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Impurity-Driven Phase Behaviour Changes and Risk of Phase Separation in CO_2 Transport and Storage

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ABSTRACT

The integration of carbon capture and storage (CCS) into climate mitigation strategies demands a comprehensive understanding of the phase behaviour of CO_2, especially when transported and injected with impurities. Industrial CO_2 streams are rarely pure and typically contain varying amounts of gases such as nitrogen (N_2), methane (CH_4), oxygen (O_2), sulphur dioxide (SO_2), hydrogen sulphide (H_2S), argon (Ar), and water vapor (H_2O). These impurities significantly alter the thermophysical properties and phase behaviour of CO_2, affecting its compressibility, viscosity, density, and critical point. Impurities can shift the phase envelope, increase the risk of two-phase flow, and cause phase separation during transport and injection, potentially leading to operational inefficiencies, increased corrosion risk, and mechanical stress on infrastructure. This review critically analyses how different impurities influence CO_2 phase behaviour under pipeline and reservoir conditions. Emphasis is placed on the implications of phase instability for flow assurance, pipeline integrity, and reservoir performance. Additionally, we discuss current modelling approaches and experimental findings that aid in predicting and managing impurity-driven phase transitions. Understanding these effects is essential for designing safe and efficient CCS systems, especially under high-pressure, high-temperature subsurface conditions.

Keywords: *CO_2 Impurities, Phase Behaviour, CCS, Pipeline Transport, Phase Separation, Injection Risk, Flow Assurance, Thermodynamic Modelling.*

1. INTRODUCTION

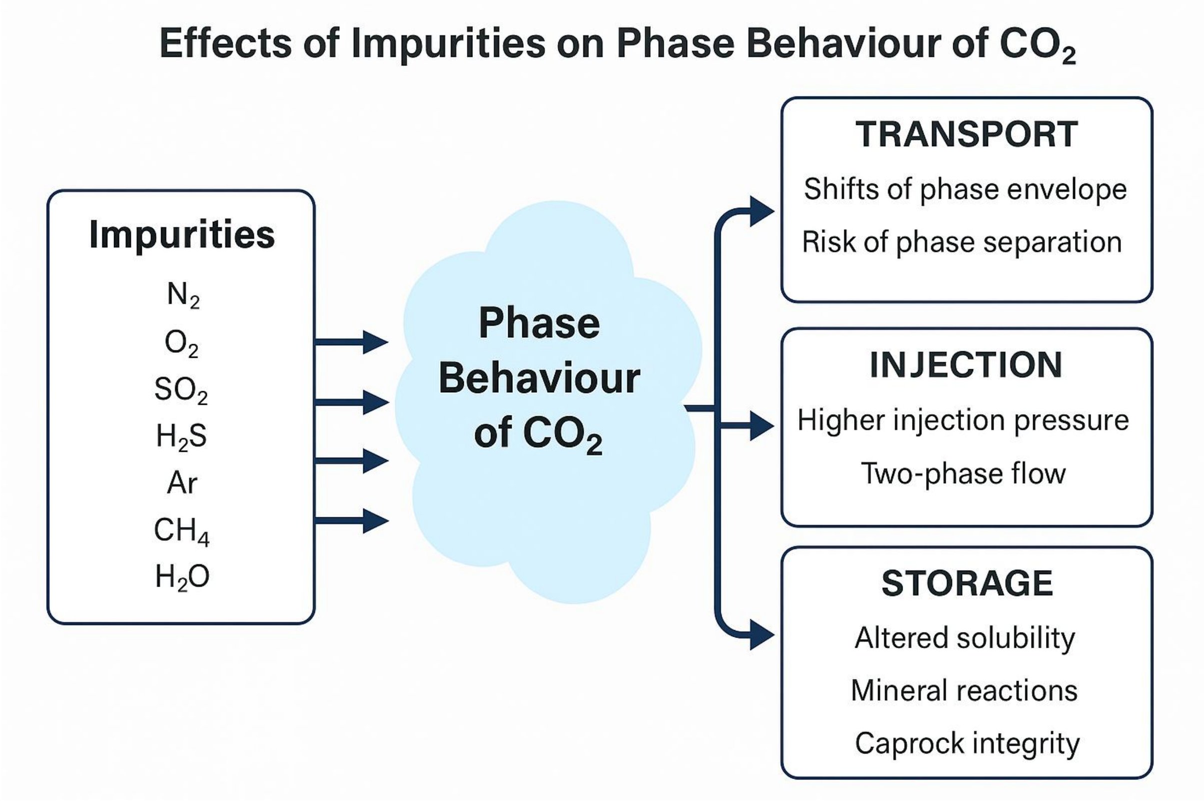
Carbon capture and storage (CCS) has emerged as a vital technological pathway to mitigate global CO_2 emissions and address climate change. While the majority of research and commercial focus has traditionally emphasized CO_2 capture and storage capacity, the transport and injection stages are equally critical for the successful deployment of CCS systems. In real-world industrial applications, the captured CO_2 stream is rarely pure and often contains a range of gaseous impurities such as nitrogen (N_2), oxygen (O_2), sulphur dioxide (SO_2), hydrogen sulphide (H_2S), argon (Ar), methane (CH_4), and water vapor (H_2O), depending on the capture method and feed source. [1] These impurities significantly influence the phase behaviour of CO_2, altering its thermophysical properties and presenting challenges in both pipeline transport and geological injection. Even small concentrations of non-condensable or reactive impurities can shift the phase envelope, lower the critical temperature, and increase the risk of phase separation. Such shifts may lead to the formation of gas-liquid two-phase flow regimes, which compromise flow assurance, reduce energy efficiency, and increase the likelihood of operational disruptions such as pressure drop fluctuations, hydrate formation, and internal corrosion. Moreover, impurities can affect the compressibility, density, and viscosity of the CO_2 stream, directly impacting injection pressure requirements and storage efficiency. These issues are particularly problematic in pipelines designed to operate under supercritical or dense-phase..

