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IMPACTS: economic trade-offs for CO₂ impurity specification

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Abstract

The IMPACTS project has a stated broad objective to develop the knowledge base of CO₂ quality required for establishing norms and regulations to ensure safe and reliable design, construction and operation of CO₂ pipelines and injection equipment, and safe long-term geological storage of CO₂. More specifically for this paper, the project sets out to reveal the impacts of relevant impurities in the CO₂ stream on the design, operation and costs of the capture, transport and storage infrastructure and to provide recommendations for optimized CO₂ quality through techno-economic assessments (amongst other considerations). This paper gives an overview of the work being carried out to investigate the impact of CO₂ quality in various areas including corrosion, water content in the CO₂ stream and the injection and storage processes. The paper reports on the derived impacts of the above mentioned aspects of CO₂ quality. These impacts are combined with estimates of the cost of measures to mitigate or prevent these impacts from affecting the operation of the CCS system, or of adapting of CCS system design. Thus, the impacts can be set out as a set of cost functions relating to Capex and Opex and including the effects of overall availability and process efficiency changes. A specifically designed CCS chain model is used to assess the impacts on a number of reference CCS chains, carrying out comparative economic trade-offs to both understand the full-chain whole-life economics of certain CO₂ impurities at different levels and then to potentially optimize a purity specification for various sets of circumstances.

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1. Introduction

The IMPACTS project has a stated broad objective to develop the CO₂ quality knowledge base required for establishing norms and regulations to ensure safe and reliable design, construction and operation of CO₂ pipelines and injection equipment, and safe long-term geological storage of CO₂. More specifically for this paper, the project sets out to reveal the impacts of relevant impurities in the CO₂ stream on the design, operation and costs of the capture, transport and storage infrastructure and to provide recommendations for optimized CO₂ quality through techno-economic assessments (amongst other considerations).

This paper gives an overview of the work being carried out to investigate the impact of CO₂ quality in various areas including:

- corrosion in the transport, injection system and storage. In each of these circumstances, different impurities in a typical CO₂ stream can play a dominant role.
- water content in the CO₂ stream, which is a vital issue on its own and in combination, with requirements to avoid free water anywhere in the transport system or the possibility of hydrate formation at any anticipated physical conditions in the process.
- the injection process, which is sensitive to the phase behaviour of the CO₂ mixture; hydrogen, nitrogen and methane are among those impurities that strongly affect mixture phase behaviour and density.
- the storage process, with key issues such as reactions with the reservoir formation and fluid, especially in carbonate reservoirs, biological anaerobic souring and impacts on the ability to achieve enhanced hydrocarbon recovery (if any) such as minimum miscibility pressure.

The paper reports on the derived impacts of the above mentioned aspects of CO₂ quality. These impacts are combined with estimates of the cost of measures to mitigate or prevent these impacts from affecting the operation of the CCS system, or of adapting the CCS system design. Thus, the impacts can be set out as a set of cost functions relating to Capex and Opex and including the effects of overall facility availability and process efficiency changes.

These data are applied using a specifically designed CCS chain economic model which includes the ability to set up user-driven CCS chains and CO₂ impurity choices while maintaining through-chain physical and chemical integrity. Derived cost functions can be added in and standard comparator economic parameters can be produced. In order to highlight the key issues for real European situations, a set of representative CCS chains have been selected and used as benchmarks for the analysis. These include a variety of capture types, both power generation and industrial, on-shore and off-shore pipelines and shipping and different storage formations of various geological types. Both stream mixing and multiple storage connections are also included.

Using the derived data, comparative economic trade-offs are carried out both to understand the influences on full-chain whole-life economics of certain CO₂ impurities at different levels and then potentially to optimize a purity specification for various sets of circumstances. There is also the possibility within the IMPACTS project of providing more generalized results which, when combined with other factors, such as Health and Safety considerations, can provide suggestions for CO₂ specifications which can optimize the technical design of wider CCS infrastructures for use by multiple sources and sinks.

