REPORT

A2.1.1: Literature review on hydrogen and carbon dioxide for primary reference materials for decarbonised gas grids

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This report was written as part of activity A2.1.1 from the EMPIR Metrology for Decarbonising the Gas Grid project. The three year European project commenced on 1st June 2021. For more details about this project please visit www.decarbgrid.eu.

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Introduction

This report is a brief survey of the recently published (2016–2021) review papers and governmental documents on pure hydrogen and pure carbon dioxide for CCS and CCUS. The intention of this document is giving a handout for discussions to identify gaps in primary reference materials for hydrogen and CCUS and to decide on the mixtures to be prepared in the activities A2.1.3, A2.1.4, and A2.1.5.

Literature Survey on Hydrogen

— H. Meuzelaar et al., Trace level analysis of reactive ISO 14687 impurities in hydrogen fuel using laser-based spectroscopic detection methods, *International Journal of Hydrogen Energy* 45, 34024–34036, 2020. DOI: https://doi.org/10.1016/j.ijhydene.2020.09.046

This paper by authors from VSL is on measurement standards and laser-based spectroscopic methods for the reactive compounds formaldehyde CH_2O, formic acid CH_2O_2, hydrogen chloride HCl, and hydrogen fluoride HF. The specifications refer to the standard ISO 14687 (specification for hydrogen in fuel cells) and the measurement results comply with the requirements given in ISO 14687 (see Table 1). Preparation methods for measurement standards based on permeation techniques are reported.
The authors have localized future research needs with mutual compatibility between analyzer setup and target compound and the development of a reliable (and to be mobile in prospective) multispecies analyzing technique.
An important paper cited therein is:
K. Arrhenius et al., Development and evaluation of a novel analyser for ISO14687 hydrogen purity analysis, *Measurement Science and Technology* 31, 075010, 2020. DOI: https://doi.org/10.1088/1361-6501/ab7cf3. In this paper, a method consisting of a gas chromatograph combined with cavity ring down spectroscopy to analyze the complete set of impurities mentioned in ISO 14687. An estimation of the costs for the analyzer is also given.

— C. Beurey et al., Review and survey of methods for analysis of impurities in hydrogen for fuel cell vehicles according to ISO 14687:2019, *Frontiers of Energy Research* 8, 615149, 2021. DOI: https://doi.org/10.3389/fenrg.2020.615149

This key paper by authors from both NMIs (NPL, VSL, RISE, CEM) and industry (Air Liquide) is a comprehensive survey of analysis methods and capabilities that are available and approved to execute analysis campaigns of gaseous compounds according to ISO 14687. The method performance with each impurity compound and the corresponding detection limits

are assessed. A cost estimation for a total analysis using the best-practice methods is also given.
The following future research needs are localized: halogenated compounds (definition of key halogenated compounds), switch from “sum or total” to “individual” compounds for sulfur-containing and halogenated species and for hydrocarbons; alignments of the – at now strongly differing and often cost-intensive – analysis methods, implementation of on-line methods (since most established methods are operated as off-line methods).

— T. A. Aarhaug et al., Assessment of hydrogen quality dispensed for hydrogen refuelling stations in Europe, *International Journal of Hydrogen Energy* 46, 29501–29511, 2021. DOI: https://doi.org/10.1016/j.ijhydene.2020.11.163

This paper by authors from NPL, two fuel cell companies from Norway and Germany, and a German research institute deals with hydrogen quality from refuelling stations. Samples from different stations were analyzed for impurities in an interlaboratory comparison according to the specifications given in ISO 14687 and SAE J2719.

— A. Murugan and N. Hart, Presentation “ISO TC 197 WG27 Task 3 Revision of ISO 14687 Grade A (and B)” by NPL, 2021.

Different hydrogen fuels according to the constitution from four different standards are given in this presentation:
(a) ISO 14687 Grade A, (b) ISO 14687 Grade B, (c) CEN TC 234 NWIP (HyQual), (d) BSI PAS 4444 (Hy4Heat)

The composition given in CEN TC 234 NWIP has been proposed for a candidate in corresponding WP of the DECARB project.

H_2 minimum mole fraction	98 cmol/mol
Total non-hydrogen	—
CO	1000 ppm (µmol/mol)
Total mercury	—
H_2S	—
Total sulfur (including H_2S)	10 mg/m^3
CH_4	—
CO_2	—
Total hydrocarbons	—
Hydrocarbon dewpoint	–2 °C
H_2O	50 mg/m^3
O_2	10 ppm
Ar	—
N_2	—

He	—
NH_3	10 mg/m^3
Halogenated compounds	< 0.05 ppm
Other impurities	Technically free

Analysis methods are existing for all impurities listed in ISO 14687 that can cope with the detection limits assigned to each compound.

Drawbacks: multiple methods required, sophisticated preparation and extended analysis times, detection limits often very close to the control threshold (operating at a method's limits can introduce disqualifying uncertainties)

Potential research targets: to analyze more compounds with one single method; less specified but more general methods; methods that are cheaper, faster, and have an easier handling; specification of mutual effects on the analysis results from the presence of multiple compounds – can another technique eclipse such effects?