conditions, where stability is crucial for economic and technical feasibility. The potential for phase separation also introduces additional complexity in subsurface injection processes, where sudden changes in phase can hinder injectivity, damage reservoir integrity, and reduce long-term storage security. [2] This review examines the impurity-induced modifications to the phase behavior of CO_2 and evaluates their consequences on transport and injection processes. By synthesizing thermodynamic studies, experimental findings, and modeling efforts, the paper highlights the key challenges, safety concerns, and engineering considerations necessary for the development of robust, impurity-tolerant CCS systems

Effects of Impurities on Phase Behaviour of CO2

Carbon capture and storage (CCS) is considered a crucial technology for reducing carbon dioxide (CO_2) emissions. Among the various components of CCS, the capture process accounts for the highest cost. Depending on the technology used, captured CO_2 streams often contain impurities such as nitrogen (N_2), oxygen (O_2), sulphur dioxide (SO_2), and hydrogen sulphide (H_2S). While complete separation of these impurities is technically possible, it significantly increases operational costs. Therefore, co-injection of CO_2 along with its associated impurities is a more cost-effective alternative. In some cases, integrated capture and storage of multiple atmospheric pollutants alongside CO_2 is also pursued. However, the presence of impurities adversely impacts the transport, injection, and storage stages of CCS. Non-condensable gases like N_2, O_2, and argon (Ar) elevate the saturation pressure and lower the critical temperature of CO_2, thus necessitating additional pressure and lower temperatures to prevent phase separation in pipelines. [3] These impurities also raise the injection pressure and reduce storage efficiency by decreasing the overall density of the CO_2 stream. Additionally, acidic impurities such as SO_x and NO_x can interact chemically with reservoir and cap rocks, potentially compromising injectivity and long-term storage integrity. In the case of a leak, the release of hazardous impurities poses significant environmental risks.