2. CO₂ compositions

The starting point in the IMPACTS project is an inventory of typical combinations of large-scale processes that produce CO₂ and the capture technologies that can be used to obtain the produced CO₂ in a processed form. Typical impurities that can be found in the CO₂ stream have been quantified based on a combination of publicly available literature data and the experience of the IMPACTS consortium partners. A comparative analysis of the gathered data

4. Techno-economic set up

4.1. Model principles

The IMPACTS techno-economic model has a standard and deliberately quite rudimentary project cash flow model at its core to allow the derivation of key economic indicators over a project lifetime. It allows the user to model CCS chains by incorporating capture, transport and storage modules and linking them to form a source-to-sink network, including joins and branches as required. A graphical representation of the chain is provided for verification. Key parameters (size, technical specifications, Capex, Opex etc) for each module are input by the user and the model checks for continuity of conditions and mass flow. CO₂ stream purity is specified for each capture unit, but can then be flexed as described below.

To facilitate analysis of specific impurity impacts, key components affected by impurities can be set up in detail and technical limitations can be created. The sensitivities of these key components to varying impurities are then included using cost functions. These functions encode data derived from key work packages within the IMPACTS project and also from public / partner data. As a simple example, if further conditioning equipment is needed to reduce H₂O levels below, say, 200 ppm then the function will include the Capex and Opex costs associated with this equipment if the CO₂ stream water content is set below 200 ppm but leave it out above this level.

4.2. Model usage

Once the input parameters and cost functions are set up, the model can be used to derive economic parameters over a range of CO₂ stream impurity levels. Initially this can be used to look at the sensitivities of the resulting economics to various key components or processes across an impurity range. This then allows parts of the IMPACTS project to be focused on the most important influences. Ultimately, the model can be used to search for optimal combinations of impurity specifications which result in the best overall project economics, for the circumstances defined. These outcomes will also be overlaid by other risk considerations including health and safety (see section 9 below).

4.3. Benchmark chain elements / the Shopping List

Benchmark CCS chains have been established both to reflect the most common expected elements in future CCS chains in Europe, and also to illustrate important aspects of capture, transport and storage where impurities will have key influences. In order to produce the most useful results, a “shopping list” of particular areas of concern has been established as a means of dialogue between the more fundamental research elements of the IMPACTS project and the techno-economic analysis and risk assessment work.

5. Pipeline transport

The required compression power will be a main driver for a typical CCS transport system. Opex will be driven by power consumption which can be estimated by assuming an isentropic efficiency, θ (-), for the actual compression work, W_A (J/kg/s). Given a isentropic efficiency the compression work reduces to a thermodynamic relation,

$$W_A = \theta W_S,$$

where, W_S (J/kg/s), is the enthalpy change of a isentropic compression path. In order to calculate Capex, the compression power requirements must be broken down to actual compression units, and a possible need for redundancy must be taken into consideration.

The need for compression power depends on pipeline boundary conditions, e.g., the capture and storage pressure, storage injectivity, the elevation profile of the pipeline giving rise to static pressure changes and the friction pressure loss in the pipeline. The boundary conditions will be given for a specific case, while the elevation and friction effects will depend on fluid properties affected by impurities of the CO₂. The pressure drop due to friction losses resulting from fluid motion in circular pipes can be calculated using the Darcy-Weisbach equation,

$$\Delta P_{\text{fric}} = \int_0^L f_D \rho \left(\frac{v^2}{2} \right) \frac{dL}{D}$$

Here, ΔP (Pa), is the pipeline pressure drop, f_D (-), is the Darcy friction factor, L (m), is the pipe length, D (m), is the pipe diameter, v (m/s), flow velocity and ρ (kg/m^3) is the fluid density. The use of this relation assumes single phase flow, or homogeneous flow of multiple phases. An isothermal integration along the pipeline, or pipe sections, will in most cases be sufficient. The heat transfer between the pipeline and its surrounding environment will produce the ambient temperature in pipeline. The extent to which this assumption is valid must be addressed on a case by case basis.

As seen from the above, the Opex of transportation can be estimated using mixture thermodynamics together with a model for dynamic viscosity. In this estimation good density predictions are vital. Phase equilibria and densities will be calculated using the TREND thermodynamics library [5].

