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CO₂QUEST: Techno-economic assessment of CO₂ quality effect on its storage and transport

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Abstract

Presented is an overview of the CO₂QUEST project that addresses fundamentally important issues regarding the impact of typical impurities in the gas or dense phase CO₂ stream captured from fossil fuel power plants on its safe and economic transportation and storage. Previous studies have mainly investigated the impact of CO₂ stream impurities on each part of the carbon capture and storage (CCS) chain in isolation. This is a significant drawback given the different sensitivities of pipeline, wellbore materials and storage sites to the various impurities. The project brings together leading researchers and stakeholders, to address the impact of the typical impurities upon safe and economic CO₂ transportation and storage. State-of-the-art mathematical models, backed by laboratory and industrial-scale experimentation, are implemented to perform a comprehensive techno-economic assessment of the impact of impurities upon the thermo-physical phenomena governing pipeline and storage-site integrities.

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1. Introduction

The ultimate composition of the CO_2 streams captured from fossil fuel power plants and other CO_2 intensive industries and transported to a storage site using high pressure pipelines will be governed by safety, environmental and economic considerations.

So far, most studies performed on this topic have been limited in scope, primarily focusing on investigating the impact of the CO_2 stream impurities on each part of the carbon capture and storage (CCS) chain in isolation. This is a significant drawback given the markedly different sensitivities of the pipeline, wellbore materials, and storage sites to the various impurities. For example, trace elements such as lead, mercury and arsenic in the CO_2 stream are of far greater concern in an aquifer storage site than compared to the pipeline given the risk of water table contamination. On the other hand, even small concentrations of water in the CO_2 stream are detrimental to the pipeline due to corrosion, but of benefit even at high concentrations during storage given the immobilisation effect of water on CO_2. It is clear, therefore, that the optimum composition and concentration of the impurities in the captured CO_2 stream involves a delicate balance between the different requirements within the CCS chain, spanning capture, transportation and storage, with cost and safety implications being the over-arching factor.

CO_2QUEST brings together key partners from the EC FP7 CO_2PipeHaz (CO_2 pipeline transportation) and MUSTANG (CO_2 geological storage) projects [1, 2], as well as other leading researchers and major stakeholders, to address the important and urgent issues regarding the impact of typical impurities in the gas or dense phase CO_2 streams captured from fossil fuel power plants on its safe and economic transportation and storage.

The present paper describes the main objectives, methodology and some recent findings of the CO2QUEST project. In particular, Section 2 defines the project scope and methodology, Section 3 characterizes the CO_2 stream impurities and their physical properties, Sections 4 and 5 are focused upon the project's analysis of the impacts of CO_2 stream impurities on the pipeline transportation/compression and storage, whilst the methodology of the techno-economic and risk assessment are presented in Section 6, which is followed by conclusions in Section 7.

2. Project Methodology

The CO_2QUEST project involves the determination of the important CO_2 mixtures that have the most profound impact upon the pipeline pressure drop, compressor power requirements, pipeline propensity to ductile and brittle facture propagation, corrosion of the pipeline and wellbore materials, geochemical interactions within the wellbore and storage site, and ensuing health and environmental hazards. Based on a cost-benefit analysis and whole system approach, the project will provide recommendations for tolerance levels, mixing protocols and control measures for pipeline networks and storage infrastructure thus contributing to the development of relevant standards for the safe design and operation of CCS.

The CO_2QUEST project has five technical Work Packages (WP). Fig. 1 gives a schematic representation of the WPs relationship to the CCS chain. In particular, in WP1 the fluid properties and phase behaviour are characterised
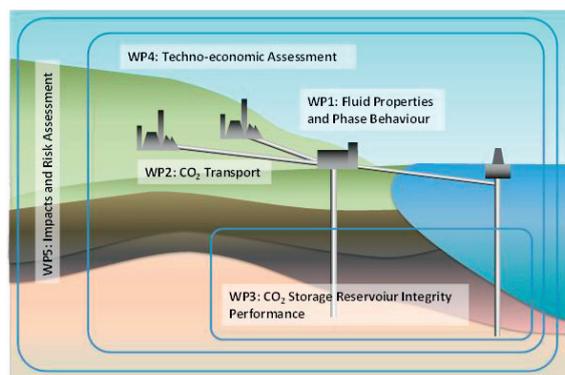

Fig 1. Schematic representation of the CCS chain, highlighting the different Work Packages in the CO_2QUEST project.

for CO_2 streams from different capture technologies. This work package provides the thermodynamic and physical properties data needed for the models to be developed under WP2 and WP3, focused on CO_2 pipeline transport (WP2) and CO_2 storage reservoir integrity performance (WP3). The latter work packages seek to generate validated modelling methods and tools for the assessment of pressure drop, compressor power, pipeline design and well design in the presence of impurities. In turn, these models will be utilized in WP4 to assess the techno-economic impact of common impurities. WP5 will demonstrate the usefulness of the tools by identifying potential environmental and health hazards.