Natural Resources Canada (NRCan) plays a leading role in the country's federal CCS initiatives. In addition to conducting R&D on CO_2 capture from coal-fired power plants and other sources, NRCan actively collaborates on projects related to CO_2 storage, including injection practices, monitoring and verification systems, storage integrity assessments, and estimation of storage capacity. [4] Given the limited literature on how impurities affect factors such as storage capacity, integrity, and injectivity—especially in saline formations—NRCan, with support from the IEA Greenhouse Gas Programme (IEA GHG), has undertaken detailed studies to address these gaps. Selected findings from these investigations are discussed herein.



Effects of Impurities on Phase Behaviour of CO_2

The phase behaviour of carbon dioxide (CO_2) is a critical factor in the design and operation of carbon capture and storage (CCS) systems. Industrial CO_2 streams are seldom pure and often contain impurities such as nitrogen (N_2), oxygen (O_2), sulphur dioxide (SO_2), hydrogen sulphide (H_2S), methane (CH_4), and water vapor (H_2O), depending on the capture source and technology used. These impurities significantly alter the thermophysical and phase properties of CO_2, impacting its performance in transport, injection, and storage processes.

Non-condensable impurities like N_2, O_2, and Ar increase the saturation pressure and reduce the critical temperature of the CO_2 mixture. This leads to a higher risk of phase separation during pipeline transport, requiring more stringent pressure and temperature control to maintain a single-phase flow. [5] The presence of these gases also reduces the overall density of the CO_2 stream, lowering the storage efficiency of geological formations.

Acidic impurities such as SO_2 and NO_x introduce additional complications. They can react with brine and rock minerals, altering reservoir chemistry and potentially compromising caprock integrity. Furthermore, these impurities may increase the corrosion rate of pipelines and injection wells, posing operational and safety challenges.

Thermodynamic Impact of Impurities on CO_2 Phase Behaviour

When impurities are present in a CO_2 stream, they alter the thermodynamic properties of the mixture significantly. These changes affect how the CO_2 behaves under various temperature and pressure conditions, especially during transport and injection phases in Carbon Capture and Storage (CCS) operations. The key thermodynamic impacts include:

1. Shift in Critical Temperature and Pressure

Pure CO_2 has a critical temperature of approximately 31.1°C and a critical pressure of 7.38 MPa (73.8 bar). This is the point above which CO_2 exists as a supercritical fluid—neither a true liquid nor gas with properties ideal for pipeline transport and deep injection. [6]

When impurities are introduced:

Non-condensable gases like N_2, O_2, and Ar tend to lower the critical temperature and increase the critical pressure of the CO_2 mixture.

This means the CO_2 mixture requires higher pressure and/or lower temperature to remain in a supercritical or dense phase.

As a result, pipelines must operate under more stringent pressure and cooling conditions to avoid phase separation, which could lead to unstable two-phase flow.

2. Altered Phase Envelope and Vapor-Liquid Equilibrium (VLE)

The phase envelope describes the conditions (pressure vs. temperature) under which a fluid mixture exists in a single phase (liquid or gas) or two phases (vapor + liquid). Impurities modify this envelope in several ways:

Impurities expand the two-phase region, making the mixture more prone to vapor-liquid separation at operating conditions.

The bubble point and dew point curves shift, which can cause phase instability during decompression or pressure drops along pipelines.

For example, adding methane (CH_4) or nitrogen (N_2) increases the range of conditions where gas-liquid separation occurs, complicating flow assurance.

This behaviour is crucial for pipeline design, as it determines the safe range of operating pressures and temperatures to avoid two-phase conditions. [7]

3. Impact on Density, Viscosity, and Compressibility

These transport properties are critical for designing compressors, pipelines, and injection systems:

Density

The density of supercritical CO_2 is typically high (~600–800 kg/m³), allowing more CO_2 to be stored per unit volume.

Impurities like N_2 and CH_4 significantly reduce the density of the mixture, which:

Decreases storage efficiency in geological formations.

Requires larger volumes to be injected to store the same amount of CO_2.

Affects buoyancy forces, possibly increasing leakage risks.

Viscosity

Viscosity determines flow resistance and affects pumping power.

Some impurities slightly lower CO_2 viscosity, while others (like H_2S or SO_2) may increase it depending on concentration and temperature.