A limited amount of supercritical and liquid viscosity data for CO_2 -rich mixtures is available in the literature [e.g., 6]. The mixture viscosity predicted by available models, will therefore be associated with uncertainty. Initial work done in the IMPACTS project indicates that the TRAPP method [7] can be used to estimate high pressure viscosity for CO_2 mixtures.

In general, impurities more volatile than CO_2 (e.g., N_2 , Ar, H_2) will reduce the fluid density and give a higher compression cost. Also the inclusion of impurities will increase the flow rate, giving an increased power consumption and Opex.

Fig. 1 shows compression work and pressure drop along a 100 km pipeline as a function of nitrogen content in the CO_2 . A significant increase in compression power is required for CO_2 with a relatively low amount of N_2 .

Impurities will also affect the boundaries of the phase line/envelope. Volatile components typically elevate the cricondenbar, making it more difficult to maintain single phase flow in the pipeline. As a result the distance between (re-)compression stations might decrease, or the operating pressure must increase. How CO_2 impurities will affect the dynamic viscosity is topic for further study.

A main Capex driver for CO_2 transport is the pipe wall thickness. The wall thickness is normally governed by operating pressure containment, but will also be affected by other factors such as corrosion and possibility of running ductile fracture. Compared to natural gas pipelines, CO_2 pipelines are more vulnerable to running ductile fracture [3].

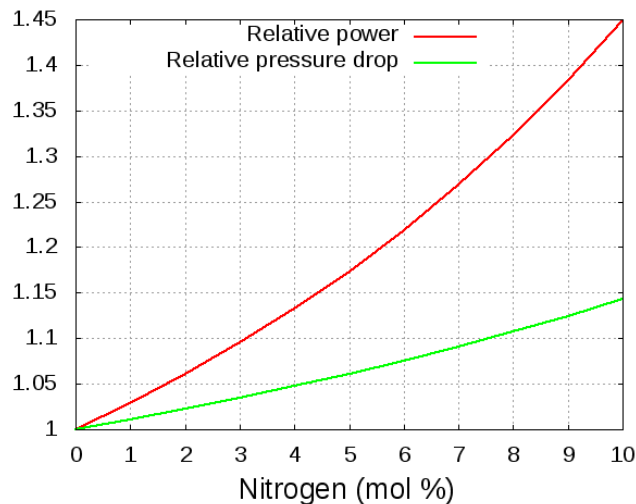


Fig. 1. The impact of nitrogen impurity in CO_2 on pipe friction and compression work for a 100 km transport pipeline, with a pipe diameter of 0.2 m. The pressure drop and compression work is plotted relative to pure CO_2 transport. Exit pressure is set to 120 bar, and a fluid temperature of 300 K is assumed.

6. Corrosion

The available know-how on CO₂ corrosion issues is strongly related to the oil and gas industry sector in which this topic has been widely investigated. This experience can supply general information on corrosion and stress corrosion processes but cannot be transposed directly to the CO₂ transportation pipelines. This is due to the fact the CO₂ pipelines are in dense phase and the transported mixtures present components and conditions strongly different from oil and gas ones.

Some specific research activities on supercritical and dense CO₂ phase have been identified, also if these works do not cover the whole scenario of CO₂ transportation conditions. In some cases the activities carried out by different laboratories have produced conflicting findings. For these reasons a further effort is required in testing activity with the aim to cover the lack of data and confirm specific important findings. In particular for the corrosion issues the main topics that require further experimental activities are:

- Effect of water content in presence of different CO₂ mixtures;
- Effect of temperature;
- Effect of flow rate;
- Effect of O₂ in the mixture;
- Effect of NO_x and SO_x in the mixture;
- Effect of H₂S in the mixture.

These results could be used to validate numerical models for general corrosion so that corrosion rates may be predicted. This model may then be used in design/evaluation of pipeline systems carrying CO₂ mixtures. For the stress corrosion issues the main topics that require further experimental activities are:

- Effect of water content in presence of different CO₂ mixtures;
- Effect of temperature;
- Effect of NO_x and SO_x in the mixture;
- Effect of H₂S in the mixture.

