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LEVERAGING DIGITAL TWINS FOR HYDROGEN LOSS MITIGATION IN LARGE SCALE SALT CAVERN HYDROGEN STORAGE

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ABSTRACT

As hydrogen continues to emerge as a key solution to decarbonise the global energy sector, interest in efficient storage solutions increases to meet rising energy demands and to ensure energy security. Large scale hydrogen storage salt caverns look to be a promising solution for hydrogen storage due to their ability to store large volumes of gas safely, as proven when storing natural gas in underground salt caverns. Hydrogen stored in underground salt caverns exhibits losses due to reasons such as gas migration, and the active chemistry they possess in addition to leaks due to damage caused by the cyclic loading on the cavern. Understanding the hydrogen loss pathways could help reduce financial losses and mitigate any safety risks imposed. Using SSE's Aldbrough Hydrogen Pathfinder project, based in the UK Humber region as a case study, this paper aims to demonstrate how a digital twin can be utilised to evaluate and forecast hydrogen leaks by incorporating real time and historical data from sensors, geological information, and environmental factors to provide a holistic view of the cavern's dynamics. This research aims to facilitate early detection of failures and highlight possible intervention mechanisms and strategies for underground salt cavern storage used for green hydrogen storage.

Keywords: Hydrogen, Digital Twin, Hydrogen Storage

1. INTRODUCTION

To address the dynamic pressures of the rapidly changing business landscape across various industries, including energy production, many companies are adapting their digital strategies to adopt more Industry 4.0 technologies in their operations. This paradigm shift is being steered by evolving customer expectations, increased competition, and the need for more sustainable practices. Within the energy sector, the oil and gas

industry has introduced various digital technologies to enhance effectiveness and overall efficiencies within companies. These have been particularly focussed on aiding in maintenance, maximising production capacity and in the design and implementation of new investments that are to be made [1]. Digital twins (DT) were identified as a promising tool as they can provide insights for asset management in addition to lifecycle planning.

Since the Paris Agreement, global efforts have gone into increasing the use of renewable energy sources such as wind and solar. However, despite progress in the industry, fossil fuels continue to dominate the energy landscape, particularly in transportation and heating. Due to the inherent intermittent nature of renewable energy, shifting to rely on them makes it challenging. However, interest in green hydrogen has increased in recent times as a low-carbon fuel alternative to conventional fossil fuels and as a versatile energy carrier, which is likely to help decarbonise challenging sectors such as transport and heating. Green hydrogen is produced through electrolysis using electricity generated from renewable energy. Electrolysis is the splitting of water (H_2O) into oxygen (O_2) and hydrogen (H_2) using electricity (see Figure 1). Therefore, it allows surplus renewable electricity to be converted into hydrogen which can be stored and reconverted into energy as and when needed. This could also help overcome limitations in transmission grid capacity and reduce renewable curtailment. Low-carbon hydrogen was highlighted as a key part of the UK Government's Net Zero Strategy to transition into a low-carbon future.

For various commercial applications currently, approximately 100 million tons of hydrogen is produced [2]. Most of this hydrogen is derived from steam methane reforming or coal gasification; both of which are carbon intensive processes. It is

predicted that hydrogen could account for 20% of European electricity demand and 10% globally by 2050 [3].