Changes in viscosity affect pressure drop calculations and pipeline sizing.

Compressibility

Compressibility defines how volume changes with pressure.

A mixture with high compressibility will have greater volume fluctuations, complicating pressure regulation.

Impurities usually increase the compressibility factor (Z), deviating the mixture behaviour from ideal gas laws. [8]

Table 1: Impact on Density, Viscosity, and Compressibility

Property	Effect of Impurities	Implications
Critical Temperature	↓ (lowered by N_2, O_2, CH_4)	Harder to keep in supercritical phase
Critical Pressure	↑ (increased by impurities)	Requires higher pressure for injection
Phase Envelope	Expanded, shifted bubble/dew points	Increased risk of phase separation
Density	↓ (less dense mixtures)	Reduced storage capacity, altered buoyancy
Viscosity	↑ or ↓ depending on impurity	Affects pumping efficiency and flow stability
Compressibility	↑ (higher Z factor)	More difficult to predict volume/pressure behavior

In saline aquifers, the presence of impurities affects key storage mechanisms—including solubility trapping and mineralization—by changing CO_2 solubility and fluid-rock interactions. The implications are particularly significant for long-term containment and leakage risk. Understanding impurity-driven changes in phase behaviour is essential for optimizing CCS system design, ensuring pipeline integrity, maintaining injectivity, and securing long-term storage. Continued experimental research and advanced thermodynamic modelling are vital to predict and manage the impact of impurities on CCS performance. [9]

Risk of Phase Separation in CO_2 Pipelines

In Carbon Capture and Storage (CCS) operations, the safe and efficient transport of carbon dioxide (CO_2) is critically dependent on maintaining the fluid in a stable, single-phase—typically in a supercritical or dense liquid state. However, the presence of gaseous impurities such as nitrogen (N_2), oxygen (O_2), methane (CH_4), argon (Ar), and hydrogen sulphide (H_2S) significantly alters the phase behaviour of the CO_2 stream. These impurities lower the critical temperature, shift the vapor-liquid equilibrium (VLE), and narrow the operational stability range, thereby increasing the risk of phase separation under pipeline conditions.

Phase separation can occur when temperature or pressure in the pipeline deviates from the optimal range required to maintain a single-phase state. Pressure drops along the pipeline due to frictional losses or elevation gradients may cause the fluid to cross the dew point or bubble point, resulting in vaporization or condensation of CO_2. Similarly, cooling caused by environmental exposure or Joule-Thomson expansion during decompression can move the system into a two-phase region of the phase envelope. [10] The likelihood of these transitions is exacerbated by impurities, which expand the two-phase region and reduce the critical stability margin of the CO_2 mixture. Once two-phase flow initiates, a number of operational issues emerge. These include flow regime instabilities such as slug flow and annular flow, which can induce pressure pulsations, vibration damage, and control difficulties. Pressure drops across the pipeline increase significantly in two-phase flow, raising recompression costs and reducing energy efficiency. An especially critical risk is the formation of CO_2 hydrates in the presence of residual water under low temperature and high pressure. Hydrate formation can obstruct flow, damage pipeline components, and lead to catastrophic failures if not mitigated effectively.

Several case studies highlight the importance of managing phase behaviour risks. The COORAL project in Germany demonstrated that even low concentrations of N_2 (as low as 2%) significantly reduced the range of safe, single-phase operation. In the Weyburn-Midale project in Canada, impurity-driven phase behaviour shifts necessitated operational adjustments during enhanced oil recovery (EOR) injection. Similarly, the In Salah CCS project in Algeria experienced flow assurance challenges due to impurity variability in the transported CO_2. Laboratory and simulation studies in Norway showed that rapid decompression of impure CO_2 can lead to two-phase flashing, reinforcing the need for robust thermodynamic modeling and safety protocols. To mitigate these risks, CCS operators must employ rigorous impurity control standards, real-time monitoring of pressure and temperature, and use of phase diagrams for dynamic flow simulations. [11] Design considerations such as pipeline insulation, hydrate inhibition, and pressure control valves play a vital role in maintaining operational integrity. As CCS expands globally, addressing phase separation risks is essential to ensure the long-term safety and reliability of CO_2 transport networks.

