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REVIEW PAPER - EXPLORATION ENGINEERING

Physical and chemical effect of impurities in carbon capture, utilisation and storage

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Abstract

Deployment of carbon capture, utilisation, and storage (CCUS) technologies to mitigate climate change and overturn CO_2 emissions growth would require transformational changes comprehensively. The primary focus of this manuscript is on the impurities standards and limitation that can ensure project feasibility in the long run. There is a need in the industry for guidance on purity analysis prior to capture, shipment, and storage of carbon dioxide. This is because the cost to capture and separate the stream is proving to be very costly that can make the project to be unfeasible to operate. Following this further, this manuscript discusses the previous research and best practices that establish standards for acceptable impurities that might present in the stream and its effects towards the CCUS system. Consequently, this manuscript also provides better understanding on the impurities effects towards CCUS technology system in general. Understanding these limitations, may provide cost effective solution for CCUS problems that revolves around the impurities in CO_2 stream. Impurities can affect some components of the carbon capture and storage process. It is clear that even a little number of impurities can cause the carbon dioxide stream properties to change. There are two primary factors discussed in this manuscript that affect how a CCUS system responds to a CO_2 stream that contains impurities: a physical and chemical effects.

Keywords CCUS · Carbon capture · Carbon dioxide · CO_2 impurities

Abbreviations

°C	Degree Celcius
F	Buoyancy forces for CO2 with impurities
F0	Buoyancy forces for pure CO2
M	Mass of CO2with impurities
MCO2	Mass of pure CO2
m	Mass flow per unit area for CO2 with impurities
mCO2	Mass flow per unit area for pure CO2
ρ	Densities of CO2 with impurities
ρ0/CO2	Densities of pure CO2
ρH2O	Densities of formation water
ρm	Densities of plume
µ	Viscosities of CO2 with impurities
µ0	Viscosities of pure CO2
∑	Summation

Introduction

The greenhouse gas emissions (GHG) have continuously rise since the nineteenth century and every year, it managed to reach historic high where reports show that the annual rate for 2021 has increase beyond the 2011–2020 average (Lamb et al. 2021; Raza et al. 2019; Shreyash et al. 2021; World Meteorological Organization 2021). As shown in Fig. 1, the dangerous greenhouse gas composed of multiple gases where carbon dioxide CO_2 contributed the most emission at 76%, followed by methane (CH_4) at 16% emission and nitrous oxide (N_2O) at 6%. The least emission is fluorinated gases (F-gas) such as hydrofluorocarbons (HFCs) and sulfur hexafluoride (SF_6) at 2% (Intergovernmental Panel on Climate Change 2015; United States Environmental Protection Agency 2022). Due to the emission percentage and long life of CO_2, it has a direct impact towards global warming

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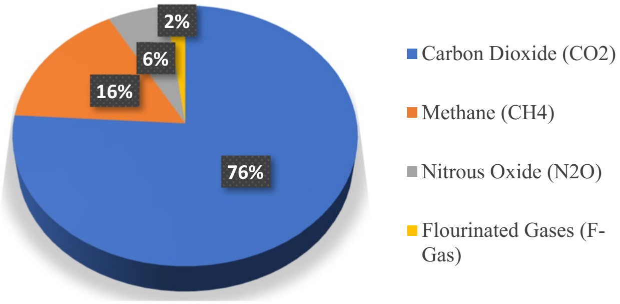


Fig. 1 Greenhouse gas (GHG) Global emission percentage by gas (Intergovernmental Panel on Climate Change 2015)

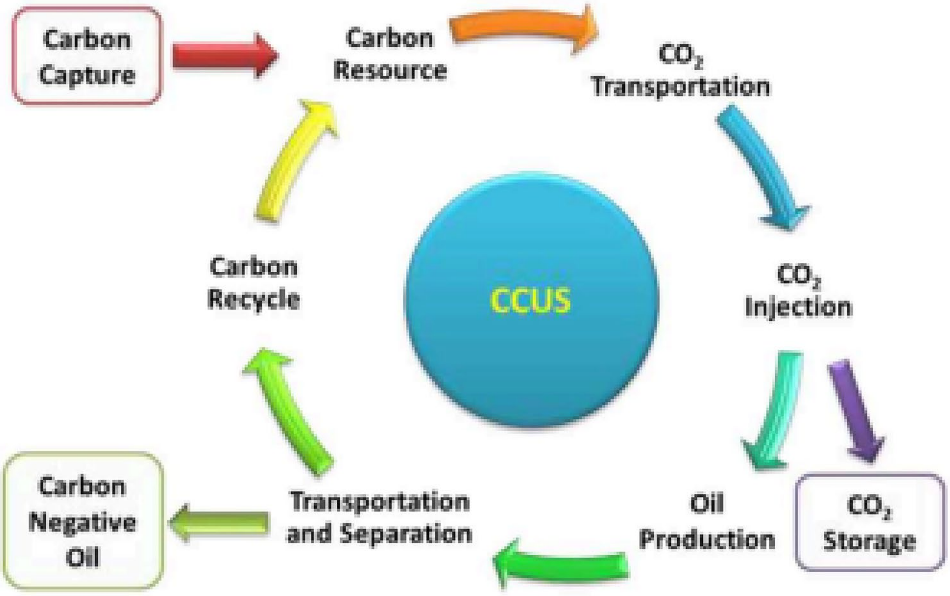
through the constant rise of temperature which indirectly cause frequent extreme weather with the rise of sea level and acidity (Li 2008; World Meteorological Organization 2021). These changes cause significant changes in natural ecosystems and society that require modifications in natural resource management and allocation. The growing vulnerability of natural and human systems underscores the need to mitigate climate change's effects in order to avoid extreme and pervasive events mentioned above.

