Selexol	Selexol	- Guillian
8 585555	1					6	7	8	9	10	11				15
											Design Books	2010	Design Basis	Design Basis	
						Design Basis		Design Basis		Design Basis	Design Basis	Design Basis	Design Basis		
		Recommended CO <sub>2</sub>	Recommended CO	Recommended CO	Recommended CO	AND	Design Basis	SESSION CONTRACTOR	Design Basis	CCS or EOR, Oxyfuel.	CCS or EOR, Oxyfuel.	CCS or EOR, Post	CCS or EOR, IGCC,	CCS or EOR, IGCC, German Lignite	
		Sequestration Design Basis	Sequestration Design	Sequestration Design	Sequestration Design	CCS, Oxyfuel, Decker Coal	CCS, Oxyfuel, Decker	CCS, Oxyfuel, Decker Coal	CCS, Oxyfuel, Illinois #6	German Lignite	German Lignite	Combustion, German Lignite	German Lignite	1840 00 000	Design Basis
		N25000	Basis	Basis	Basis	9/4869	Coal	0.00000 0.0000000000000000000000000000	coal	Compression and	Compression and	19/5//e825	Compression and	Compression and drying, Selexol process,	Carbon Steel piping
	Current Systems	Remote EOR	Adjacent EOR	Remote Geological	Adjacent Geological	Compression and drying	Partial Condensation	Part. Cond. And Distillation	FGD,ESP,FF,Compres	drying, SO <sub>2</sub> removal	drying, CO <sub>2</sub> and SO <sub>2</sub> co- sequestration	Compression and drying, MEA Absorption	drying, Selexol process, H;S removal	CO2 and H2S co-	transporting CO <sub>2</sub>
	Analysis Guidelines CO <sub>2</sub> Specification	Carbon Sequestration	Carbon Sequestration	Carbon Sequestration	Carbon Sequestration		7th Annual conference	000000000	sion and drying	Vattenfall Utvecking,	Water Little Comment	CONTRACTOR SOCIO	W	sequestration	(*Pipeline Design and
	Specification	Systems Analysis Technical Note No. 10,	Systems Analysis	Systems Analysis	Systems Analysis	7th Annual conference on CCS (2008).	on CCS (2008),	7th Annual conference on CCS (2008),	ASME Turbo Expo	Stockholm, Sweden	Vattenfall Utveckling, Stockholm, Sweden	Vattenfall Utveckling, Stockholm, Sweden	Vattenfall Utveckling, Stockholm, Sweden	Vattenfall Utveckling.	Construction* ASME publication M
		Revised March 2007,	Technical Note No. 10, Revised March 2007,	Technical Note No. 10, Revised March 2007,	Technical Note No. 10, Revised March 2007,	*Considerations for	"Considerations for Treating Oxy-	"Considerations for	2007, "Impact of Gas	"CO <sub>2</sub> quality requirement for a	*CO <sub>2</sub> quality	"CO <sub>2</sub> quality	"CO <sub>2</sub> quality	Stockholm, Sweden "CO2 quality	Mohitpour)
		NETL Contact: Jared Ciferno	NETL NETL	NETL NETL	NETL NETL	Treating Oxy- Combustion Flue Gas	Combustion Flue Gas	Treating Oxy- Combustion Flue Gas	Phase Impurities on CO <sub>2</sub> Compression	system with CO <sub>2</sub>	requirement for a system with CO <sub>2</sub>	requirement for a system with CO2	requirement for a system with CO:	requirement for a	
		Caerno.	200000		CSAONE	Prior to Sequestration"	Prior to Sequestration*	Prior to Sequestration"	CO <sub>2</sub> Compression	capture, transport, and	capture, transport, and	capture, transport, and	capture, transport, and	system with CO <sub>2</sub>	
										storage.	storage.	storage.	storage.	capture, transport, and storage.	