Literature Survey on Carbon Dioxide (CCS, CCUS)

— R. T. J. Porter et al., Techno-economic assessment of CO_2 quality effect on its storage and transport: CO_2QUEST An overview of aims, objectives and main findings, *International Journal of Greenhouse Gas Control* 54, 662–681, 2016. DOI: https://doi.org/10.1016/j.ijggc.2016.08.011

This paper by multiple authors gives an overview of the objectives and findings of the European project CO_2QUEST. The techno-economic approach executed was based on a realistic-scale experimental test program accompanied with mathematical modelling. The main objectives were how to deal with typical CO_2 impurities from power plants, impact of CO_2 impurities on pipeline transport and geological storage using adapted test facilities, multicomponent CO_2-containing mixtures at CCS conditions investigated, and data for model improvement. An overview of CO_2 impurities from different capture technologies are given in Table 2.
The authors emphasized that methods have to be validated with highly accurate mixtures that qualify as reference materials.
Important reference for further reading:
R. T. J. Porter et al., The range and level of impurities in CO_2 streams from different carbon capture sources, *International Journal of Greenhouse Gas Control* 36, 161–174, 2015. DOI: https://doi.org/10.1016/j.ijggc.2015.02.016
This paper by authors from the University of Leeds, UK, reports CO_2 compositions in great detail with corresponding tables of composition and references.

— V. E. Onyebuchi et al., A systematic review of key challenges of CO_2 transport via pipelines, *Renewable and Sustainable Energy Reviews* 81, 2563–2583, 2018. DOI: https://doi.org/10.1016/j.rser.2017.06.064

This review paper by authors from Cranfield University, UK, is a holistic assessment on component impurities. Knowledge gaps are identified, recommendations for CO_2 quality are given (see Table 2), expected impurities from different CO_2 capture technologies, and the influence of impurities on phase behavior – for example, the change of the critical pressure – are reviewed and discussed.
CO_2 containing SO_2, NO_2, O_2, and H_2O is a particular challenge; there are few data on O_2, SO_2, Ar present in CO_2; uncertainty in the universally allowable free water concentration; effect of other impurities on the solubility of water; the authors strongly advocate investigations of multicomponent mixtures.

"In summary, there has been considerable work carried out on the effect of each impurity on both critical point and pipeline repressurisation distances. Most research on the effect of impurities on the thermodynamics of transported CO_2 is largely based on mono, binary and ternary considerations. For this reason, it is essential to quantify the holistic impacts of CO_2 impurities on transport line performance. This should be conducted at different impurity contents, for example, up to 20 %."

References for further reading: nos. 91, 92, 93 on thermophysical properties; no. 111 on moisture content in CO_2 pipelines; no. 114 managing the corrosion in pipeline steel; no. 231 on determination of dew points for CO_2 with impurities.

— US Department of Energy, National Energy Technology Laboratory, Quality Guidelines for Energy System Studies, CO_2 impurity design parameters, January 2019, NETL-PUB-22529
ESPA Authoring Template (doe.gov) (www.netl.doe.gov)

This document is a comprehensive survey of CO_2 contaminants and research needs (an individual section in the report) for CCUS from the perspective of the US Government. Exhibit (Table) 2-1 on page 12 lists the recommended maximum (or minimum when noted) CO_2 impurities for enhanced oil recovery (EOR) or saline reservoir CCUS.

— J. F. D. Tapia et al., A review of optimization and decision-making models for the planning of CO_2 capture, utilization and storage (CCUS) systems, *Sustainable Production and Consumption* 13, 1–15, 2018. DOI: https://doi.org/10.1016/j.spc.2017.10.001

This review by authors from the Philippines, Taiwan, and Malaysia provides a survey of process integration methods for CCUS technology. SO_x and NO_x are identified as crucial impurities for processes.
Reference for further reading: Mohd Nawi et al., 2016b

— Y. Xiang et al., Role of residual 2-amino-2-methyl-1-propanol and piperazine in the corrosion of X80 steel within an impure supercritical CO_2 environment as relevant to CCUS, *International Journal of Greenhouse Gas Control* 82, 127–137, 2019. DOI: https://doi.org/10.1016/j.ijggc.2019.01.006

The subject of this paper is corrosion behavior of pipeline steel by supercritical CO_2, with view on residuals from the CO_2 capture process using alkanolamines (e.g., 2-amino-2-methyl-1-propanol AMP, piperazine PZ). Corrosion tests and material characterization are discussed. The corrosion inhibition mechanisms of AMP and PZ with regards to the corrosion behavior of X80 steel in the supercritical CO_2 phase with impurities were investigated. The effect of different amines, amine concentration, and flow conditions were considered. An experimental CO_2 matrix for corrosion tests is given in Table 1.