As part of the efforts to limit global warming, various CO_2 reduction schemes and technologies have been proposed by multiple international organization and government which is initiated by the United Nations (Mohd Pangi and Md Yusof 2022). One of the recent initiatives was the Paris Climate Accords where the main objective revolves around limiting the release of GHG into the atmosphere and control the temperature rise by 1.5 to 2 °C each year (United Nations 2016). It is also listed the carbon capture, utilisation, and storage (CCUS) strategy as an essential technology to help the mitigation of CO_2 emissions and contribute to the goal of achieving net zero anthropogenic greenhouse gas emissions by 2050 (Budinis et al. 2018; Kearns et al. 2021; Wang et al. 2011).

CCUS technology is defined as technology that can capture, transport, store, and utilize carbon (Khalid 2021). Capturing of CO_2 from a variety of point source would be required for geological storage of CO_2 and this capture and separation technology is the most expensive steps in the CCUS chain which account 75% of the total overall cost (Nicot et al. 2013). When carbon is captured, it will be accompanied with impurities and the separation of the impurities can give a significant impact on the project cost (Khalid 2021; Wang et al. 2011). In transport section, the carbon stream is transported by either pipelines, ships, or trucks from the capture points to storage and utilization (enhanced oil recovery). In storage, the CO_2 is injected into reservoir of rock formations deep under the seabed or in saline aquifer. For short-to-medium period of storage, deep saline aquifer provides the best solution to CCUS compared to order method (Jiang 2011). The remaining amount of CO_2 is then used for utilization, where it can be converted into chemicals and also for enhanced oil recovery (EOR) (Khalid 2021). This complete CCUS chain process is depicted clearly in Fig. 2.

The CCUS technology incorporated waste to wealth system which is beneficial not only to the stakeholders but also to the environment sustainability (Khalid 2021). However, the development of these technologies is slower than anticipated and does not meet the Paris Agreement's carbon reduction commitments (International Energy Agency 2021b). In 2021, there are only 20 commercial CCUS that operate worldwide but this is expected to grow (International Energy Agency 2021a,

Fig. 2 CCUS chain process by (Wang et al. 2019)



2021b, 2021c). The slow progress is due to the high cost of developing and utilizing CCUS compared to other mitigation approaches. This technology, however, can be very reasonable in the long run (Budinis et al. 2018; Nicot et al. 2013). However, this can be overcome with a solid collaboration model between government and private sector for investment plus scaling up purposes where this can be seen with at least 100 new CCUS projects that have been announced so far and the worldwide project pipeline for CO_2 capture capacity is expected to grow by four-fold (International Energy Agency 2021b; Khalid 2021).

Due to technical and economical constraints, there are different types of impurities could come together with CO_2 in the stream and lead to a major concern on CO_2 transport, injection and also storage (Wang et al. 2011; Wetenhall et al. 2014). The impurities are anticipated to have a major impact on the phase behaviour of CO_2 streams, which has consequences for pipeline and injection well design and operation. Most of the impurities found are classified as non-condensable impurities which can affect the temperature and properties of the stream. As an example, nitrogen (N_2), oxygen (O_2) and argon (Ar) would increase the saturation pressure of liquid CO_2 and decrease the critical temperature which in turn can cause overpressure and for transportation and injection. Other than that, impurities like sulphur oxides (SO_x) may have acidic reaction with the cap rock which can cause problems in the storage structure and injectivity (Wang et al. 2011).

Despite the importance of impurities presence in CO_2, there remains a paucity of evidence on the acceptable impurities' percentage for CO_2 transport and storage. Many uncertainties still exist about the relation between impurities and CO_2 on design and operation of pipelines as well as its impact on geochemical and petrophysical changes during storage in the geological media. This paper assesses the significance of CO_2 impurities and its effects on the CCUS system. The first section of this paper gives a brief overview of standards and regulations by various authorities on acceptable impurities level for CCUS project. It will then go on to classification of impurities and analyze its physical impacts (phase behavior, storage capacity, injectivity, buoyancy) and chemical impacts (fluid-rock interactions and surface material). Therefore, this study makes a major contribution to advance the understanding of impurities in CCUS system. With better understanding on the matter, a guidelines or best practice are needed to make sure that the CCUS system can work seamlessly, effectively and at cost effective structure.

Standard for CCUS

There are a variety of impurities that could be present together with CO_2 and it is almost impossible to completely remove the impurities from CCUS system. Thus, standards of acceptable impurities are required to ensure that project is feasible while obeying to the rules and regulations setup by regulators (Anheden et al. 2005; Harkin et al. 2017). These specifications usually in form of upper and lower limit was developed from tons of data where it is classified into components and its application such as transport (pipelines), storage (carbon sequestration) or utilisation (enhanced oil recovery) (Harkin et al. 2017; Shirley and Myles 2019). This quality requirement can be use as guidance to meet the CO_2 capture technology validation and recommendations (Det Norske Veritas 2010).