The knowledge of the corrosion and stress corrosion behaviour will be used in the design of components to be used in the CCTS chain. In particular concerning the capture section of chain, in these plants there is an extensive use of stainless steel and corrosion resistant alloy (CRA) materials that are selected on the base of corrosion environment and local conditions (pressure and temperature) for each point of the plant. The knowledge/availability of resistance material for harsh environments is high and there is no problem to identify the right one. But the use of stainless steel and CRA materials in pipelines implies a large increase of costs for those components in particular when the corrosion conditions are severe (see Fig. 2).

Concerning the transportation stage, the amount of steel material required is large and the increase of cost in material procurement affects strongly the Capex cost of project. For this reason the selection of material for CO₂ pipelines starts with the most used carbon-manganese steel if the water level can be maintained at low value and if the corrosion effects of other impurities have been evaluated. The use of sour service materials (at different levels of conditions) can be adopted in case H₂S values require these types of materials. In case of very harsh transported mixture the use of internally clad or lined pipes can be taken into account.

Concerning the storage stage, the injected CO₂ fluid is assumed to be dry and non-corrosive, following from the fact that usually it has been transported by carbon steel pipes (which require the CO₂ to be dry and non-corrosive), so during the injection phase the well is not subject to corrosion and standard low alloy carbon steels could be used for all the well components, considering only the injection phase of the well life. But this ideal condition can fail in different cases, for example at the interface of the brine and the injected fluid within the formation, there will be a rapid dissolution of CO₂ and other injected components into the water phase. For these reasons it may be necessary to consider CRA materials for the tubing if it is envisaged to be exposed to the aggressive water over the long term. Anyway, even if expensive materials have to be used, the amount of materials required in well is lower than that in transportation pipelines and the impact of cost on project is consequentially much lower.



Fig. 2. Materials range in terms of average price and availability (<http://www.parker.com/>).

7. Injection

An existing analytical tool [4] has been extended and modified to investigate the impact of impurities on the storage capacity and the injectivity of CO₂. The properties of mixtures were added by connecting the RefProp database (<http://www.nist.gov/srd/nist23.cfm>). In addition, descriptions for a saline aquifer and an oil reservoir were added to the already existing formulas for gas reservoirs. Specifically for the oil reservoir, several assumptions were made, such as a choice between miscible- and immiscible-EOR, a typical primary and secondary oil production fraction. A sensitivity analysis was conducted with varying depths (800, 900, 2000 and 3400 m), leading to changes in the reservoir temperature and pressure. For these conditions, properties of the CO₂ mixtures (up to three components), such as density, viscosity and the Z factor, were taken from the RefProp software. The boundary conditions were set at the initial pressure for the hydrocarbon reservoirs, while for aquifers this value was set at 10% above the initial reservoir pressure.

Up to three of the most dominant impurity components per capture technology were considered. The modelling results of the mixtures were always compared to the prediction with pure CO₂ in the same reservoir. Since actual storage compartments served as examples, it is not possible to compare the storage capacity in the aquifer with those in the hydrocarbon reservoirs. Table 2 shows some examples of various capture-storage site combinations.

Table 2. The effect of impurity levels in the CO₂ stream on storage capacity (Mt), for different CO₂ streams and three types of storage reservoir. Computations have been made at several depths; the maximum effects are observed at depths near 800 m.

Depth (m) reservoir	Selexol based adsorption Oil field			Post combustion ammonia Aquifer			Natural gas processing Gas reservoir		
	Pure	Mixture	Diff (%)	Pure	Mixture	Diff (%)	Pure	Mixture	Diff (%)
800	9.2	4.7	-48.9	14.1	13.9	-1.4	6.0	3.1	-48.3
900	5.2	3.9	-25	15.9	15.7	-1.3	5.2	3.3	-36.5
2000	4.9	4.7	-4.1	34.2	34.2	0	5.0	4.5	-10.0
3400	4.0	3.9	-2.1	57	56.8	-0.3	4.0	3.8	-5.0

As expected the largest impact of impurities can be found at a depth of 800 m. This can be attributed to changes to the critical points and the associated significant changes in properties (such as density) of the CO₂ mixtures with respect to the pure CO₂. Further away from the critical conditions at greater depths, the impact of impurities is far

smaller. At still greater depths, the storage capacity again reduces for gas and oil reservoirs. This is due to the compressibility Z factor, which increases again after a minimum value around 200 bar for both mixtures and pure CO_2 . For aquifers, the storage capacity increases with depth. This is due to the boundary conditions of limiting pressure to 10 % above initial pressure for aquifers, which leads to an increase of additional allowed pressures with depth.