Table 2: Risk of Phase Separation in CO_2 Pipelines

Risk Factor	Effect	Mitigation Strategy
Pressure drop	Causes condensation/vaporization	Maintain high pressure, reduce pipeline length
Temperature drop	Moves CO_2 into two-phase region	Thermal insulation, temperature control
High impurity concentration	Alters phase envelope, lowers stability margin	Set impurity specifications, real-time monitoring
Two-phase flow formation	Causes slug flow, instability	Design for worst-case flow regimes
Hydrate formation	Pipeline blockage	Use of dehydration units and inhibitors

Impurity Effects on CO_2 Injection Dynamics

The injection dynamics of carbon dioxide (CO_2) into geological formations are significantly influenced by the presence of gaseous impurities in the CO_2 stream. These impurities, such as nitrogen (N_2), methane (CH_4), oxygen (O_2), and hydrogen sulphide (H_2S), alter key injection parameters—namely pressure, temperature, phase behaviour, and miscibility with in-situ reservoir fluids. [12] One of the primary effects is the increase in required injection pressure, as non-condensable gases reduce the density and compressibility of the CO_2 stream, making it more resistant to compression and flow under reservoir conditions. In parallel, the shift in phase envelope caused by impurities can reduce the temperature window for single-phase injection, necessitating additional cooling or heating infrastructure to maintain operational stability. Moreover, impurities affect the miscibility between CO_2 and reservoir fluids, which is especially critical in enhanced oil recovery (EOR) scenarios. Pure CO_2 has favorable miscibility with hydrocarbons, facilitating efficient oil displacement. However, the presence of N_2 or CH_4 can raise the minimum miscibility pressure (MMP), potentially making the CO_2 stream partially or completely immiscible with the reservoir fluids. This results in reduced sweep efficiency, lower oil recovery, and increased gas breakthrough risks. In saline aquifer storage or depleted gas reservoirs, impurities reduce the injectivity—the ease with which fluids can be injected—due to their impact on fluid properties such as viscosity and density, which in turn affects flow through porous media. Lower-density CO_2 mixtures may exhibit reduced mobility and uneven front advancement, creating injection inefficiencies and flow diversion. [13]

Another critical concern is the local cooling effect near the injection wellbore, especially during high-rate injection or pressure drops. The Joule-Thomson effect, enhanced by certain impurities, can cause rapid cooling that may drop temperatures below hydrate formation thresholds or even cause thermal stress-induced cracking of wellbore cement and surrounding rocks. This can compromise well integrity, reduce sealing efficiency, and accelerate infrastructure degradation if not properly accounted for during well design. [14] Furthermore, impurity-driven changes in CO_2 phase behavior can affect the utilization of available pore space within the reservoir. Due to decreased density of the impure CO_2 mixture, more volumetric space is required for the same mass of CO_2, thereby reducing the effective storage capacity. Additionally, if phase separation occurs during or after injection, gas exsolution or condensation can create multiphase flow conditions that limit the long-term containment and reduce capillary trapping efficiency. [15] These effects are compounded in heterogeneous reservoirs, where impurities can amplify flow channelling or bypassing of target zones. Addressing impurity effects on injection dynamics requires advanced reservoir simulation tools that incorporate real-fluid equations of state (EOS), impurity-specific phase diagrams, and formation-specific data. Adaptive injection protocols, robust monitoring, and flexible surface facilities are essential for optimizing injection performance and ensuring the long-term safety and efficiency of CO_2 storage.