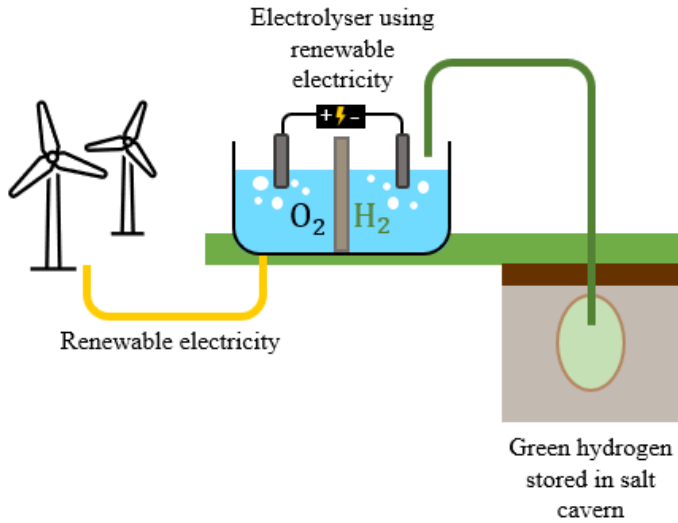


FIGURE 1: SCHEMATIC DIAGRAM OF GREEN HYDROGEN PRODUCTION AND SALT CAVERN STORAGE

As the adoption of green hydrogen is set to increase, subsurface salt caverns are being explored as a promising option for large-scale and seasonal hydrogen storage to facilitate the large-scale production. Geological gas storage has been used for many years to store large volumes of gases like natural gas and town gas across countries such as the United States, Germany, France, China and the UK [4]. For hydrogen, there are currently four operational salt caverns that store hydrogen. Details of these can be found in Table 1. A challenge with geological gas storage is leak management and the seal of the cavern. During operations, the gas storage cavern is subject to cyclic injection, brine erosion, and corrosion for extended time periods. This leads to gas loss through various pathways and poses health and safety concerns in addition to economic losses that can be difficult to quantify.

Digital twins have been proposed in the field of pipes and wells within the oil and gas industry for early detection of future faults and carry out predictive maintenance in addition for well integrity management [1]. To aid in cavern maintenance, this paper aims to review hydrogen leakage pathways in salt cavern storage and explore how digital twins may be used to aid in the operation of such caverns to reduce gas loss, limit economic losses and apply it for overall product lifecycle management [5].

TABLE 1: OPERATIONAL SALT CAVERN HYDROGEN STORAGE SITES [3,6,7]

Location	Clemens (USA)	Moss Bluff (USA)	Spindletop (USA)	Teesside (UK)
Geology	Domal Salt	Domal Salt	Domal Salt	Bedded Salt
Operator	Conocco Phillips	Praxair	Air Liquid	Sabic Petroleum
Established	1983	2007	2016	1972
Hydrogen Content (%)	95	95	95	95
Volume (m ³)	580,000	566,000	906,000	210,000
Depth (m)	930	>822	1340	350
Pressure Range (MPa)	7 – 13.5	5.5 – 15.2	6.8 – 20.2	4.5
Hydrogen Capacity (GWh)	81	123	274	25

2. SALT CAVERN INTEGRITY FOR HYDROGEN STORAGE

During large scale gas storage operations, any unplanned gas loss poses economic, safety and environmental concerns. Therefore, geological gas storage sites, namely salt caverns, are closely monitored to manage the integrity to ensure operation as intended, with minimal loss. Salt cavern integrity, hence, gas storage capabilities of salt caverns may deteriorate over time due to various factors. These include abiotic (geochemical reactions) and biotic interactions (microbial activities) with the hydrogen present and impurities that occur in salt deposits in addition to faults and fractures that may be exasperated because of cyclic hydrogen injection and withdrawal that takes place.

2.1. Hydrogen Loss from Salt Caverns

Hydrogen loss in salt cavern storage sites can broadly be classified as chemical and physical losses. Figure 2 shows the various hydrogen loss pathways.

2.1.1. Geochemical (Abiotic) Interactions

Hydrogen stored in salt caverns can react chemically with impurities found in the cavern. These consist of reactions between hydrogen and minerals found in rocks in addition to hydrogen reactions under the action of microorganisms.

Geochemical interactions greatly impact the loss of hydrogen in salt caverns. Salt caverns used for hydrogen storage are strongly reducing environments. The minerals in the rock salt that form the caverns consist of rock salt (NaCl), carbonate (CaCO₃), sulphates (K₂SO₄, MgSO₄), gypsum (CaSO₄), carnallites (KCl, MgCl₂), magnesium oxide (MgO) and aluminium oxide (Al₂O₃) [7]. Hydrogen losses due to the dissolution of calcite can be

substantial [3]. Hydrogen injection into a cavern where brine is present stimulates the dissolution of water and hydrogen. At high temperatures and pressure, an increase in pH is observed due to the presence of OH^- ions from the water. The alkaline solution triggers the dissolution of calcite in brine making carbonate ions available to react with hydrogen ions to produce carbon dioxide (CO_2) and methane (CH_4). The consumption of H^+ ions further increase the pH, further accelerating the loss of hydrogen. This reduces the purity of the hydrogen found in the cavern. Furthermore, the carbon dioxide produced reduces the life of the wellbore and the pipeline due to corrosion. If unmitigated, the corroded pipeline poses a failure risk. To combat this issue, special coatings can be applied in the casing and pipeline to reduce both the electrochemical and erosive corrosion due to the presence of carbon dioxide [7]. Additionally, the formation of methane can lead to the formation methane hydrates under low temperature and high-pressure conditions. This can lead to pipeline blockages and impact the injection and withdrawal rate from the cavern. Methods of prevention include insulating the well head, adding inhibitors and fungicides [7].

