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Techno-economic issues and trade-offs for CO₂ purity in CCS

chains

Charles Eickhoff^a*, Andy Brown^a, Filip Neele^b

^aProgressive Energy Ltd, Stonehouse, United Kingdom ^bTNO, Princetonlaan 6, 3508 TA, Utrecht, the Netherlands

Abstract

The IMPACTS project has the objective to develop the knowledge base of CO_2 quality required for establishing norms and regulations to ensure safe and reliable design, construction and operation of CO_2 pipelines and injection equipment, and safe long-term geological storage of CO_2 . More specifically for this paper, the project sets out to reveal the impacts of relevant impurities in the CO_2 stream on the design, operation and costs of the capture, transport and storage infrastructure and to provide recommendations for optimized CO_2 quality through technoeconomic assessments. The areas covered include corrosion from water content in the CO_2 stream in combination with other impurities and the influences of impurities on transport, injection and storage processes and include estimates of the cost of measures to mitigate or prevent these impacts, or of adapting of CCS system design. A specifically designed CCS chain model is used to assess the impacts on a number of reference CCS chains, evaluating economic trade-offs to both understand the full-chain whole-life economics of certain CO_2 impurities at different levels and then to potentially optimize a purity specification for various sets of circumstances.

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* Corresponding author. E-mail address: charles@progressive-energy.com

1. Introduction

The IMPACTS project [1] has a stated broad objective to develop the CO_2 quality knowledge base required for establishing norms and regulations to ensure safe and reliable design, construction and operation of CO_2 pipelines and injection equipment, and safe long-term geological storage of CO_2 . More specifically for this paper, the project sets out to reveal the impacts of relevant impurities in the CO_2 stream on the design, operation and costs of the capture, transport and storage infrastructure and to provide recommendations for optimized CO_2 quality through techno-economic assessments and risk assessment guideline (amongst other considerations). An example of a techno-economic assessment of the full CCS chain, using results from the IMPACTS project, has been presented by Skaugen et al [2]. A similar project into CO_2 quality and impacts of impurity on CCS system behaviour was undertaken in Germany [3].

This paper provides an overview of the work undertaken in the project to investigate the technical and economic impact of CO_2 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.
- storage capacity, 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.
- storage process, with key issues such as reactions with the reservoir formation and fluid, especially in carbonate
 reservoirs, biological anaerobic souring and impacts on formation / caprock stability.

The technical impact aspects of CO_2 quality were derived in the more fundamental sections of the IMPACTS project (e.g., [4-7]). These impacts are combined in this paper 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 to cope with the outcomes. Thus, the impacts can be set out as a set of cost functions relating to Capex and Opex of the full CCS chain, including the effects of overall facility availability and process efficiency changes.

These data are analysed using a specifically designed CCS chain economic model, described below. 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 (pre-combustion, post-combustion and oxyfuel) applied to both power generation and industrial plant, on-shore and off-shore pipelines and shipping combined with different storage formations of various geological types. Both stream mixing and multiple storage connections are also included.

A Techno-economic Analysis, such as in IMPACTS (see, e.g., [8]), is usually performed to provide insight into cost-benefit decisions about projects and involves two basic elements:

- The technical requirements to achieve a defined outcome;
- The economic changes that this implies.

These two elements can be combined into a standard project financial model with the capability to:

- model the technical issues;
- vary the assumptions to look for optimal solutions.

Using the derived data, comparative economic trade-offs have been carried out to both understand the influences on full-chain whole-life economics of certain CO_2 impurities at different levels and then to potentially optimize a purity specification for various sets of circumstances. These results are used within the IMPACTS project to provide a Toolbox [9] with more generalized guidelines when combined with other factors, such as Health and Safety considerations, and suggestions for CO_2 specifications which can optimize the technical design of wider CCS infrastructures for use by multiple sources and sinks.

2. CO₂ compositions

2.1. Impurity of realistic combinations of emission points and capture technologies

The starting point in the IMPACTS project was an inventory of common large-scale processes that produce CO_2 and the capture technologies that can be used to obtain the produced CO_2 in a purified form. Typical levels of various impurities were identified for a large number of combinations of emission source type and capture technology. Seven combinations were identified, that together cover the ranges of capture technologies and largescale CO_2 emitting processes. Where multiple cases were found, a high average concentration of impurities was selected. Thus, the set of CO_2 mixtures shown in Table 1 represents a realistic view on CO_2 purity levels for current capture technologies, with concentrations for specific mixture components biased to high levels. The CO_2 concentration of the streams is given by the balance of the impurities.