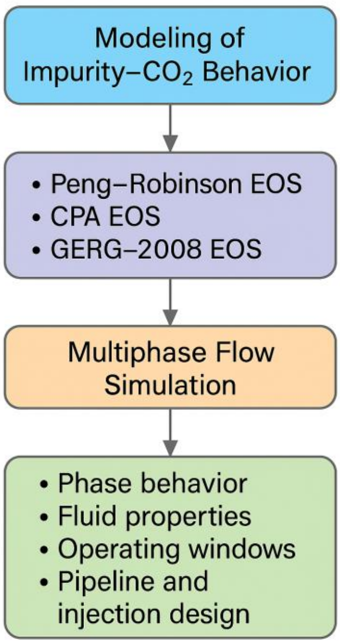
Material and Infrastructure Challenges

The transportation and injection of CO_2 streams containing acidic impurities such as sulphur dioxide (SO_2) and hydrogen sulphide (H_2S) introduce significant challenges to the integrity of pipelines and subsurface infrastructure. These impurities, when dissolved in the presence of water, form strong acids like sulphurous acid and hydro sulfuric acid, which are highly corrosive to conventional pipeline and well materials. This corrosive environment accelerates the degradation of carbon steel, which is commonly used in pipeline construction, leading to thinning of pipe walls, development of leaks, and potential catastrophic failure if not properly managed. [16] A major concern is material compatibility, particularly in injection well casings and tubing, which are constantly exposed to high-pressure, high-temperature CO_2 mixtures. Standard materials may suffer from stress corrosion cracking, especially under fluctuating pressure and temperature conditions. Additionally, localized corrosion phenomena such as pitting and crevice corrosion can initiate in micro-defects or weld seams, leading to structural weakness over time. Acidic impurities also promote hydrogen embrittlement, which reduces the ductility and strength of metal components, making them more susceptible to fatigue and failure.

To address these risks, the industry employs a variety of preventive strategies. One common approach is the use of corrosion-resistant alloys such as stainless steels (e.g., 316L) or nickel-based alloys (e.g., Inconel), which exhibit superior resistance to acid attack and are capable of withstanding aggressive chemical environments. However, these materials come at a significantly higher cost and may not be feasible for long-distance pipelines. In such cases, internal coatings such as epoxy linings or polymeric films can serve as protective barriers, preventing direct contact between the corrosive fluid and the pipeline wall. [17] Another widely adopted technique involves the continuous or batch injection of chemical corrosion inhibitors, which form passivating layers on metal surfaces and minimize reaction rates with acids. Proper design and monitoring protocols are equally important. Pipelines carrying impure CO_2 must be designed to accommodate the specific composition of the gas stream, including pressure ratings that consider impurity-driven changes in fluid properties. Monitoring systems such as corrosion coupons, inline sensors, and pigging tools are used to detect early signs of corrosion and material loss. In critical zones such as wellheads and downhole components, dual-barrier systems and redundant seals are recommended to enhance operational safety. Ultimately, ensuring infrastructure integrity in the presence of impurities requires a multidisciplinary approach, combining materials science, fluid chemistry, and engineering design. [18] As CCS deployment scales up, particularly in industrial clusters where impurity-rich CO_2 streams are more common, these material and infrastructure considerations will become even more vital to project viability and long-term containment assurance.

Modelling and Simulation of Impurity–CO_2 Mixtures

Accurate modelling and simulation of impurity-laden CO_2 mixtures are essential for designing safe and efficient carbon capture, transport, and storage (CCS) systems. The presence of impurities such as nitrogen (N_2), oxygen (O_2), sulphur dioxide (SO_2), and hydrogen sulphide (H_2S) significantly alters the thermodynamic behaviour of CO_2 streams. To capture these effects, advanced equations of state (EOS) and simulation models are employed to predict phase behaviour, fluid properties, and system performance under various operating conditions. Among the most widely used thermodynamic models is the Peng–Robinson (PR) EOS, favoured for its simplicity and reasonable accuracy in estimating vapor–liquid equilibrium (VLE) for binary and multicomponent mixtures. [19] However, for more complex or highly polar components, the Cubic Plus Association (CPA) EOS offers improved predictions by accounting for hydrogen bonding and association effects, especially relevant for impurities like water and alcohols. Another robust framework is the GERG-2008 EOS, developed specifically for multicomponent natural gas-like systems. GERG-2008 is particularly suitable for CO_2-rich mixtures with a broad range of impurities, as it combines high-fidelity data with empirical corrections to model compressibility, density, and caloric properties across wide pressure–temperature domains. These EOS models serve as the foundation for multiphase flow simulations, helping engineers evaluate conditions for phase separation, hydrate formation, or supercritical behaviour, which are critical to the integrity and safety of CO_2 transport pipelines and storage sites. [20]