Many international standard bodies such as Det Norske Veritas (DNV) and International Organization for Standardization (ISO) have come up with a guidelines or best practice that present a systematic approach in evaluating CCUS capture technology from fossil fuel production. These standards need to be updated frequently as the content is not always sufficient to adapt with the rapid development of CO_2 capture technology (Det Norske Veritas 2010). Due to this reason, many major governmental bodies set their own standards of purity and impurities composition that are deemed reasonable and safe towards the environments. For example, in the United States of America (USA), the US Department of Energy convened all stakeholders such as industry players, subject matter experts, governmental and non-governmental official for at least once a year. This meeting is for sharing and exchange of information with the possibility of collaboration with the end goal of standardizing the CCUS throughout United State of America (National Energy Technology Laboratory 2017).

Other than that, The People's Republic of China (PRC) which is the world largest energy consumer have recently published a standard to CCUS process that focuses on monitoring, measurement, performance, and risk. This standard was in collaboration between the government and a nonprofit scientific organization called The Chinese Society for Environmental Sciences (CSES). These standards were tabulated because nearly 90% of the energy consumption in this country was produced by fossil fuel, thus a significant action is taken by the authority to ensure that the country obeys to low-carbon emission towards ecological civilization goal (Asian Development Bank 2015). Table 1 listed the CCUS standards produced by various authority that can act as a guideline for a safe and reliable CCUS projects.

Impurities in CCUS

CO_2 can be captured using several methods, and the stream contains gaseous pollutants that is unfavourable to the stream (Walspurger 2012). Some of the impurities discovered consist of water (H_2O), hydrogen (H_2), hydrogen sulfide (H_2S), carbon monoxide (CO), nitrogen (N_2), oxygen (O_2),

Table 1 Standard for CCUS by various authorities and ongoing projects

Authority	Title
(Anheden et al. 2005)	CO_2 quality requirement for a system with CO_2 capture, transport, and storage
(Forbes et al. 2008)	Guidelines for carbon dioxide capture, transport, and storage
(Det Norske Veritas 2010)	Qualification procedures for CO_2 capture technology
(National Energy Technology Laboratory 2017)	CO_2 impurity design parameters
(Wetenhall et al. 2014)	Impact of CO_2 impurity on CO_2 compression, liquefaction and transportation
(Asian Development Bank 2015)	Roadmap for carbon capture and storage demonstration and deployment in the People's Republic of China
(National Energy Technology Laboratory 2017)	Siting and regulating carbon capture, utilization and storage infrastructure
(Harkin et al. 2017)	Development of a CO_2 specification for a CCS Hub network
(Zitelman et al. 2018)	Carbon capture, utilization, and storage: technology and policy status and opportunities
(Murugan et al. 2019)	Purity requirements of carbon dioxide for carbon capture and storage
(International Organisation of Standardisation 2020)	ISO/TC 265: Carbon dioxide capture, transportation, and geological storage
(Health and Safety Executive 2020)	EH40/2005: Workplace exposure limits
(Chinese Society of Environmental Sciences 2021)	T/CSES 41-2021: Terms of carbon dioxide capture, utilisation, and storage (CCUS)

methane (CH_4), argon (Ar), sulphur oxides (SO_x), and many others (Nicot et al. 2013; Wang et al. 2011). The type and composition structure of the unwanted gasses are varied depending on various factors such as capture technology and source (International Energy Agency 2021b; Wang et al. 2011; Wetenhall et al. 2014). CCUS process can be divided into four major process which is production, capture and transport, storage and lastly utilization. In each process, the purity varied from one to another. The goal of this section is to identify the probable impurities that is produced together with H_2O by a variety of CO_2 capture processes. Figure 3 can provide a basic understanding on the maximum limit of impurities that could present in CO_2 capture process.

Before carbon can be captured, it must be produced first. This carbon production process can be divided into two major methods, which is pre-combustion and post-combustion. In pre-combustion methods, the carbon is removed before the fuel can be converted into energy. This can be achieved by converting fuel to syngas by reforming or gasifying process depending on the raw materials. Additional to that, the utilization of water gas shift may help in getting additional hydrogen from the water. One of the advantages for these methods is low impurities that can expected at the end results because carbon dioxide is removed before combustion (De Visser et al. 2008). However, the downside for these methods is the presence of H_2S as impurities. The purity for the carbon captures with these methods ranging from 95 to 99% (Intergovernmental Panel on Climate Change 2015; Kather 2009).

In contrast to pre-combustion, post-combustion methods refer to the process of carbon production after the fuel converted into energy where it can be divided into three types

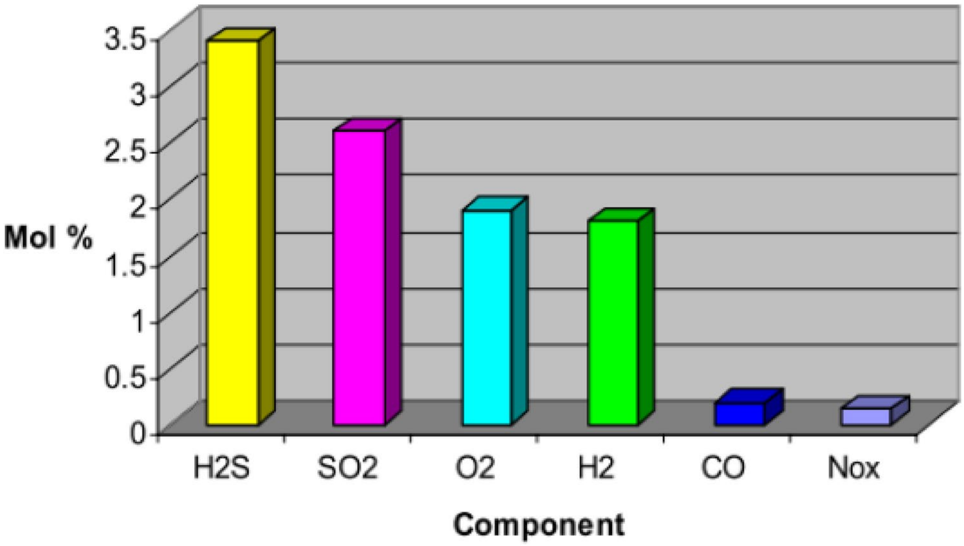


Fig. 3 Possibility on the maximum level of impurities that could be obtained from CO_2 captured processes (Murugan et al. 2020)