2.1.2. Microbial (Biotic) Interactions

The presence of microbial interactions is recognised as a key factor which can affect the viability of many underground storage resources such as hydrocarbon reservoirs, aquifers, and underground hydrogen storage. One of the main causes of hydrogen loss in underground reservoirs are microbial metabolism, making it a key concern when considering large scale hydrogen storage in salt caverns. Microorganisms can be introduced into subsurface gas storage sites through natural processes such as sedimentation or through construction activities like drilling [3]. Various factors affect the growth of these microorganisms underground, these include temperature, pressure, pH, salinity and chemical concentrations [3].

Microorganism colonies found in the caverns belong to Actinobacteriota, Halobacterota, Desulfobacterota, Firmicutes, Halanaerobiaeota, Proteobacteria, and Bacteroidota [7]. During the biotic interactions, nitrates, sulphates, iron (III), and carbon dioxide get reduced during the oxidation of the hydrogen. Bacteria gain energy for metabolism through chemical oxidation/reduction therefore requiring electron donors (hydrogen) and electron acceptors (sulphates, carbon dioxide, sulphur, nitrates, iron (III) and oxygen). The microbial hydrogen consumption reactions are summarised in Table 2. Assuming all the listed substrates are present in the cavern whilst hydrogen concentration is high, all microbial reactions are likely to occur simultaneously with methanogenesis, sulphate reduction and acetogenesis being the main processes [3].

Sulphate reduction is highlighted as one of the main concerns in underground hydrogen storage due to formation of hydrogen sulphide (H_2S). This is primarily because minimal amounts of hydrogen sulphide can impact the gas quality and lead to increased health and safety concerns and corrosion. The presence of iron has been shown to inhibit hydrogen sulphide production to an extent as pyrrhotite (FeS) precipitates form when the sulphate produced reacts with dissolved iron. The dissolved iron (II) can also lead to the formation of ferrihydrite, goethite and magnetite precipitates in the presence of low oxygen and nitrate concentrations due to iron oxidising microorganisms[3].

In salt caverns, as the surface contact between the injected gas and rock is low due to the presence of the salt, the microbial interactions should be lower in comparison to porous gas storage reservoirs. This is because the lack of surface contact stops the formation of the microbial biofilm. The salinity in the brine also induces higher osmotic stresses in the cells which can encumber microbial activity (except for halophilic bacteria) [3]. Nevertheless, in certain instances, it has been demonstrated that the formation of hydrogen sulphide can be notable at the gas-brine interface in the presence of sulphates. Consequently, while increased salinity may affect the diversity of microorganisms, it does not necessarily diminish the consumption of hydrogen[3,8].

Therefore, the safety and stability of salt cavern hydrogen storage can potentially be impacted by microbial interactions. A

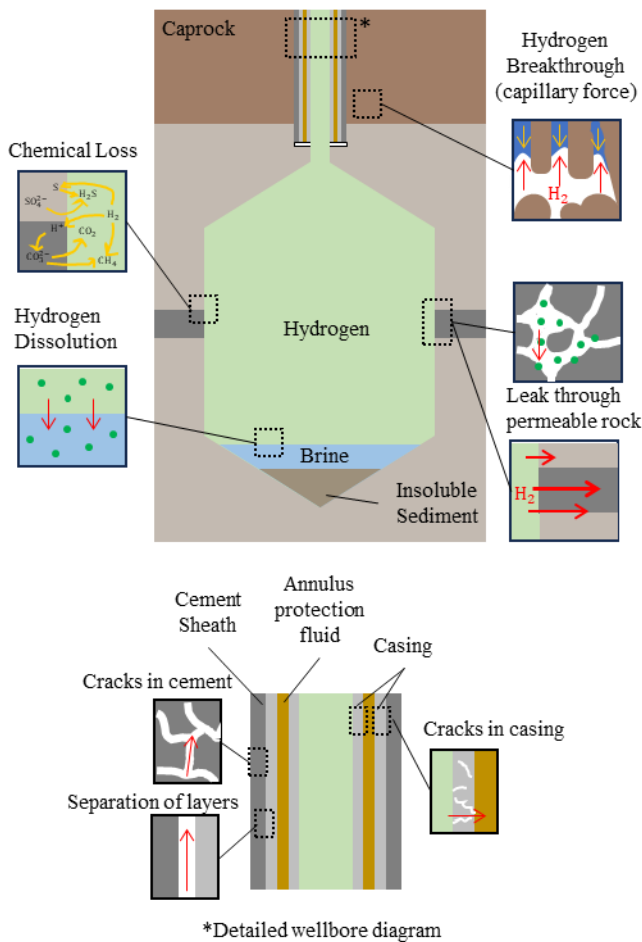


FIGURE 2: LEAKAGE PATHWAYS IN AN UNDERGROUND SALT CAVERN (ADAPTED FROM REF [7])