To operationalize these models, a range of simulation tools is used in academia and industry. Software platforms such as Aspen Plus, OLGA, PVTsim, and TOUGH2 allow for dynamic and steady-state simulations of CO_2 injection and flow through pipelines and porous formations. These tools integrate EOS calculations with transport models, enabling detailed predictions of phase envelopes, Joule–Thomson effects, and flow regimes in the presence of impurities. Moreover, they assist in identifying safe operating windows, designing compressor stations, optimizing injection protocols, and estimating storage capacity. Ultimately, thermodynamic modelling of impurity–CO_2 mixtures forms a critical backbone for CCS project planning, risk assessment, and long-term monitoring. [21, 22]

Risk Mitigation and Design Considerations

Effectively managing the challenges posed by impurities in CO_2 streams requires a multifaceted approach that combines robust system design, regulatory guidance, and continuous monitoring. One of the primary strategies involves defining safe and reliable operating envelopes that accommodate the thermodynamic shifts caused by impurities. These envelopes are developed using advanced modeling tools and phase behavior data to ensure the system remains within a single-phase regime during transport and injection. By understanding the phase boundaries of CO_2 mixtures with varying impurity concentrations, engineers can avoid conditions that lead to vapor–liquid separation, hydrate formation, or flow instabilities in pipelines and wells. To limit these risks, impurity specification standards have been developed, such as ISO 27913, which provides guidelines for the acceptable composition of CO_2 streams used in pipeline transport. [23, 24] These specifications help standardize impurity thresholds for components like N_2, O_2, SO_2, and H_2S, thereby ensuring compatibility with materials, operational pressures, and environmental safety requirements. Adhering to these limits reduces the likelihood of corrosion, phase separation, and integrity loss during long-term storage or enhanced oil recovery operations.

In addition to standardization, the incorporation of real-time monitoring systems is essential for early detection of operational anomalies. Pressure sensors, temperature monitors, and phase detectors are strategically placed along pipelines and near injection wells to track system performance and detect any deviation from optimal conditions. These sensors provide critical data to control systems that can trigger automated responses or alert operators in the event of hydrate formation, pressure drops, or two-phase flow onset. Finally, adaptive equipment design further enhances system resilience. [25, 26] Compressors and pipeline components are selected and sized based on a wide range of operating conditions, with the flexibility to handle varying impurity levels and changing flow characteristics. This includes the use of variable-speed drives, anti-surge protection, and modular pipeline sections that allow for expansion or retrofit as needed. Altogether, these risk mitigation and design considerations ensure the safe, efficient, and long-term viability of CO_2 transport and storage networks, even when dealing with complex and impurity-rich gas streams. [27]

Knowledge Gaps

Despite significant advances in carbon capture and storage (CCS) research, several critical knowledge gaps remain, particularly concerning the effects of impurities in CO_2 streams. One of the major limitations is the scarcity of experimental data for multicomponent CO_2 mixtures under high-pressure and high-temperature conditions. While binary systems (e.g., CO_2–N_2, CO_2–SO_2) have been somewhat characterized, data on complex, real-world mixtures involving multiple impurities are limited. [28] This lack of empirical information makes it challenging to validate thermodynamic models, predict phase behaviour accurately, and design safe operating envelopes for CO_2 transport and injection. Another significant area of uncertainty is the long-term geochemical and geomechanically impact of impurities on reservoir formations. Acidic impurities such as SO_2 and H_2S can react with formation brines and minerals, potentially altering rock permeability, porosity, and caprock integrity. However, the full extent of these interactions—particularly over decadal to centennial timescales—is not well understood. This limits the ability to predict storage performance and assess risks related to leakage or reduced injectivity in saline aquifers and depleted hydrocarbon reservoirs.