According to the EU CCS Directive [10], stored CO_2 has to consist "overwhelmingly of carbon dioxide". This definition is often translated into a minimum required CO_2 concentration of 95%. All seven cases in the table meet this minimum requirement, except coal-fired oxyfuel combustion. In a complex CCS infrastructure with multiple sources of captured CO_2 , this specification could be met by mixing lower-purity CO_2 with higher-purity streams. The CO_2 stream shown for oxyfuel combustion is one with a relatively high CO_2 purity.

No water concentration is defined in Table 1, because it is mainly determined by the chosen dehydration specification. For coal-fired power plants, only cases including desulfurization have been taken into account.

Table 1: Overview of typical CO₂ stream compositions of six CO₂ source and capture technology combinations that are responsible for the most extreme impurity levels. The concentrations are given on a volume basis (ppm where not labelled as %). See also [8].

CO ₂ source;	Coal-fired pp	Coal-fired pp	Coal-fired pp Selevol-	Coal-fired pp	Natural gas proc.	Synthesis gas proc.	Cement industry	Ketzin injection
Capture technology	absorption	based abs.	based abs.	Amine-based absorption	Rectisol- based abs.			
CO_2	99.8%	99.8%	98.2%	95.3%	95%	96.7%	83%	95%
N_2	2000	2000	6000	2.5%	5000	30	11%	
O_2	200	200	1	1.6%		5	6%	
Ar	100	100	500	6000				
NO_x	50	50		100				
SO_x	10	10		100				
СО	10	10	400	50		1000		
H_2S			100		200	9000		
H_2			1.0%			500		
CH_4			1000		4.0%	7000		
C_2+					5000	1.5%		
NH ₃	1	100						
Amine	1							

2.2. Concentrations of individual impurities

Table 2 shows a different representation of the levels of impurities listed for combinations of CO_2 emission processes and capture technologies. Ranges of impurity levels were derived from the literature data on existing or planned capture projects; the benchmark levels represent a purity level that can be expected based on the technologies used in these projects. Minimum and maximum levels of each major impurity were also set to limit the scope of interest of the project. The ranges given in Table 2 were used in the IMPACTS project to study the range of physical effects given in Section 1 above.

Impurity	H ₂ O	N ₂	O ₂	Ar	NOx	SOx	CO	H_2S	H₂	CH_4	C2+	Cl	NH₃
General limits	(some only	applicable	e in spec	ific case	s) includi	ng Post-	combustic	on:					
Max	1000	5%	300	600	250	250	200	200	5000	1000	2000	20	300
Benchmark	100	2000	100	20	100	100	20	100	50	500	1000	5	50
Min	0.001	100	2	1	20	20	10	20	20	20	100	1	10
Adjusted For C	Dxyfuel:												
Max		5%	5%	5%			1500						
Benchmark		2%	3%	2%			50						
Min		1%	2	100			10						
Adjusted For P	re-combust	ion:											
Max		5%	30	600	250	250	1500		2%	100			
Benchmark		2%	10	200	10	10	400		1%	50			
Min		1%	2	100	10	10	50		20	20			
Adjusted For G	ias Processi	ng:											
Max										5%			
Benchmark										4%			
Min										20			

Table 2: Impurity concentration ranges (in ppm, when not indicated as percentages). These impurity ranges are used in the research areas covered in the IMPACTS project (transport, corrosion, injection and storage).

3. Cost functions

3.1. Use of cost functions

A major task in the IMPACTS project has been investigating the technical effects of impurities in the CO_2 stream on the materials, operations and efficiency of parts of, and then ultimately the whole, CCS chain. In order to make use of this data in a techno-economic analysis, the effects have to be translated into equivalent costs at varying levels of impurity for the CCS chain. This is done by using cost functions which are effectively the partial differential of chain cost by individual impurity. They are expressed as a linear function of cost (Opex or Capex) against level of impurity in ppm. These cost functions can be applied as relevant to the benchmark chains (see Section 4.3, below) in order to understand the variations in overall costs with varying quality of CO_2 stream.