3. CO_2 Streams Composition

Given the number of potential sources for CO_2, both from the power and non-power sectors, it will be necessary to consider in the cost-benefit analysis of CCS the CO_2 source and also the capture technology with which it will be matched. There are three main options for the decarbonisation of electricity generation: pre-combustion, post-combustion and oxy-fuel combustion. Whilst both pre-combustion and post-combustion technologies typically produce a CO_2 stream which is in excess of 98% pure, oxy-fuel combustion technologies can produce a CO_2 stream where the composition varies in the range of 74 to 99 vol%. This is illustrated in Table 1 [3] below.

In view of the above, and given the importance of accurate modelling of the thermodynamic properties and phase behaviour of CO_2 mixture properties, an extensive literature review of experimental data available for the properties of CO_2 mixtures with the impurities highlighted has been carried out. The review covered the vapour-liquid equilibria (VLE), volumetric and derivative thermodynamic properties and transport properties. As a result, knowledge gaps for the majority of CO_2 mixtures with impurities and properties of interest to CCS technology were identified. In particular, it was found that for binary CO_2 mixtures little data is available on derivative thermodynamic properties and transport properties, while the only property extensively studied in the literature is the VLE pressure of saturation as depicted in Fig. 2. As the complexity of the mixtures increases in terms of the number of components and conditions, the data become scarcer. In fact, the experimental data for isothermal compressibility found for the system CO_2-N_2-CH_4-H_2 [4], as well as the phase envelope, density, and viscosity for the system CO_2-N_2-O_2-Ar [5], are the most complex cases of CO_2 mixtures with gases that exist in the literature.

Table 1. Summary of CO_2 impurities from different capture technologies [3].

|	Oxy-fuel Combustion			Pre-combustion	Post-combustion
	Raw/ dehumidified	Double flashing	Distillation		
CO_2 % v/v	74.8-85	95.8-96.7	99.3-99.4	95-99	99.6-99.8
O_2 % v/v	3.21-6	1.05-1.2	0.01-0.4	0	0.0035-0.015
N_2 % v/v	5.8-16.6	1.6-2.03	0.01-0.2	0.0195-1	0.045-0.29
Ar % v/v	2.3-4.5	0.4-0.61	0.01-0.1	0.0001-0.15	0.0011-0.021
NO_x / ppmv	100-709	0-150	33-100	400	20-38.8
SO_2 / ppmv	50-800	0-4500	37-50	25	0-67.1
SO_3 / ppmv	20	-	20	-	
H_2O / ppmv	100-1000	0	0-100	0.1-600	100-640
CO / ppmv	50	-	50	0-2000	1.2-10
H_2S/COS / ppmv				0.2-34000	
H_2 / ppmv				20-30000	
CH_4 / ppmv				0-112	
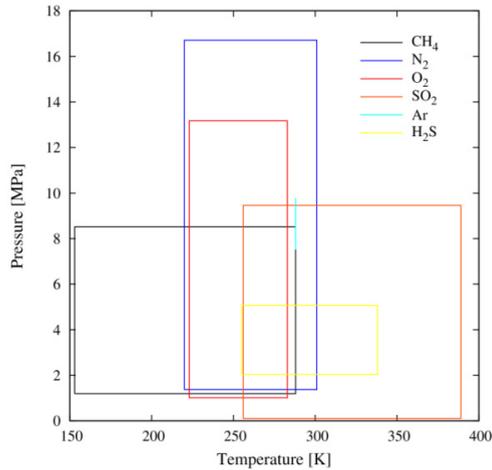
Fig. 2. Range of conditions of data for binary VLE data [6].

4. CO$_2$ Compression and Transport

Minimising the pressure drop and avoiding two-phase flows in CO$_2$ pipeline networks are essential for reducing compressor power requirements. This is critically important given that the compression penalty for CO$_2$ capture from coal-fired power plants is estimated to be as high as 12% [7].