depending on the type of air reacting with the fuel. In these methods, the fuel is combusted with a gas without the refining process (reforming or gasifying). For the fuel combusted with normal air, it is known as normal post-combustion methods where lots of impurities such as N_2, O_2, SO_x and many other is expected (De Visser et al. 2008). If the normal air is change to pure oxygen for combustion, it is known as oxy-fuel methods. With the absence of N_2, this can greatly reduce the consumption of fuel needed for combustion. The impurities present in this method is quite similar to post-combustion with the addition of other nitrogen-based gasses such as nitrogen monoxide, nitrogen dioxide and carbon monoxide (The Global CCS Institute 2012). Lasty, instead of fuel reacting with air or oxygen gas, the methane is reacted with water where this is known as steam methane reforming. This reaction can produce a steady stream of H_2 and CO_2. For the post-combustion methods, the purity of carbon captures ranging from 95 to 99.9% (Intergovernmental Panel on Climate Change 2015; Kather 2009; White et al. 2009). From previous reports and studies, the range of impurities produce from each of this process is listed in Table 2.

In many of the CO_2 capture method studied, it is possible to increase the purity of the CO_2 produced. CO_2 transport and storage systems are likely to have a trade-off between improving CO_2 purity and creating a system that is able to manage some impurity in the stream. Overall, this manuscript should significantly contribute to the body of knowledge that CCUS project developers can use to decide the optimal techniques to manage CO_2 impurities within CCUS systems.

Impurities requirement in CCUS

This section discussed the recommended limit and impurities effects towards CCUS projects based on standards and best practice all around the world. As discussed previously, these impurities need to be removed from the stream as it can cause problems not only to the CCUS system but also towards the environment. The quality of captured carbon is crucial in determining the CCUS process efficiently. These impurities can be classified into two components which is condensable and non-condensable components. Where in non-condensable impurities, can be broken down further to three class which is major impurities (more than 0.5%), minor impurities (usually in ppm level but less than 0.5%) and micro impurities (particulate matters) with different composition percentage (Fig. 4). Other than the H_2O, CO, Nitrogen (N_2), Oxygen (O_2), Argon (Ar), Sulphur Oxides (SO_x) and Hydrogen Sulphide (H_2S), there are other impurities that possibly presented in the stream, but the composition is considered insignificant.

Table 2 Typical Impurities Present in CCUS System (Intergovernmental Panel on Climate Change 2015; Kather 2009; White et al. 2009)

Impurities	Pre-combustion (cmol/mol)	Post-combustion (cmol/mol)
H_2O	0–2.8	< 0.1
CO	0.04	< 0.1
N_2	0–1.5	0.1–4.1
O_2	0–1.5	0.1–4.1
Ar	0–1.5	0.1–4.1
SO_x	< 0.1	< 0.5
H_2S	0–0.6	–

Water (H_2O)

Water is known to be the side product for combustion (Anheden et al. 2005; De Visser et al. 2008; Det Norske Veritas 2010; Forbes et al. 2008; SNC-Lavalin Inc 2004). This compound is harmless on its own, but it can cause problem to the system when it reacts with other impurities present in the stream. The presence of large amounts of water in CO_2 streams is the most difficult problem to manage which creates many problems in transportation (pipelines) and storage (injection). The water level should be kept as low as possible to avoid excessive and stress corrosion as well as hydration production (Neele et al. 2017). For example, when H_2O reacts with CO_2 itself, it will produce carbonic acid (H_2CO_3), chemical equation is shown in (1), which is a type of dibasic acid which easily decomposed at certain temperature and pressure (Forbes et al. 2008; Wang et al. 2016).

$$CO_2 + H_2O \rightarrow H_2CO_3 \tag{1}$$

Other than that, H_2O also can react with H_2S to produce a very corrosive acid called sulphuric acid (H_2SO_4), chemical equation as in (2) (De Visser et al. 2008; Intergovernmental Panel on Climate Change 2015; Schwartz 1989; SNC-Lavalin Inc 2004).

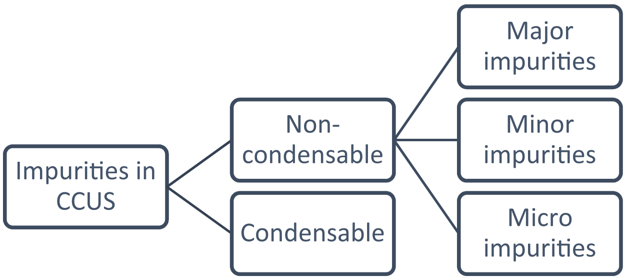


Fig. 4 Classification of impurities in CCUS

$$H_2S + H_2O \rightarrow H_2SO_4 \quad (2)$$

This acid can cause significant problem towards the pipelines and equipment due to its corrosive nature which are known as sour corrosion (Bai and Bai 2019). Furthermore, H_2O also can form hydrates when reacts with hydrocarbons component in the systems. These hydrates can cause disruption to the stream flow as at certain temperature and pressure, it will adhere to the pipeline and by time it can block the pipelines (Anheden et al. 2005; Husein et al. 2021; International Organisation of Standardisation 2020).