CO2		>95 vol%	>95 vol%	not limited	not limited	72.2 mol%	94.5 mol%	99.7 mal%	89.019 mol%	91 vol%	90 vol%	99.8 vol%	97.8 voP%	95.6 vol%	
	233°K (-40°F) dew point	150 ppmv	150 ppmv	150 ppmv	no free water	l				1400 ppmv	1400 ppmv	1400 ppmv	1400 ppmv	1400 ppmv	380 - 650 ppmv
Water	028 86 48		- 100								17-32-4		2000		
N <sub>2</sub>	<300 ppmv	<40000 ppmv	<40000 ppmv	not limited	not limited	198000 ppm wt	328000 ppm vA	0 mol%	19420 ppm wt	6100 ppmv	6000 ppmv	210 ppmv	300 ppmv	300 ppmv	
02	<40 ppmv	<40 ppmv	<40 ppmv	<100 ppmv	<100 ppmv	48500 ppm wt	10800 ppm wt	0 mol%	47590 ppm wt	16000 ppmv	16000 ppmv	30 ppmv	unknown	unknown	
Ar	<10 ppmv	<10 ppmv	<10 ppmv	not limited	not limited	3.03 mol%	0.9 mol%	0 mol%	4.281 mol%	5.7 vol%	5.6 vol%	0.021 vol%	0.05 vol%	0.049 vol%	
CH4		<0.8 vol%	<0.8 vol%	<0.8 vol%	<4.0 vol%								350 ppmv	350 ppmv	
H <sub>2</sub>		uncertain	uncertain	uncertain	uncertain								1.7 vol%	1.7 vol%	
co		<10 ppmv	<10 ppmv	not limited	not limited	200 ppm wt	0 mol%	0 mol%		unknown	unknown	10 ppmv	1700 ppmv	1700 ppmv	
<b>H</b> ₂S		<1.3 vol%	<1.3 vol%	<75 vol%									0.01 vol%	2.3 vol%	
SO <sub>2</sub>		<40 ppmv	<40 ppmv	30000 ppmv	30000 ppmv	1600 ppm wt	2300 ppm wt	2500 ppm wt		760 ppmv	15000 ppmv	10 ppmv			
NO										2500 ppmv	2400 ppmv	20 ppmv	unknown	unknown	
NO <sub>2</sub>		uncertain	uncertain	uncertain	uncertain	0.03 mol%	400 ppmwt	500 ppm wt							
TOTAL Hydrocarbons		<5 vol%	<5 vol%	<5 volNi	<5 vol%							30 ppmv	unknown	unknown	
NH <sub>3</sub>		<10 ppmv	<10 ppmv	not limited	not limited					trace	frace	unknown	30 ppmv	30 ppmv	
HCI										trace	trace	trace	trace	trace	
HF										trace	trace	trace	trace	trace	
HCN										trace	trace		<5 ppmv	<5 ppm∨	
cos													<5 ppmv	<5 ppmv	
TOTAL Sulfur															
C₂H <sub>6</sub>															
C₀H₀															
C <sub>2</sub> +													2		
C3+												1		-	
volatile hydrocarbons															
TOTAL Inerts			-												
Hg										trace	frace	trace	trace	trace	
Metals										trace	frace	trace	trace	trace	
Particulate										<1 ppm	<1 ppm	<1 ppm	<1 ppm	<1 ppm	
Glycol															
MEA						i						unknown			1
Selexol													unknown	unknown	
Delivery Pressure	152 bar														
Delivery Temperature															
, + statute		0													1

Type Application	Generic	EOR	EOR	EOR	EOR	EOR	EOR	EOR	EOR	PIPE SPECI	FICATIONS EOR	Generic	Generic	Generic	Generic
Misc	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
	Design Basis DYNAMIS quality recommendation (Enka de Visser, "Dynamis CO; quality recommendations")	Design Basis  ENCAP WP 1.1 EOR Godelines ("Oxy*fuel Combustion: Progress and Remaining Issues", A. Sarofim)	Design Basis ENCAP WP 1.1 Severe Limt Case ("Oxy-fuel Combustion: Progress and Remaining Issues", A. Sarofm)	Kinder Morgan Pipeline Specification For EOR (Kinder Morgan CO <sub>2</sub> Company, 2003)	PCOR Bell Creek Pipeline Specification for EOR Coal Fired, Post Combustion (DNV-RP-J202 recommend practice by DNV 2010)	PCOR Bell Creek Pipeline Specification for EOR Coal Fired, Pre Combustion (DNV-RP-J202 recommend practice by DNV 2010)	PCOR Bell Creek Pipeline Specification for EOR Coal Fired, Oxyfuel (DNV-RP-J202 recommend practice by DNV 2010)	PCOR Bell Creek Pipeline Specification for EOR Gas Fired, Post Combustion (DNV-RP-J202	PCOR Bell Creek Pipeline Specification for EOR Gas Fired, Post Combustion (DNV-RP-J202 recommend practice by DNV 2010)	PCOR Bell Creek Pipeline Specification for EOR Gas Fired, Oxyfuel (DNV-RP-J202	Dixon Consulting EOR August 2001 (Air Products presentation at 2006 gastification conference)	Dynamis specification for concertration limits as presented at the CCS conference Trondhelm in 2007 (OosterKamp Presentation 2008 - R&D Foundation Polytec)	R&D Foundation Polytec Ppeline Specification Amine (OosterKamp Presentation 2008 - R&D Foundation Polytec)	R&D Foundation Polytec Pipeline Specification Oxyfuel (CosterKamp Presertation 2008- R&D Foundation Polytec)	R&D Foundation Polytec Pipeline Specification Pre-combustion (CosterKamp Presentation 2008 - R&D Foundation Polytec)
CO2	>95.5%	>90 vol%	>95 vol%	>95 vol%	g:							>95%	>99 vol%	>90 vol%	>95.6 vol%
Water	500 ppm	<500ppm	<5 ppm	<650 ppmv				10			<-5C dp @ 300 psia	500 ppm	N/A	N/A	N/A
N <sub>2</sub>			-7	<40000 ppmv	100 ppmv	300 - 6000 ppmv	37000 ppmv	100 ppmv	13000 ppmv	<42000 ppmv	<2.0% N2 & H2	<40000 ppmv	<0.17 vol%	70000 ppmv	6000 ppmv
02		100 ppm	100 ppm	<10 ppmw	100 ppmv	300 - 6000 ppmv	37000 ppmv	100 ppmv	13000 ppmv	<41000 ppmv	<2.0 ppmw	Storage <4 vol%, EOR <100 ppm	<100 ppmv	<30000 ppmv	trace
Ar					0.01 vol%	0.03-0.6 vol%	3.7 vol%	0.01 vol%	1.3 vol%	<41000 ppmv		<4 vol%	trace	<5 vol%	<0.05 vol%
CH4	Storage <4 vol%, EOR <2 vol%				0	0.01 vol%	0	0	2.0 vol%	0	<1.0%	Storage <4 vol%, EOR <2 vol%	<100 ppm	-	350 ppm
H <sub>2</sub>					0	0.8-2.0 vol%	0	0	1 vol%	0	<1.0%	<4 vol%	trace	trace	<3 vol%
co	2000 ppm			1000	0	300-4000 ppmv	0	0	400 ppmv	0		2000 ppm	<10 ppm	trace	4000 ppmv
H₂S	200 ppm	<50 ppm	<5 ppm	<20 ppmw	0	0.01-0.6 vol%	0	0	<0.01 vol%	0	<100 ppmw	200 ppm	trace	trace	<3.4 vol%
SO <sub>2</sub> NO		<50 ppm	<5 ppm <5 ppm		100 ppmv 100 ppmv	0	5000 ppmv 100 ppmv	100 ppmv 100 ppmv	0	100 ppmv 100 ppmv	50000 ppmv	100 ppm	<10 ppm	25000 ppmv	
NO <sub>2</sub>			Орри		100 ppint		тоо рршу	100 ppiliv		тоо рршу		100 ppm	<50 ppm	2500 ppmv	
TOTAL Hydrocarbons				<5 vol%		1.									
NH <sub>3</sub>															
HCI HF															
HCN			5 ppm			-									
cos		<50 ppm	10 ppm												
TOTAL Sulfur											<300 ppmw				
C₂H₅ C₀H₅											<1.0%				
C <sub>2</sub> +													<100 ppm		<0.01 vol%
C3+											<1.0%				
volatile hydrocarbons					2										10
TOTAL Inerts	<4 vol%	<4 vol%	<4 vol%												
Hg Metals															
Particulate															
Glycol				46 ppbv											
MEA															
Selexol Delivery Pressure															
Delivery Temperature															