In the past, three main options for compression of CO$_2$ from gas to supercritical pressures have been recommended for a pure CO$_2$ stream, including those using conventional multistage centrifugal compressors (option A), supersonic axial compressors (option B) and compressors combined with liquefaction followed by pumping (option C). Amongst these, option C was found to be the most efficient [8] and practically attractive, since pumping of a liquid is less energy demanding than gas-phase compression, whilst the relatively high boiling point of pure CO$_2$ (ca 20 °C at 60 bar) allows using utility streams for the liquefaction process. Supersonic shock-wave compressors can be used for compression of large amounts of fluid, and have the benefit of lower capital costs than traditional centrifugal compressors.

In the case of industrial-grade CO$_2$, however, the presence of impurities is inevitable and hence the choice of strategy and costs associated with compression will depend on the physical properties of the particular CO$_2$ mixture, such as fluid compressibility, density and saturation data. Fig. 3 illustrates the impact of impurities on the phase envelope for differing mixtures of compositions as defined in Table 1, in addition to pure CO$_2$. It can be observed
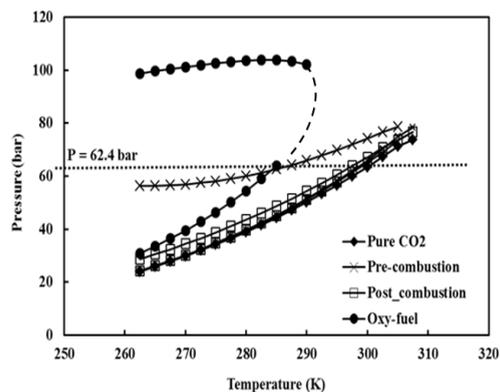

Fig. 3. Boundaries of VLE region in pressure-temperature phase diagram for pure CO$_2$ and oxy-fuel, pre- and post-combustion CO$_2$ mixtures calculated using the Peng-Robinson equation of state.
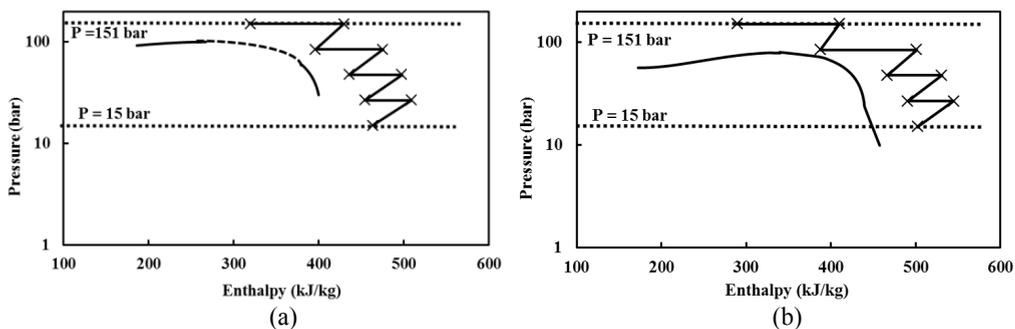
Fig. 4. The thermodynamic paths for compression of pure CO_2 (a), and CO_2 mixtures from oxy-fuel (b) using compression and pumping with subcritical liquefaction.

that the saturation pressures for oxy-fuel and pre-combustion mixtures diverge significantly from the saturation pressure for pure CO_2 and post-combustion mixtures.

The compression work, and hence the penalty incurred by the presence of impurities, has been calculated for the above-mentioned compression options and CO_2 stream compositions of Table 1. As an example, Fig. 4 shows the thermodynamic paths of four-stage compression with intercooling relative to the phase envelopes for pure CO_2 (a) and oxy-fuel (b) mixtures, whilst Fig. 5 shows the power consumption for each compression strategy (options A-C) for mixtures indicative of all capture technologies.

In agreement with the data published in the literature, the study shows that the integration of the multi-stage compression with liquefaction and pumping can greatly decrease the total power consumption (combining the power of compression and inter-cooling) as compared to conventional gas-phase compression. This option is particularly attractive for compression of almost pure CO_2, when liquefaction can be achieved using utility streams at 20 °C for post-combustion mixture of purity 99.46 vol%, and 8 °C for pre-combustion mixture (CO_2 purity about 98 vol%). At the same time, the cryogenic temperatures required for liquefaction of oxy-fuel CO_2 stream carrying 74-85 vol% of impurities (Table 1), may require use of extra power for refrigeration. Clearly, such information forms the foundation for practical optimization of CO_2 compression, which should be performed not in concert with other processes involved in CCS chain, such as the CO_2 capture and transport.