key challenge for future hydrogen cavern storage will be to understand the interactions between geochemical and microbial reactions and how they contribute to salt cavern integrity and hydrogen storage performance. In addition to the reactions that compromise the gas composition, it can also lead to issues such as corrosion of steel casings and/or wellbore materials induced by microbial interactions. This may compromise the integrity of the hydrogen storage infrastructure increasing the risk of gas leakage and environmental contamination in addition to health and safety concerns. Furthermore, microbial activities may induce changes in the salt caverns geomechanical properties further compromising the structural integrity of the salt cavern.

The main indicators of chemical reactions occurring in salt caverns for hydrogen storage are the production of impurity gases such as carbon dioxide and hydrogen sulphide in addition to the overall consumption of hydrogen. Therefore, effective monitoring of these concentrations and preventive measures, such as employing biocide treatments and selecting appropriate materials, are crucial for mitigating risks associated with microbes to ensure the prolonged reliability and safety of hydrogen storage in salt caverns [8].

TABLE 2: SUMMARY OF ABIOTIC AND BIOTIC CHEMICAL REACTIONS THAT TAKE PLACE IN SALT CAVERN HYDROGEN STORAGE [3,7].

Reaction	Chemical Reaction
<i>Geochemical</i>	
Carbonates	$\text{CO}_3^{2-} + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{OH}^- + \text{H}_2\text{O}$
Sulphates	$\text{SO}_4^{2-} + 4\text{H}_2 \rightarrow \text{H}_2\text{S} + 2\text{OH}^- + 2\text{H}_2\text{O}$
Sulphides	$\text{FeS}_2 + \text{H}_2 \rightleftharpoons \text{FeS} + \text{H}_2\text{S}$
Ferric iron	$\text{Fe}_2\text{O}_3 + \text{H}_2 + \text{H}_2\text{O} \rightleftharpoons \text{Fe}(\text{OH})_2$ $3\text{Fe}_2\text{O}_3 + \text{H}_2 \rightleftharpoons 2\text{Fe}_3\text{O}_4 + \text{H}_2\text{O}$
<i>Microbial</i>	
Methanogenesis	$\text{HCO}_3^- + 4\text{H}_2 + 4\text{H}^+ \rightarrow \text{CH}_4 + 5\text{H}_2\text{O}$
Acetogenesis	$2\text{HCO}_3^- + 4\text{H}_2 + \text{H}^+ \rightarrow \text{CH}_3\text{COO}^- + 4\text{H}_2\text{O}$
Sulphate reduction	$\text{SO}_4^{2-} + 4\text{H}_2 + \text{H}^+ \rightarrow \text{HS}^- + 4\text{H}_2\text{O}$
Iron reduction	$2\text{FeOOH} + \text{H}_2 + 4\text{H}^+ \rightarrow 2\text{Fe}^{2+} + 4\text{H}_2\text{O}$
Denitrification	$2\text{NO}_3^- + 5\text{H}_2 + 2\text{H}^+ \rightarrow \text{N}_2 + 6\text{H}_2\text{O}$
Sulphur reduction	$\text{H}_2 + \text{S} \rightarrow \text{H}_2\text{S}$
Aerobic H ₂ oxidation	$2\text{H}_2 + \text{O}_2 \rightarrow \text{H}_2\text{O}$

2.1.3. Physical Losses

Hydrogen exhibits high fluidity which makes it prone to leakage from underground salt cavern storage. Figure 2 illustrates the leakage pathways of hydrogen from underground salt cavern storage; these include losses from the wellbore, caprock and the cavern itself.