In order to understand the cost consequences of specifying different levels of purity for the CO_2 stream, the equipment and resources required to reduce each impurity of interest has been estimated for each of the capture technologies and applications. The additional costs (or savings in the case of purity relaxation) from the benchmark position have been assessed by the partners using both proprietary and public information. These data have then also been converted into cost functions to feed into the model library.

Figure 1 shows an illustrative example. Here the blue line shows cost of increasing purity at source, whilst the red line shows changing downstream Transport and Storage costs with changing impurity levels.

There is a clear optimum position of minimum total cost at 450 ppm in this illustrative diagram.



Fig. 1: Illustrating the use of conditioning and consequential cost functions

3.2. Example cost function: water content and capture cost

As a simple example, if conditioning equipment is needed to reduce H_2O levels below, say, 250 ppm then the function will include the Capex and Opex costs associated with this equipment if the CO_2 stream water content is set below 250 ppm. Figure 2 shows how an illustrative series of values is translated into the cost function.



Figure 2: Simple illustration of the derivation of a cost function for the water content in a CO₂ stream.

4. Techno-economic model

4.1. Model principles

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

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 the relevant information from a library of cost functions. Similar functions for the costs of purifying the CO_2 stream are also included, as relevant to the capture technology being used.

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 CO_2 stream impurity levels. By only introducing limited sets of cost functions, this can be used to look at the sensitivities of the resulting economics to various key components or processes across an impurity range. This was used to focus on the most important influences. The model was then set up with all the relevant cost functions in place and the impurity specifications flexed down the whole CCS chain as set up. This enabled a search for the optimal combinations of impurity specifications which result in the best overall project economics, as defined by standard project financial parameters, such as levellised costs or rate of return. These economic outcomes were also overlaid by other risk considerations including health and safety limitations (see section 7 below).

4.3. Benchmark chains

Benchmark CCS chains have been established to both reflect the most common expected elements in future CCS chains in Europe, but also to illustrate important aspects of capture, transport and storage where impurities will have key influences. These have been used to provide illustrative results of optimal specifications in certain defined circumstances.

In all reference chains, storage reservoirs are located offshore and include depleted fields, oil fields and saline formations. Transport distances vary from 20 km to 400 km. One of the reference chains links several sources to multiple storage locations, to study issues such as mixing of CO_2 streams and the impact on storage cost of impurities.

5. Example trade-offs

5.1. Impurities and storage costs

The effects of impurity levels on storage capacity have been studied for each geological case occurring in a benchmark chain and for the Ketzin site. The seven CO_2 compositions presented in Table 1 were used to compute the error made in estimating static storage capacity in either a saline formation or oil field, when using the properties for pure CO_2 . In addition to these seven cases, the rightmost column in the table represents the mixture that was used in a recent experiment at the Ketzin pilot storage site in Germany, in which 95% CO_2 mixed with 5% N_2 was injected [4].

The storage capacity (in Mt) in a specific subsurface compartment was calculated from the volume of available pore space and the density of the injected fluids in that volume. This density depends on the composition of the CO_2 phase and on the pressure and temperature conditions. Impurities in CO_2 can come from a variety of sources and have an impact on the PVT behaviour of the injected fluid. Methane can be present, coming from residual gas or oil in the reservoir. The CO_2 may also strip components from the storage compartment itself or from crude oil in case of a CO_2 -EOR process. In addition, depending on the kind of capture technique, various impurities are also introduced during the capture process, as described above (Tables 1 and 2).

The storage capacity was calculated for various depths to investigate the sensitivity of pressure and temperature. The results are presented in Table 3, which shows the relative difference between the storage capacity as computed for the impure CO_2 mixture and that computed for pure CO_2 , relative to the capacity for pure CO_2 , as a percentage. Negative values represent lower storage capacity for the impure CO_2 . Also given in the table is the weight percent of the impurities in the CO_2 . The change, often a reduction, in storage capacity is sum of two effects. The first is displacement of the CO_2 by the impurities, the second is the change in the density of the mixture due to the presence of impurities. Some impurities, such as SO_2 , increase the mixture density (e.g., [11]); however, this increase is more than offset by the displacement effect and the net result for the mixtures considered here is a decrease in storage capacity that is disproportionally larger than the impurities total weight fraction.