In addition, there is currently a lack of universally accepted standards for impurity limits across different CCS applications and geographic regions. While some frameworks (e.g., ISO 27913) exist, they are often generalized and may not account for specific reservoir characteristics, regional regulations, or project-specific objectives such as enhanced oil recovery (EOR). The absence of standardized, application-specific impurity guidelines hinders consistency in CCS design and complicates cross-border CO_2 transport and storage initiatives. Addressing these knowledge gaps will require targeted experimental studies, long-term pilot-scale field trials, and collaborative standardization efforts involving regulatory bodies, academia, and industry stakeholders. Closing these gaps is essential for enabling the widespread, safe, and cost-effective deployment of CCS technologies worldwide. [29]

Future Directions

As carbon capture and storage (CCS) continues to evolve into a cornerstone technology for global climate mitigation, addressing the challenges posed by impurities in CO_2 streams becomes increasingly important. Future research must focus on expanding high-quality experimental data for multicomponent CO_2 mixtures under reservoir-relevant pressures and temperatures. This includes not only the acquisition of thermodynamic and transport property data, but also detailed studies on long-term chemical interactions between impurities and geological formations. Such data are essential for refining equations of state (EOS) and improving predictive accuracy of simulation tools used in CCS design. [30-32] Another critical direction involves developing impurity-specific operational guidelines and regulatory frameworks that reflect differences in geological storage types (e.g., saline aquifers, depleted oil fields) and capture technologies. This includes updating and regionalizing standards like ISO 27913 to better accommodate varying impurity profiles across industries and locations. Standardizing impurity limits for diverse CCS applications would help streamline pipeline and infrastructure development, enhance cross-border CO_2 trade, and ensure environmental safety.

Materials science advancements also hold promise. Research into cost-effective, corrosion-resistant alloys, polymer linings, and chemical inhibitors tailored for impurity-rich CO_2 streams could significantly improve the safety and longevity of transport infrastructure. Similarly, smart materials with self-monitoring or self-healing properties may play a role in next-generation pipeline and well designs. [33] Finally, there is growing need for integrated modelling platforms that combine thermodynamics, geochemistry, geomechanics, and risk assessment in real time. These digital tools, possibly powered by machine learning and cloud-based monitoring, could offer predictive insights and adaptive controls for CCS networks operating under variable impurity conditions. [34-36] The future of CCS lies in bridging current knowledge gaps through multidisciplinary collaboration, technological innovation, and the development of globally harmonized standards ensuring that impurity management does not become a bottleneck in the large-scale deployment of CO_2 mitigation strategies.

2. CONCLUSION

The successful deployment of Carbon Capture and Storage (CCS) technologies hinges not only on capturing and storing CO_2 effectively but also on understanding and managing the influence of impurities within the CO_2 stream. This review highlights that impurities such as N_2, O_2, H_2S, SO_2, CH_4, and Ar can significantly alter the thermodynamic behavior, phase stability, and transport dynamics of CO_2. Their presence can lead to operational challenges including phase separation, pressure fluctuations, and corrosion of infrastructure, ultimately affecting the safety, efficiency, and economic feasibility of CCS projects. While progress has been made in modeling the phase behavior of CO_2 mixtures using equations of state (e.g., Peng–Robinson, CPA, and GERG-2008), substantial knowledge gaps remain—particularly concerning multicomponent systems under reservoir conditions. Experimental validation, standardized impurity thresholds, and robust simulation tools are essential to address these challenges. Additionally, material compatibility, wellbore integrity, and corrosion mitigation strategies must be carefully considered during the design phase of CO_2 transport pipelines and injection systems. To ensure safe and reliable CCS deployment, future research should focus on developing more accurate multiphase models, establishing internationally harmonized impurity specifications, and conducting long-term field-scale studies. Holistic system design that incorporates adaptive infrastructure, real-time monitoring, and flexible operational protocols will be crucial for mitigating the risks posed by impurities and enhancing the long-term viability of CCS as a climate mitigation tool.

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