Hydrogen leakage from the wellbore can occur through to cracks caused by corrosion and the mechanical failure of the wellbore, it is often the largest source of leakage. The wellbore of a hydrogen storage salt cavern consists of a casing and cement surrounding it. Wellbore corrosion occurs because of hydrogen embrittlement in the steel casing which leads to the reduction of mechanical properties in addition to displaying hydrogen

induced cracking and blistering [7]. The cement sheath surrounding the casing is also subject to corrosion, hence cracking failure, due to the accumulation of acid gases like carbon dioxide and hydrogen sulphide (see sections 2.1.1 and 2.1.2). Tobermorite, a calcium silicate hydrate (CSH), ($3\text{CaO} \cdot 2\text{SiO}_2 \cdot 3\text{H}_2\text{O}$) and portlandite (CSH($\text{Ca}(\text{OH})_2$)) are the two components of cement that control the strength [7]. When they react with carbon dioxide to form calcium carbonate, initially it strengthens the cement; however, further acidification leads to the formation of calcium bicarbonate ($\text{Ca}(\text{HCO}_3)_2$), a soluble salt reducing the cement strength. Similarly, in the presence of hydrogen sulphide, ettringite is formed which increases the internal force in the cement leading to further crack formation in the cement [7]. The carbonation chemical reactions are summarised in Table 3.

TABLE 3: CHEMICAL REACTIONS OF CEMENT IN SALT CAVERN HYDROGEN STORAGE (ADAPTED FROM REF [7])

Reaction	Chemical Reaction
Cement Carbonation	$3\text{CaO} \cdot 2\text{SiO}_2 \cdot 3\text{H}_2\text{O} + 3\text{CO}_2 \rightarrow 3\text{CaCO}_3 \cdot 2\text{SiO}_2 \cdot 3\text{H}_2\text{O}$ $\text{Ca}(\text{OH})_2 + \text{CO}_2 \rightarrow \text{CaCO}_3 + \text{H}_2\text{O}$ $3\text{CaO} \cdot 2\text{Al}_2\text{O}_3 \cdot 3\text{CaSO}_4 \cdot 3\text{H}_2\text{O} + 3\text{CO}_2 \rightarrow 3\text{CaCO}_3 + 3\text{CaSO}_4 \cdot 2\text{H}_2\text{O} + 2\text{Al}(\text{OH})_3 + 9\text{H}_2\text{O}$ $3\text{CaO} \cdot \text{SiO}_2 + 3\text{CO}_2 + \text{nH}_2\text{O} \rightarrow \text{SiO}_2 \cdot \text{nH}_2\text{O} + 3\text{CaCO}_3$ $2\text{CaO} \cdot \text{SiO}_2 + 2\text{CO}_2 + \text{nH}_2\text{O} \rightarrow \text{SiO}_2 \cdot \text{nH}_2\text{O} + 2\text{CaCO}_3$
Further Acidification	$\text{CaCO}_3 + \text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{Ca}^{2+} + 2\text{HCO}_3^-$ $\text{CaCO}_3 + 2\text{H}^+ \rightarrow \text{Ca}^{2+} + \text{H}_2\text{O} + \text{CO}_2$
H ₂ S corrosion	$8\text{Fe}(\text{OH})_3 + \text{HS}^- \rightarrow 8\text{Fe}^{2+} + \text{SO}_4^{2-} + 5\text{H}_2\text{O} + 15\text{OH}^-$ $6\text{Ca}^{2+} + 2\text{Al}(\text{OH})_4^- + 4\text{OH}^- + 3\text{SO}_4^{2-} + 26\text{H}_2 \rightarrow \text{Ca}_6[\text{Al}(\text{OH})_6]_2 \cdot (\text{SO}_4)_3 \cdot 26\text{H}_2\text{O}$

As hydrogen is considered as a green energy carrier, salt caverns which store hydrogen are subject to a higher frequency of injection and withdrawal than those that store other gases, causing varying cycles of cavern pressure. As a result of the cyclic loading, the wellbore of hydrogen storing salt caverns well bores are more prone to mechanical failure During the operational life cycle of a hydrogen storage salt cavern, the cement strength decreases because the cyclic loading leads to the formation of radial cracks and micro annulus allowing hydrogen to leak out of the cavern [7].

Another contributing factor to wellbore hydrogen leakage is due to the separation that occurs at the interface between the different layers of the casing and the cement sheath. As hydrogen is injected and withdrawn, the stress exerted on the cavern and wellbore are not uniform due to varying elastic moduli. This leads to a concentration of damage at the casing – cement interface leading to the eventual separation of the two. The separation is further impacted by the subsurface geomechanics. Throughout long term operation, salt caverns decrease in volume as the rock salt exhibits creep in an axial direction and the internal pressure is lower compared to the surface stress [9]. As

a result of the shrinkage, the tensile stress leads to separation between the cement and the rock salt [7].