Carbon monoxide (CO)

Carbon monoxide is a colourless and tasteless gas that is produced when carbon in fuel is not completely burned (Wilbur et al. 2012). However, the percentage for this compound can be very low percentage. Excessive CO composition in a stream may affect sequestration and utilization process. For sequestration, due to the nature of this gas to be classified as GHG, the concern revolves around storage leaks and exposure to the atmosphere. In addition to that, CO have the ability to increase the minimum miscibility pressure (MMP) that are used in utilisation process by enhanced oil recovery. If the compound present in the stream is more than 5%, it may negatively affect the EOR overall performance (SNC-Lavalin Inc 2004). From previous study, the acceptable CO range that is deemed safe and acceptable for feasible project is between 900 and 5000 µmol/mol (Harkin et al. 2017).

Nitrogen (N_2), oxygen (O_2), and argon (Ar)

Nitrogen, oxygen, and argon are known as the air gasses because these are the main composition of dry air. Even though these gases are known as light gas, it still can pose some problems in CCUS process especially in storage and utilization segments. For example, these light gasses have the ability to lower the stream density in which can limit the CO_2 storage capacity (International Organisation of Standardisation 2020; SNC-Lavalin Inc 2004). Other than that, the presence of O_2 may present some threat to the storage integrity as it may dissolve caprock (Pearce et al. 2016). However, in order it to pose significant threat to the storage structure, large quantity of oxygen is needed thus, to prevent such nature, 10 µmol/mol of oxygen is often used to be the maximum allowable limit in the stream (Wang 2015). In term of utilization segment, likewise with carbon monoxide, the presence of these gasses also can boost the minimum miscibility pressure (MMP) thus can affect the EOR performance (SNC-Lavalin Inc 2004). Other than that, the presence of oxygen may pose as fire hazard and also can increased bacteria growth in the field (Forbes et al. 2008; Shirley and Myles 2019; White et al. 2009).

Sulphur oxides (SO_x) and hydrogen sulphide (H_2S)

SO_x and H_2S are colourless gases that have a bad odor (Bai and Bai 2019). These gasses have the ability to cause damage in the CCUS system especially to the production equipment and pipelines by either turning sour on its own or by reacting with water to produce corrosive sulphuric acid (H_2SO_4) (De Visser et al. 2008; Intergovernmental Panel on Climate Change 2015; Schwartz 1989; SNC-Lavalin Inc 2004). Usually, when fossil fuel or coal is combusted, it will produce a high concentration of these acidic gas which if it is release to the atmosphere, it can cause acid rain (Mohajan 2019). Thus, a strong and stable storage are needed to prevent leak, as it will release toxic gases to the atmosphere and endanger everything in the surrounding (Intergovernmental Panel on Climate Change 2015; SNC-Lavalin Inc 2004). Other than that, one study found that the presence of H_2S in the stream can cause pore blockage at the storage site, this is unfavourable as it may limit the efficiency of the storage (Wang 2015). Due to the dangerous consequences that these gasses may cause, the standards or common practice for the maximum allowable limit for H_2S is very low when compared to other impurities at 50 µmol/mol (Forbes et al. 2008).

Impurities effects on CCUS

An important part of the CCUS safety analysis is the determination of the impurities impact towards CCUS system. All of the impurities in the system does not give the same effects toward the system where some have a more substantial effect compared to the others. For example, non-condensable impurities could alter the stream thermodynamic and other properties by raising the saturation pressure while reducing the critical temperature of CO_2 (International Organisation of Standardisation 2020; Peletiri et al. 2017; SNC-Lavalin Inc 2004; Wetenhall et al. 2014). This, in turn, can alter the behaviour of the stream and effecting the system during transportation and storage. When the stream is transported though pipelines, if the stream properties is not favourable, it needed higher pressure is needed to ensure that the flow is in single phase flow. During storage, similar problem can be observed where higher injection pressure is needed due to pore blockage, hence limiting the storage capacity (Wang 2015).

There are numerous ways that impurities could affect the CCUS operations, from design and operation of pipelines to geological and storage possibilities. Since pure CO_2 behaves in a different way when compared to normal capture stream, this is the primary reason that need to be address and understand. Impurities can have physical and chemical effects on CCUS where both have the potential to impair CCUS system from working feasibly. The effect of CO_2 stream with impurities on CCUS system can be divided into two namely, physical and chemical effects. Briefly, physical effect is due to the variation of density and viscosity however, chemical effect is due to the compound reactivity with reservoir rocks (Nicot et al. 2013). The next section will discuss in detail on the physical and chemical effect of impurities in CO_2 stream.

Physical effects of impurities

Physical impacts of impurities refer to the variations in the phase behaviour and density of pure CO_2. The density of CO_2 is affected by the presence of non-condensable impurities such as O_2, N_2 and Argon, which cannot be liquefied at ambient temperature. These non-condensable impurities, which do not compress to the same degree as pure CO_2, may also result in a loss in system capacity when pure CO_2 is replaced. Table 3 shows the typical CO_2 stream composition in CCUS system based on studies and handbook by previous researchers (Rumble et al. 2021; Wang 2015).