The required tubing head pressures are presented in Table 3 for an example where the tubing head temperature was set at 10 °C. The impact on injectivity for this example is rather limited.

Table 3. Tubing head pressures for CO_2 injection in a gas reservoir, for pure CO_2 and CO_2 with impurities ('mixture').

Year	Gas reservoir with gas processing Tubing head pressures (bar)		
	1	2	3
Pure	10	26	38
Mixture	10	26	36

Different reservoir and well pressures as a result of injection impurities are likely to have an impact on the costs of storage. Lower storage capacity leads to shorter injection periods at certain injection rates, raising the technical cost per Mt CO_2 stored. The degree of impact depends on the composition of the mixture and the depth (temperature and pressure) of the storage compartment. Cost impacts are fed into the economic modelling.

8. Storage

The objectives regarding geological storage of impure CO_2 are to analyse chemical and physical effects of impurities on CO_2 storage, on the one hand, and investigate operational and material effects of impurities in CO_2 streams, on the other. Data is generated from laboratory experiments, field tests and numerical simulations of geochemical reactions.

The laboratory experiments cover both fundamental systems with binary gas mixtures (e.g. CO_2+SO_2) and limited chemical complexity and much more complex systems with ternary (e.g. $\text{CO}_2+\text{SO}_2+\text{NO}_2$) and/or multicomponent gas mixtures (e.g. $\text{CO}_2+\text{SO}_2+\text{NO}_2+\text{O}_2$). A work-plan for laboratory experiments was initially defined including a selection of mineral and rock samples, P-T conditions, run durations, brine compositions, and impurity species next to respective impurity concentrations. A wide range of P-T conditions were selected in order to cover real reservoir conditions for a large variety of typical European storage sites. Solid samples comprise mineral separates of siderite and illite, whole rock reservoir and cap rock samples from the Ketzin (Germany) and Hontomín (Spain) pilot CO_2 storage sites, as well as cement samples that have been used for well completion at Hontomín and well abandonment at Ketzin, respectively. The Hontomín site is a carbonate reservoir with a marl seal formation, whilst at Ketzin, CO_2 is stored in a sandstone formation with a mudstone seal. Thus, both carbonate and siliciclastic materials are considered in the project. In addition, typical chalk samples of North Sea hydrocarbon reservoir rocks are included in the work plan.

Expected results include individual mineral reaction rates for precipitation and/or dissolution processes as a function of impurity level, changes in porosity and permeability, individual effects of chemically aggressive impurities (e.g. SO_2), as well as an evaluation of the combined effects of several impurities and associated effects on mineral dissolution-(re-) precipitation processes.

Field tests comprise a large-scale N_2 tracer test at Ketzin and a CO_2 injection-extraction test at Hontomín. For the Ketzin field test, expected results comprise the analysis of chromatographic effects of the $\text{CO}_2\text{-N}_2$ mixture, isotopic effects between injected CO_2 and brine and pressure feedbacks (both wellhead and reservoir pressure) due to the injection of an impure CO_2 stream. For the Hontomín field test, expected results include the evaluation of the contribution of dissolution and capillary trapping mechanisms, and rates for solubility of the various gaseous and aqueous phases, including CO_2 and different reactive and inert tracers that are used as analogues for impurities.

Geochemical reactions of impure CO_2 are simulated based on batch and reactive transport models that are set up for Ketzin and Hontomín reservoir rocks and cap rocks as well as wellbore cement. The chemical influence of varying SO_2 concentrations in the CO_2 stream and related changes in porosity on different time scales are of major

concern. While short-term mineral reactions (days to tens of years) are prioritized for reservoir rocks, both short- and long-term mineral reactions (decades to hundreds of years) are analyzed for cap rocks. For each case a base scenario is defined, and sensitivity (i.e. influence of temperature) as well as uncertainty (i.e. kinetic mineral dissolution parameter) analyses are performed to underline simulation reliability. The models are being calibrated based on experimental results obtained during IMPACTS project.