The table shows that the presence of impurities affects the storage capacity. As expected, the largest impact of impurities can be found at a depth of 800 m. This can be attributed to shifts of the critical points and the associated changes in density of the CO_2 mixtures with respect to pure CO_2 . Away from the critical conditions, at greater depths, the impact of impurities decreases. Due to a positive effect on density for some impurities, the net effect on

storage capacity can be lower than expected, based on the impurity weight percentage. An example of this is the 'Ketzin' injection case, where over 7 wt% impurities (SO₂) result in only 1.5% or 3.3% capacity decrease at depths of 2000 m and 3400 m, respectively.

Table 3: Storage capacity of pure CO_2 versus CO_2 fraction of mixtures at various depths in various storage compartments. The top row gives the source of the CO_2 considered (see Table 2 for the corresponding mixtures); the second row gives the storage reservoir (saline formation or oil field)

non)										
CO_2	Coal-fired pp	Coal-fired pp	Coal-fired pp	Coal-fired pp	Natural gas	Synthesis	Cement	Ketzin		
source;	Amine-based	Ammonia-	Selexol-	Oxy-fuel	proc.	gas proc.	industry	injection		
Capture technology	absorption	based abs.	based abs.		Amine-based absorption	Rectisol- based abs.				
Storage type	Oil field	Saline formation	Oil field	Saline formation	Oil field	Oil field	Oil field	Saline formation		
wt % impurities	0.24	0.05	0.21	1.28	0.93	0.41	4.99	7.37		
800 m	-2.8	-0.5	-5.3	-16.0	-15.1	-9.7	-53.0	6.6		
900 m	-2.0	-0.3	-4.1	-11.4	-11.0	-7.4	-41.3	5.0		
2000 m	-0.7	-0.2	-1.7	-4.4	-4.2	-3.1	-12.2	-1.5		
3400 m	-0.7	-0.2	-1.2	-3.2	-3.1	-2.2	-7.5	-3.3		

The results strongly suggest that effects of impurities need to be included in the assessment of storage capacity, to prevent unexpected effects during the storage process.

A real example of the cost impact of an impurity on storage costs is shown in Figure 3. This shows the effect of nitrogen on the cost of CO_2 storage at various formation depths. In each case the cost goes up with increasing nitrogen content as the space for pure CO_2 is reduced. In the case at 2500 m depth, the pure $CO_2 \operatorname{cost} (\mathcal{C}/t)$ is greater due to the additional well costs etc. but the effect of the nitrogen is smaller as the formation pressure is high enough to avoid the mixture bubble point. In the 800 m case, however, although the pure cost is lower, the effect of the nitrogen outweighs this at higher impurity levels because of the lower density of the nitrogen and hence the larger displacement of CO_2 in the formation capacity. The models used to determine these relationships were calibrated based on experimental results obtained during the IMPACTS project at the Ketzin and Hontomín sites.



Figure 3: Effect of Nitrogen on CO₂ storage cost. The cost shown (vertical axes) applies to a CCS chain with a transport distance of 400 km. which explains the unit cost of about 110 C/tCO_2 . The range in nitrogen level covers the range shown in Table 2.

If we look at the corresponding costs of reducing nitrogen content, then a good example is that of pre-combustion capture technology where relaxation of the nitrogen impurity specification can allow a cheaper Air Separation Unit

and lower energy operating costs. In contrast, tightening the specification requires the substitution of nitrogen by CO_2 as the propellant in the coal lock-hoppers causes additional expense. This is shown in Figure 4.



Figure 4: Changing costs of achieving Nitrogen impurity specification in a pre-combustion capture plant. The cost shown (vertical axes) applies to a CCS chain with a transport distance of 400 km, which explains the unit cost of about $110 \text{ } \text{C/tCO}_2$.

6. Techno-economic trade-offs

6.1. Water content

Having established the technical effects and the cost functions associated with them, the model is capable of looking for economic trade-offs down the full chain of a benchmark CCS project. In some circumstances there is a clear case for setting a very high purity standard, while in others for leaving the specification at the normally achieved level (driven in many cases by the side effects of other impurity levels).