5. CO_2 Storage Reservoir Integrity Performance

For the successful application of CCS technologies, it is critically important to understand the effects of impurities upon the performance of geological CO_2 storage operations. Various aspects of these processes are being studied, including fluid/rock interactions, leakage of trace elements, and their impacts upon the subsurface environment. Laboratory and field-scale experiments are to be performed to assess the impact of impurities in the
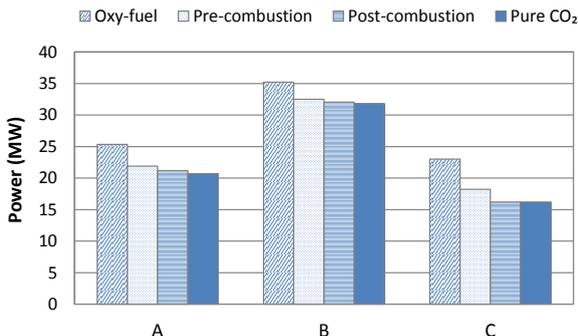

Fig. 5. Power demand for multistage compression (options A, B, and C) of pure CO_2, oxy-fuel (raw/dehumidified), pre- and post-combustion streams (Table 1).
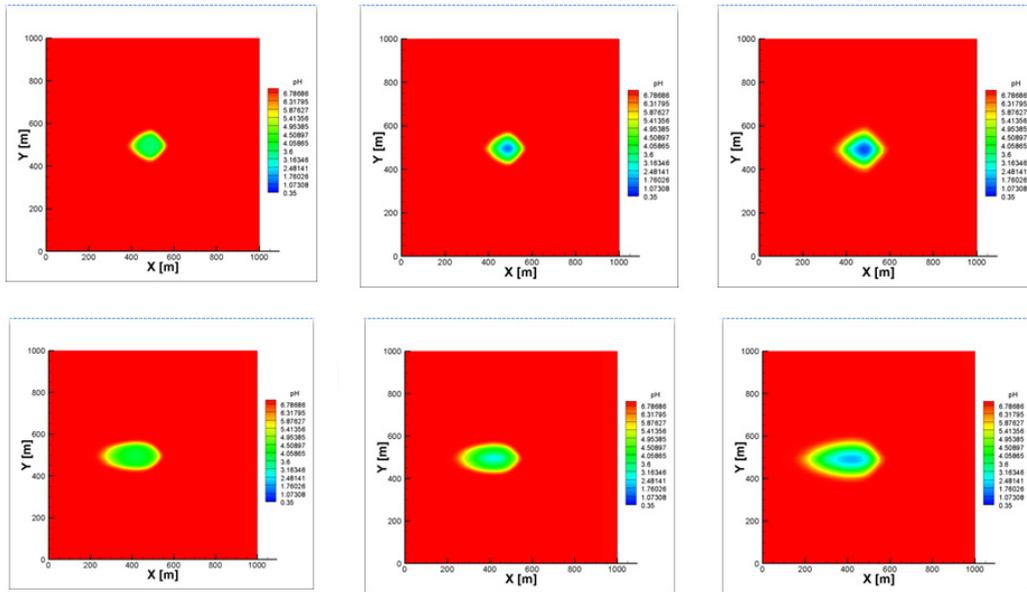
Fig. 6. Predicted pH levels for pure CO_2 (left), 2% SO_2 (middle) and 4% SO_2 (right) after 1 year (top) and after 10 years (bottom) at a height of 20 meters from the bedrock.

CO_2 stream on rock properties and its subsequent migration behaviour, and the overall effects upon the storage performance and caprock integrity. A significant component of the work will be a field scale injection experiment at Heletz, Israel [2], where CO_2 will be co-injected with impurities and the effects analysed. Simultaneously, numerical models are being developed to understand the physical and chemical processes involving impure CO_2 more clearly, and in particular, the multiphase fluid phenomenon of CO_2 spreading/trapping and the acidic chemical environment induced by impurities.

In the case of injection of impure CO_2, critical processes for the subsurface CO_2 injection are those which possibly exert negative impacts on the environment. CO_2 injection could lead to geochemical alteration and geomechanical deformation of the caprock, and alter its sealing capacity [9]. Co-injection of acidic species such as H_2S, SO_x and NO_x enhances the solubility of many minerals including those containing significant concentrations of hazardous trace elements such as As, and Pb. In the event of release with CO_2, they are likely to exacerbate the impact upon groundwater quality by the formation of strong metal-sulfide complexes [10, 11]. Also supercritical CO_2 is itself an excellent solvent for toxic organic compounds such as benzene, which can potentially be mobilized through the occurrence of a leak [12]. Impurities can also have a geochemical impact in a CCS scenario where CO_2 is injected for storage in a deep brine geological formation.