Effect on phase behaviour

From previous literature, it is found that even the slightest impurities have the ability to change the phase behaviour of CO_2 stream (Luna-ortiz 2021; Luna-ortiz et al. 2021). To ensure a stable and steady supply of CO_2 stream in pipeline, the operator must ensure that stream flow always be in a single phase in order to decrease energy usage and investment costs while also ensuring operational safety (Li 2008). Any change of phase behaviour on pipeline transportation during the supercritical phase may need the operator to increase the supply pressure in order to avoid two-phase flow from developing. This happens because the impurities increase the bubble point of the stream (Luna-ortiz et al. 2021). If this is not monitored properly, two-phase flow condition can happen in the pipelines, and this will hinder the system to work efficiently. This will cause problems towards compressor, pump and during injection process (Wang 2015; Zirrahi et al. 2010). Furthermore, CO_2 stream that contains impurities can negatively impact the stream properties in term of pressure, temperature, and composition. The permeation and buoyancy of a CO_2 plume are affected by the permeation and viscosity of a mixture's physical qualities.

Table 3 Molecular Weight and Critical Properties for CO_2 Stream (Rumble et al. 2021; Wang 2015)

Impurities	MW (g/mol)	Critical temperature (K)	Critical pressure (MPa)
CO_2	44.010	304.20	7.39
H_2	2.016	33.20	1.30
CH_4	16.040	190.82	4.64
NH_3	170.31	405.40	11.33
H_2O	18.015	647.10	22.06
CO	28.010	132.86	3.49
N_2	28.013	126.00	3.39
O_2	32.000	154.58	5.04
H_2S	34.081	373.59	9.01
Ar	39.948	151.15	4.87
SO_2	64.066	430.65	7.88
SO_3	80.066	491.45	8.49
Hg	200.590	1765.00	151.00
NO	30.00	180.15	6.48
NO_2	46.01	431.15	10.13

Due to their low critical temperatures, non-condensable impurities especially H_2, N_2, O_2 and Ar can increase bubble point and vapour liquid saturation pressure while lower critical temperature (Al-siyabi 2013; Peletiri et al. 2017; Wang 2015). Vapor–liquid equilibrium (VLE) phase studies are commonly used to better understand the phase behaviour of binary systems and multicomponent mixtures. However, the relation is non-linear as it moves closer to the VLE line due to phase change (Luna-ortiz et al. 2021).

Effect on storage capacity

Previous studies discovered that inert impurities can directly affect the structural trapping capacity by replacement of CO_2 and also reducing the density of the stream (Wang et al. 2012). This density reduction causes the stream to be less compressible compared to pure CO_2 stream, thus reduce the efficiency of the storage (Wang 2015). It is also noted that O_2, Ar, and N_2 give higher density reduction largely related to higher volume compared to H_2 in the supercritical stream (Wang 2015). This effects, however, is highly dependent on the pressure and temperature of the well. Study by IEA Greenhouse Gas R&D Programme (IEAGHG) found that the storage capacity can reduce up to 40% in 15% of non-condensable impurities present in the stream at shallow reservoir, however, at deeper reservoir of more than 3800 m, the storage capacity is approximate to the pure CO_2 streams (Wang et al. 2012; Wang 2015). Similar findings were found by another group of researchers and the results is shown by Fig. 5. Due to these reasons, it is unfeasible to store CO_2 stream with impurities at shallow reservoir (Neele et al. 2017). In order to quantify the storage capacity of reservoir, (3) is used. This is the ratio of mass CO_2 per unit volume in the stream with impurities to the pure state of CO_2.

$$\frac{M}{M_0} = \frac{\overline{\rho}}{\rho_0\left(1+\sum_i m_i/m_{CO_2}\right)} \tag{3}$$

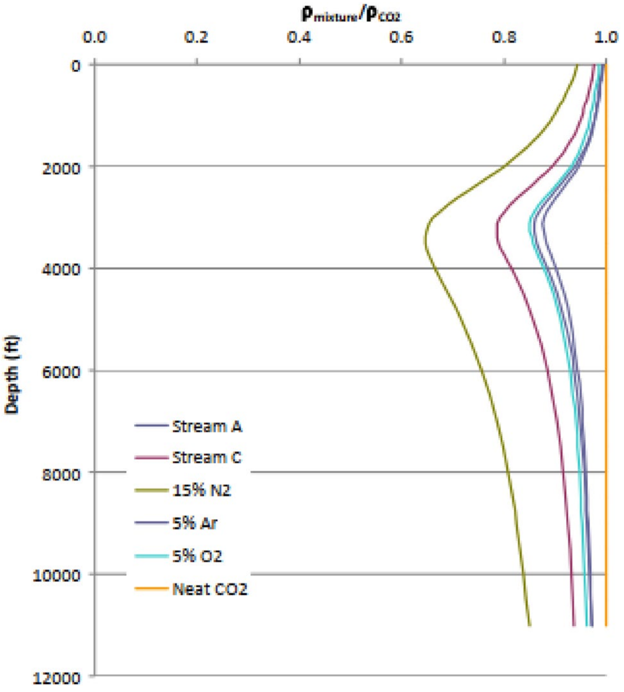


Fig. 5 Mixture density relative to the depth (Wang et al. 2012)

where M and M_0 refer to the mass of CO_2 with impurities and mass of CO_2 pure, respectively. While ρ and ρ_0 represent density of CO_2 with impurities and density of pure CO_2. Lastly, m_i/m_{CO2} represent the mass ratio between CO_2 with impurities and pure CO_2 stream.