A clear example of the derivation of a trade-off effect is obtained for the water level in a benchmark chain that combines a post-combustion capture using chilled ammonia absorption with a 20-km on-shore pipeline to a carbonate formation storage. In these circumstances the increased costs of more expensive pipeline materials to avoid excessive corrosion at higher water concentrations are well balanced with additional costs of reducing the moisture content in the conditioned CO_2 . The traditional "bathtub" cost curve that is derived for this case (Figure 5) shows an optimal specification in the 250 -350 ppmm range.



Figure 5: Economic Trade-off of water content in a CCS chain that connects a post-combustion chilled ammonia capture facility on a coalfired power plant through a 20-km onshore pipeline to a carbonate storage reservoir. At higher water levels, cost increases due to more expensive, corrosion-resistant pipeline material; equally high costs are found when decreasing the water content to below about 250 ppm.

6.2. Impurity levels and storage cost

Similarly, the effects of varying nitrogen concentration on storage capacity and on the costs of capture were derived for a CCS benchmark chain that connects amine-based capture at a coal-fired power plant through a 100-km offshore pipeline with a depleted gas field. Figure 6 shows the 'bathtub' cost curve that is obtained, with an optimal specification for the level of nitrogen in the 250 -1000 ppmm range. The storage depth used is 800 m in this example. At this range of impurity any additional costs of reducing the level of nitrogen impurity in the CO_2 are balanced by the cost impact on the cost of storage.



Figure 6: Economic trade-off for nitrogen content for a CCS benchmark chain that connects amine-based capture at a coal-fired power plant through a 100-km offshore pipeline with a depleted gas field at 800m depth. In the range 250 - 1000 ppmm, the impact of variations in the N₂ level on storage cost balances that on capture cost.

7. Safety

 CO_2 is a substance that has many everyday applications, from carbonising drinks to extinguishing fires and prolonging shelf-lives of food items. However CO_2 , if inhaled in sufficiently high concentrations, can have toxicological effects on the human body. At even higher concentrations, CO_2 can cause asphyxiation by displacing oxygen in the air.

This hazardous aspect of CO_2 , combined with the very large quantities that will be contained within CCS systems, creates the potential that a leak from a CO_2 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 CO_2 as discussed above will contain impurities such as CO, H_2O , H_2S , NO_x , SO_x , O_2 and H_2 . Such impurities can even in very low concentrations change the properties of the CO_2 stream and thus change the likelihood and/or the consequences of a CO_2 release, if it occurs.

Part of the IMPACTS project has investigated well tried and tested frameworks to manage risk associated with many industries such as bulk chemicals, gas transportation and the nuclear industry. These methodologies can be used and adapted to ensure that the CO_2 system risks are brought down to, and subsequently maintained at, acceptable levels and a framework to achieve this has been proposed by the IMPACTS project [5].

One important finding relevant to the issues addressed in this paper is that, given the assumptions made in the IMPACTS project, the toxicity of the impurities (at the range of plausible concentrations assumed) will be lower than that of the CO_2 itself for which the safety guidance is set out [12]. Hence toxicity considerations do not set any further limits on the proposed optimal economic purity levels.

8. Discussion

The IMPACTS project (2013 - 2015) focused on the impact of the quality of CO₂ on the design and operation of

CCS chains. The level of impurities in the captured CO_2 stream depends on the capture technology and subsequent conditioning steps. The aim of IMPACTS has been to develop the knowledge base required for defining recommendations to ensure safe and reliable design, construction and operation of CO_2 pipelines and injection equipment and safe long-term geological storage of CO_2 .

The relation between CO_2 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. The benchmark CCS chains considered during the project reflect these designs. A sound knowledge base is required on the impact of CO_2 quality on fluid properties and material interaction and, hence, its behaviour in the transport and storage system.

The IMPACTS project has developed such a knowledge base [9] for impure CO₂. This takes into account the economic trade-offs reported in this paper and also the risk analysis methodologies and technical results from other work-packages in IMPACTS [12]. This paper presents some key results focusing on the relation between specific impurities and the cost of the overall CCS chain; further results and conclusions regarding optimum or limiting impurity concentrations can be found in [12].

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