Depending upon the CO_2 capture process, the injected CO_2 may contain various compositions of residual O_2, SO_x, NO_x and inert gases. It is of interest to determine the environmental impact resulting from the inclusion of SO_2 in the CO_2 stream, and given the environmental and human health benefits of controlling SO_2 emissions [13], it may be economically advantageous to dispose of SO_2 together with the CO_2.

The impact of the injection of CO_2 with an impurity level of 2 vol% and 4 vol% SO_2-CO_2 has been investigated using a mathematical modelling method. The model was developed using the PHREEQC software to evaluate the sulfate ion distribution, and also the PFLOTRAN code to predict the fate of the injection streams of SO_2-CO_2 and SO_2(aq) in the target storage reservoir. This model estimates the highest impact obtained by the presence of a significant amount of SO_2 in the injection stream.

Fig. 6 shows the pH level at the ceiling of the reservoir, where the ceiling height is 20 m above the base. For the studied case of an injection period of one week, the influence on the pH level is noticeable adjacent to the injection well, but its impact is insignificant near the reservoir ceiling. In the case of long term injection of pure and impure CO_2 streams, a significant impact upon the pH level is observed. In addition, since corrosive water, having a low pH

level, can induce changes in the physical properties of the caprock, this model can serve as the basis for investigations of the effect of SO_2 impurity on the impervious cap.

6. Techno-economic Analysis and Risk assessment

For the techno-economic assessment of highly complex and inter-dependent CCS systems carrying impure CO_2 streams, a state-of-the-art methodology is being developed in WP4 of the project. The methodology uses a multi-scale, whole-systems treatment of the operation of a CO_2 capture and transport network with a view to identifying and quantifying the cost, operability and safety trade-offs that invariably exist within a network of this kind. The methodology will make use of the findings in WPs 1-3, and aims to gain an understanding of how the potential impurities may propagate in a simple linear systems and more complex collective and distributive CCS chains. The approach takes into account the chemistry implicit in mixing CO_2 rich streams from several sources, and also potential interactions between these mixtures and the pipeline materials and indeed during injection and storage.

In order to explore and quantify inherent trade-offs between the different components of the system, whole-system performance measures will be used. These will be backed up with a fit-for-purpose, model-based integrated assessment methodology [14], which is being designed using the concepts of operational envelopes and design spaces [15].

Whilst the costs of CO_2 capture depends to some extent on the desired purity of CO_2 there are benefits that come of improved purity on the performance of the transport and injection/storage system. It is therefore important to understand the relative costs and benefits associated with CO_2 purity in a CCS system. Therefore for the identified feasible operational envelopes, the cost-benefit trade-offs between the production of a high-purity stream of CO_2 (with associated high capture cost, but lower transport costs and complications) and the production of a less pure stream of CO_2 (with lower capture costs, but commensurately higher transport costs). The cost model will be developed based on the results of modelling of CO_2 compression, transport and storage in WPs 1-3 and will incorporate a 'safety and impact tool' for the qualitative assessment of industrial and environmental risks associated with CCS which is the focus of WP5.

7. Conclusions

The cost of CO_2 capture plants will increase with increases in the required degree of purification of CO_2. In contrast, pipeline transportation and storage costs increase with a decrease in the CO_2 purity. Clearly the optimum CO_2 purity requires a trade-off between these two requirements.

Based on a cost-benefit analysis and whole system approach, validated mathematical models developed and realistic-scale CO_2 pipeline transportation and storage experiments conducted as part of the CO_2QUEST project, predictions and results will be employed to provide recommendations for CO_2 purification levels, mixing protocols and control measures for pipeline networks and storage infrastructure, thus contributing to the development of relevant standards for the safe design and economic operation of CCS.

The methods and tools developed in the project will allow industry and other stakeholders involved in the implementation of CCS schemes to improve operational safety and safeguard members of the public and operators from the consequences of CO_2 leaks from transportation pipeline networks and geological CO_2 storage formations. Sharing the knowledge generated in the project with industrial and public sectors is expected to facilitate the safe and commercially advantageous deployment of CCS, as a key technology which enables exploitation of fossil fuel reserves, including coal, in Europe and the rest of the world without adding to greenhouse gas emissions.

Acknowledgements

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