The main outcome of the investigations performed on geological CO₂ storage will be geochemical-mineralogical as well as petrophysical data sets that can be fed into the techno-economic assessment models.

9. External safety

CO₂ is a substance that has many everyday applications from carbonising drinks to extinguishing fires. However CO₂, if inhaled in sufficiently high concentrations, can have toxic effects on the human body. At even higher concentrations, CO₂ may cause asphyxiation by displacing oxygen in the air.

This hazardous aspect of CO₂, combined with the very large quantities that will be contained within CCS systems creates the potential that a leak from a CO₂ system could pose a major accident hazard (MAH) (i.e. a hazard that could present significant harm to humans or the environment).

In addition, captured CO₂ unlike natural CO₂ used for EOR in the US will not be 100% pure. A CO₂ stream from a capture plant will contain substances, here referred to as stream impurities, such as CO, H₂O, H₂S, NO_x, SO_x, O₂ and H₂. Such impurities can even in very low concentrations change the properties of the CO₂ stream and thus change the likelihood and/or the consequences of a CO₂ release, if it occurs.

The methods to manage risk associated with bulk chemicals are well tried and tested across many industries. These methods can, when appropriately applied, ensure that the CO₂ system risks are brought down to, and subsequently maintained at, an acceptable level.

Several projects have developed project specific specifications for CO₂ transport in pipelines, e.g., Canyon Reef and Weyburn pipelines. However, for a multi-source and/or multi-sink arrangement (CCS cluster), the potential for conflicting stream compositions is increased. In order to understand the risks and consequences, and thus a determination of an acceptable level of risk of failure as a result of the thermodynamics of chemistry, the pipeline operator will need to exercise some control over the composition of the product being carried.

This leads to a tension between the high costs of removing impurities within the CO₂ and the high costs of providing pipelines designed to withstand the impacts of these impurities. At the one extreme, pipeline operators cannot be expected to invest in a resilient pipeline system to transport CO₂ that would corrode the pipeline, produce flow constrictions or result in unacceptable levels of harm were there to be an uncontrolled loss of containment incident. At the other extreme, the producer cannot be expected to invest in expensive equipment to produce food grade purity CO₂, enabling the pipeline operator to save costs by using low-grade materials in the pipeline, or shallow ground cover.

Recent work has indicated that non-condensable components in the CO₂ stream may have significant economic impacts for longer pipelines, and that the cost of CO₂ purification can have a significant role for the total cost of CCS, as one will need to balance the cost of purification with other costs (such as storage and transportation).

10. Discussion

The IMPACTS project (2013 – 2016) focuses on the impact of the quality of CO₂ on the design and operation of CCS chains. The level of impurities in the captured CO₂ stream depends on the capture technology and subsequent processing steps. The aim of IMPACTS is to develop the quality knowledge base required for defining recommendations to ensure safe and reliable design, construction and operation of CO₂ pipelines and injection equipment and safe long-term geological storage of CO₂.

The relation between CO₂ quality and CCS system design and performance is relevant, not only for single source – single sink project, typical for demonstration projects, but also for more complex, multi-user systems. During the design phase, the relation between CO₂ quality and system requirements should be known, to ensure safe and reliable system operation during all phases of operation, including start-up and shut-down. In addition, for all types of CCS systems, changes over time in the quality of the transported fluids may occur, either arising from changes in the capture technologies delivering to the system, or from new entrants to the transport and storage network.

A sound knowledge base is required on the impact of CO₂ quality on fluid properties and, hence, its behaviour in the transport and storage system.

It is the aim of IMPACTS to provide that knowledge base. In addition, IMPACTS will perform a techno-economic analysis, to find trade-offs, if any, between CO₂ quality requirements and full-chain, whole-life CCS system economics, potentially optimizing CCS system design and CO₂ purity requirements for various sets of circumstances.

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