The amount of CO_2 held per unit volume of storage space reduces when impurities are present in the CO_2 stream (Wang 2015). Capacity is a key factor in determining the total cost of CCUS. The cost of injection wells and the amount of CO_2 that can be permanently stored are currently considered in cost estimating methods. Reduced CO_2 storage capacity due to impurities may cause a drop in storage capacity earlier than expected, increasing storage costs later. Furthermore, N_2, O_2, Ar, CH_4, H_2S, decreased CO_2 storage capacity for solubility trapping mechanism, while SO_2 would enhance it (Kim and Song 2017; Ziabakhsh-ganji and Kooi 2014).

Effect on injectivity

The ability of a geological formation to take CO_2 injection fluids can be characterised as injectivity (Md Yusof et al. 2021). As mentioned before, the non-condensable impurities have the ability to decrease stream density, this will in turn cause mass flux to drop over the same pressure drop (Yusof et al. 2022). However, as viscosity decrease, it will increase the mass flux which eventually effecting injectivity (Wang 2015). As density and viscosity are dependent on pressure and temperature, these effects are less likely to cause problem at deeper reservoir storage (Nicot et al. 2013). Studies found that a substantial amount of non-condensable impurities can reduce injectivity by 15% at shallow or low-pressure reservoir, however, at deeper reservoir with higher pressure of more than 20 MPa, the injectivity is almost similar to pure CO_2 stream (Wang 2015). The Darcy's law of permeation flux can be used to examine effects in a single-phase flow. A normalized permeation flux formula is shown in (4).

$$\frac{M_{CO_2}}{M_0} = \frac{\rho(\mu_0/\mu)}{\rho_0(1+\sum_i m_i/m_0)} \tag{4}$$

where M_{CO2} and M_0 are the mass flow per unit area for CO_2 with impurities and pure CO_2 stream respectively, while ρ and ρ_0 are the densities of the injected stream and pure CO_2; μ and μ_0 are the viscosities of the injected fluid and pure CO_2.

The pressure and temperature of the system will have the greatest impact on the viscosity and density of the fluid. There have been a number of hypothetical simulations done to investigate the impact of injectivity on storage capacity, and the results suggest that compensation between density and viscosity has a significantly smaller impact on injectivity than previously thought (Wang 2015).

Effect on buoyancy

As impurities can alter the density and velocity of the stream, it will indirectly increase the buoyancy of the CO_2 plume in the reservoir. Previous study discovered that high level of impurities may increase the buoyancy by 50% depending on pressure and temperature. This, in turn, can also increase the velocity of the stream by three-fold (Wang 2015). Depending on the heterogeneity of reservoir, the rising velocity of the injected CO_2 plume could reduce residual trapping and increase lateral spreading of the plume at the caprock. Other than that, increase in buoyant force may make the CO_2 with impurities plume to be less broad when compared with pure CO_2 stream (Nicot et al. 2013). The buoyancy of a normalized CO_2 plume can be calculated by (5) (Wang 2015).

$$\frac{F}{F_0} = \frac{\rho_{H_2O}-\rho_m}{\rho_{H_2O}-\rho_{CO_2}} \tag{5}$$

where F and F_0 are buoyancy forces for the CO_2 mixture and pure CO_2, ρ_{H2O}, ρm and ρ_{CO2} are the densities of the formation water, plume, and pure CO_2 respectively.

Chemical effects of impurities

Most significant component that gives higher chemical effect is the condensable impurities (SO_x, NO_x, and H_2S). In contrast to the physical impacts of impurities, the chemical reactions from impurities take some time to occur and require long-term monitoring.

Effect on injectivity, caprock and reservoir capacity

The presence of SO_x with water can produce sulphuric acid which is a very acidic acid. This can lower pH and cause mineral precipitation of sulphate and dissolution of both carbonate with aluminosilicate rock in the reservoir (Wang et al. 2011; Wang 2015). This usually happen after injectivity process finished, the stream with impurities will migrate towards the caprock and reaction may occur resulting in mineral dissolution which is shown in Fig. 6. Previous study showed that with the presence of only 1.5% of SO_x in the stream, it can increase the dissolution rate up by 50% (Wang 2015). This caprock dissolution can negatively affect the caprock integrity and increasing the chance of leak to happen. Rapid dissolution and precipitation of minerals can alter the initial reservoir rock characteristics and this can block some pore and effecting the porosity which eventually can affect the reservoir capacity and injectivity (Bacon et al. 2009; Labus and Suchodolska 2017; Wang 2015). The problem can be worsened when H_2S present, this usually happen when both pre and post combustion source injected at the same reservoir. A substantial pore blockage in the formation could be caused by the deposition of sulphur compounds. Other than that, O_2 also can play role in the dissolution of rocks by reacting with pyrite forming iron sulphate which can cause acidic pockets, however, for this to happen it large amount of O_2 is needed to be present in the stream (Wang 2015). On top of that, impurities may alter the wettability of the rock, resulting in the rock requiring various sealing capabilities to hold the CO_2 with impurities (Li et al. 2005).