— T. Flechas et al., A 2-D CFD model for the decompression of carbon dioxide pipelines using the Peng-Robinson and the Span-Wagner equation of state, *Process Safety and Environmental Protection* 140, 299–313, 2020. DOI: https://doi.org/10.1016/j.psep.2020.04.033

An equation of state model for phase behavior (expansion, non-equilibrium phase transition, fluid flashing) liquid-CO_2 pipeline transport is reported in this paper by authors from Texas A&M University. The authors conclude that abrupt expansion can cause pipeline rupture and that there is a need for precise and consolidated thermodynamic properties of the medium.
In the paper by K. K. Botros et al., Measurements of decompression wave speed in binary mixture of carbon dioxide and impurities, *Journal of Pressure Vessel Technology* 139, 021301, 2017, DOI: https://doi.org/10.1115/1.4034016, results for shock tube tests on binary mixtures of CO_2 with impurity compound are reported.

— US Department of Energy, National Energy Technology Laboratory, 2020 Carbon Capture Program R&D, Compendium of Carbon Capture Technology, May 2020 https://www.netl.doe.gov/sites/default/files/2020-07/Carbon-Capture-Technology-Compendium-2020.pdf

This document gives a detailed overview on CCS projects sponsored by the US Government; a summary of each project with a lot of technical information and references is given.

— H. Lu et al., Carbon dioxide transport via pipelines: A systematic review, *Journal of Cleaner Production* 266, 121994, 2020. DOI: https://doi.org/10.1016/j.jclepro.2020.121994

This paper discusses the influence of impurities on phase equilibrium and corrosion mechanisms in CO_2 pipelines, Tables with gas qualities (Tables 12 and 13) are provided. H_2S is identified as a particular challenge, *"Some researchers think that H_2S will slow down the corrosion rate of CO_2, while some researchers show that H_2S will increase the corrosion*

rate of CO_2."
References for further reading: Porter et al., 2015 (see above); Skaugen et al., 2016; Istre, 2019 (weblink)

— H. Wang et al., Carbon recycling – An immense resource and key to a smart climate engineering: A survey of technologies, cost and impurity impact, *Renewable and Sustainable Energy Reviews* 131, 110010, 2020. DOI: https://doi.org/10.1016/j.rser.2020.110010

This paper contains a thorough overview and detailed discussion of impurity effects on CCS and CCU. Various compositions (see Tables 4, 5, and 7), impurity sources and specific technical as well economic issues are discussed. Acidic compounds (SO_x, NO_x) are identified as the most problematic impurities in CCU processes, the differences of impurity effects on CCS and CCU are discussed.
References for further reading: no. 41 (impurity effects on electrodes), no. 281 (CO_2 quality recommendations), no. 282 (source of Table 7), no. 292 (impact of impurities, weblink), no. 293 (Skaugen et al., mentioned above), no. 294 (B. Wetenhall et al., The effect of CO_2 purity on the development of pipeline networks for carbon capture and storage schemes, *International Journal of Greenhouse Gas Control* 30, 192–211, 2014, DOI: https://doi.org/10.1016/j.ijggc.2014.09.016, effect of CO_2 impurities on pipeline networks with tables of various CO_2 specification)

— K. Smith et al., Modular CO_2 Capture Processes for Integration with Modular Scale Gasification Technologies: Literature Review and Gap Analysis for Future R&D, US Department of Energy, National Energy Technology Laboratory, Pittsburgh PA, October 2020, DOE/NETL-2020/2149. DOI: https://doi.org/10.2172/1668758 Modular CO2 Capture Processes for Integration with Modular Scale Gasification Technologies: Literature Review and Gap Analysis for Future R&D (doe.gov)

This document portrays and reviews modular scale gasification processes with precombustion CO_2 capture.

"The aim of this report is to assess the potential of integrating modular scale carbon capture processes with modular scale coal gasification technologies, and to help guide future research and development efforts in this area.
This report can be used to guide future R&D of pre-combustion carbon capture technologies and ensure they are well aligned with future gasification processes and end use applications."

— A. Murugan et al., Performing quality assurance of carbon dioxide for carbon capture and storage, *C – Journal of Carbon Research* 6, 76, 2020. DOI: https://doi.org/10.3390/c6040076

This review paper published by NPL reviews publicly available reports that specifically provide threshold amount fraction limits for impurities in CO_2 for the purpose of transport and storage together with background information for these limits. A carbon dioxide purity specification plus threshold amount fractions of impurities is provided on the basis of the findings, as well as recommendations on further work required to develop a suitable gas metrology infrastructure to support these measurements. These recommendations include primary reference materials, sampling methods, and instruments for performing purity analysis. Purity specifications (with references) are given in Tables 3 (for beverages) and 5, the analysis methods recommended in Table 6.

There are more specifications of CO_2 due to the multiple sources of origin, and the CO_2 quality issues are still less standardized than the corresponding H_2 quality issues. Analysis methods are existing for most impurities. The individual impurity thresholds strongly depend on the application (CCS or CCUS).

Drawbacks: multiple methods required, analysis methods have to be adapted to the process requirements, numerous different standards are therefore required

Potential research targets: similar to those for H_2; to analyze more compounds with one single method; less specified but more general methods; methods that are cheaper, faster, and have an easier handling; specification of mutual effects on the analysis results from the presence of multiple compounds; development of standards for the processes that operate with CO_2