Effect on surface materials

The return of acidic impurities-containing water can harm well materials both during and after CO_2 injection by corrosion (Wang et al. 2019). Impurities such as SO_x and H_2S can be found in CO_2 injection streams and can exacerbate corrosion and this is a key issue in CCUS system (SNC-Lavalin Inc 2004). This is likely to happen after injection is finished because from thermochemical estimation shows that the acid impurities are more significant to the cement compared to rocks. This is because the chemical properties for SO_x is almost identical to the CO_2 (Scholes et al. 2009). This can cause a huge problem if the protective layer of the cement lost, it can affect the steel casing and can cause corrosion. Thus, to avoid this, the project needs to invest higher in improving casing quality and cement (Wang 2015). If the cement sheaths fail to protect them, the steel casings are vulnerable, Fig. 7 depicts corrosion of well components after exposure to the CO_2 stream with impurities. An addition to that, the presence of O_2 also can escalate the corrosion rates of carbon steel in water-saturated CO_2 phase (Choi et al. 2010).

Conclusions

This paper presents a comprehensive review on physical and chemical effects of impurities on the CCUS system. Based on the extensive literature analysis the following conclusions were made:

- Global standard-setting organizations have established their own recommendations or best practices for purity and the composition of impurities that are judged appropriate and safe for the environment and CCUS deployment.
- In the CCUS development chain, the presence of impurities in captured CO_2 has been considered as being a significant concern.
- CO_2 stream with impurities affects the viscosity and density variations result in physical consequences, whereas compound reactivity with reservoir rocks results in chemical impacts.

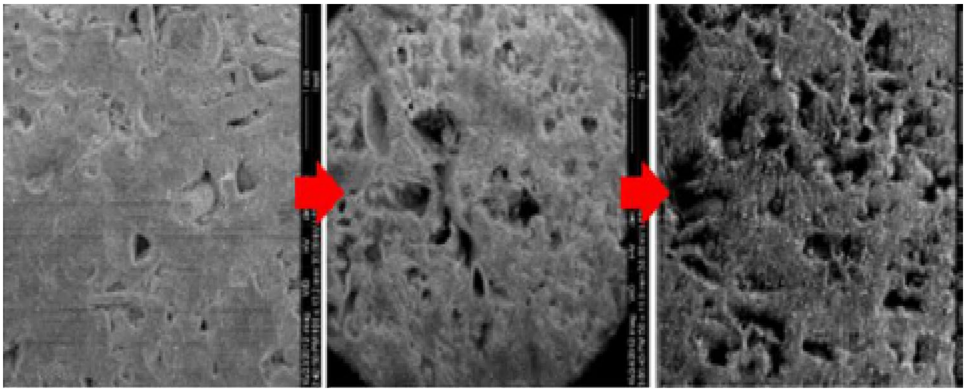


Fig. 6 Example of the dissolution of minerals on reservoir rock over time, post CO_2 injection for storage

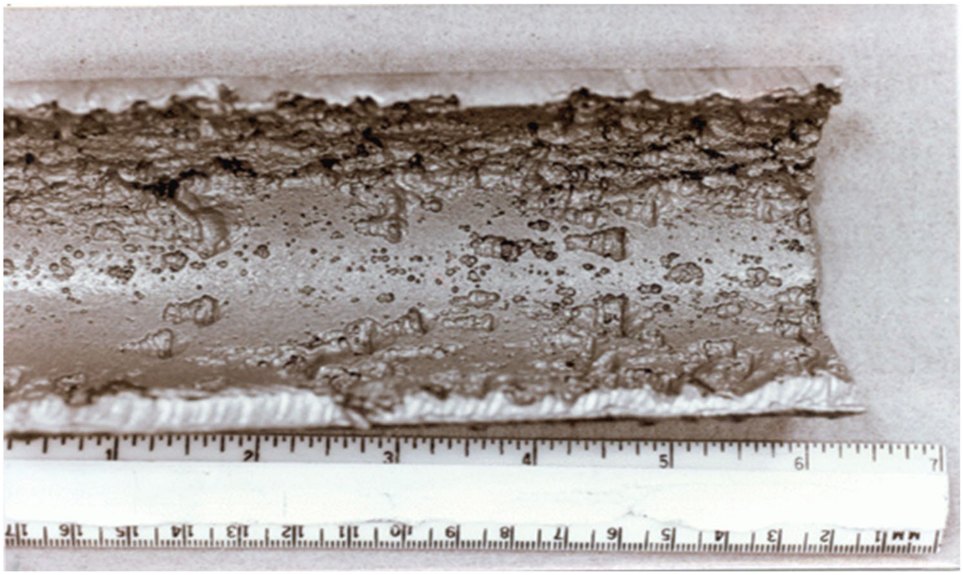


Fig. 7 Example of the corrosions occurred on the well materials, after been exposed with CO_2 with the presence of impurities

- The thermophysical characteristics of impurities are shown to have a significant impact on CCUS functioning in term of phase behavior, storage capacity, injectivity and buoyancy of the CO_2 plume in the reservoir.
- The chemical impurities knowingly affect the CO_2 storage properties such as corrosion, injectivity failure, and reservoir capacity of the geological site.

Recommendations

- As the knowledge of CCUS technologies becomes better understood, current standard and guidelines recommended to be updated regularly to incorporate new best practices as we learn more about the CCUS technologies as a whole.
- Special attention during the early deployment phase is recommended to highlight which areas that require greater investigation, as this is where the potential for future development is most obvious.
- Currently, there is limited research on how contaminants affect the geological storage of CO_2, and several of the theoretical impacts investigated in the study have not yet been supported by actual evidence.
- It is crucial that researcher stay informed about new experimental study that might confirm the consequences. The results of this investigation may have greatly contributed to this technology advancement and reap the potential advantages of CCUS technology which demonstrate that safe and permanent storage is feasible.

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Declarations

Conflicts of interest On behalf of all the co-authors, the corresponding author states that there is no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

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