The buoyancy of hydrogen also contributes to the migration of hydrogen gas from the salt cavern through the caprock. The caprock is an impermeable layer with the purpose of preventing migration of any fluids to the surface. However, hydrogen can travel through the caprock through capillary action given that the buoyancy exceeds the required pressure. This is referred to as the breakthrough pressure [7]. It has been shown that as the depth of the cavern increases, the required breakthrough pressure of the cavern decreases which decreases the tightness of the caprock. The temperature and pressure of the cavern also impacts the gas migration as it influences the density and interfacial tension of the hydrogen-brine system within the cavern [7].

Leakages from caverns can also occur due to the permeability of the rock. The leakage characteristics of hydrogen and natural gas are similar despite the key differences in gas characteristics [7,10]. Due to the ionic crystal structure of pure rock salt, hydrogen is unable to leak through because the lattice spacing of the NaCl (2.8×10^{-10} m) is smaller than the kinetic diameter of the hydrogen molecule (2.89×10^{-10} m) [7]. However, the impurities found in different salt formations can lead to gas leakage. Bedded rock salts have a higher impurity content than domal salts; these impurities can lead to hydrogen leakage channels.

Hydrogen loss in salt caverns is also possible through hydrogen dissolution and adsorption. The brine that remains in the cavern after gas injection dissolves hydrogen. The overall dissolution loss of hydrogen is equivalent to the hydrogen solubility in brine [7]; where hydrogen solubility is affected by the brine salinity, temperature and pressure. Hydrogen loss can also occur through adsorption into porous media found around the cavern. This includes shale, coal and clay. In salt cavern storage, hydrogen adsorption mainly occurs on clay due to the microstructure it possesses along with the high specific surface area. However, compared to other loss pathways, dissolution and adsorption losses are minimal and they are also difficult to control from an operational perspective [7].

2.2. Cavern Monitoring and Maintenance Practices

To successfully develop, monitor and maintain caverns, accurate characterisation is necessary. A model is developed using both static and dynamic properties which are updated throughout the operation of the cavern. Static cavern properties include facies type, porosity and permeability whilst dynamic properties include pressure, temperature and fluid saturation [11]. Using all possible data available allows the creation of more accurate models and predictions of performance and degradation. It is essential that any anomalies in behaviour are realised in advance as any maintenance and repair work that is needed would require the cavern to be out of service which would have financial implications. As it stands, standard monitoring practices mainly include monitoring the pressure and

temperature of the wellhead, surface leakage detection and well loggings and inspections at set intervals, often every 1-2 years. One of the issues with this is that any faults that develop in the time between the logs may grow. There is a trade-off between well logging frequency and costs associated with well shut down to facilitate inspections[12].

A gas storage cavern monitoring system can consist of cavern integrity tests, cavern shape assessments, temperature, pressure, and gas flow rate monitoring in addition to monitoring surface subsidence and micro-seismic activities.

Cavern integrity tests (or Mechanical Integrity Tests) evaluate the seal of the salt cavern. During the test, nitrogen is injected as a pressure test medium to identify any leaks, hence giving an indication of the seal. Throughout the test duration, small amount of nitrogen is added to the cavern at regular intervals while the gas volume change is monitored at the wellhead. Given that nitrogen and brine contact depth is sustained for extended periods, the cavern is considered well sealed [13]. In industry, these tests are repeated at least every 5 years [14].

To monitor the shape of the cavern, sonar surveys are used. The frequency of these surveys is dependent on the quality of the cavern; it can range for every one to five years. Over the course of operation, it is common for changes to occur to the shape of the cavern due to salt creep. A sonar device is lowered into the cavern by changing the vertical depth allowing the formation of a 3D shape profile of the cavern. These are compared to records from previous years to assess any changes [13].

Monitoring temperature, pressure, and flowrate downhole and at the wellhead can also provide the information needed for PVT simulations. These are critical for any estimation of the remaining storage capacity of the cavern in addition to assessment of the cavern integrity and salt creep occurring [13]. Using historic data, future predictions can be made which can be used for gas leakage alerts, optimisation of gas injection and withdrawal in addition to compressor operations.

Surface subsidence is a term used to describe the movement of the earth's surface which can be attributed to both natural and human processes. Caverns shrink over time due to volume creep. This deformation resonates through the ground to other strata leading to surface subsidence [15]. Subsidence can be monitored using GPS satellites to track ground movement over a large area and can be predicted through the use of numerical simulations [15,16].

Micro-seismic monitoring is a passive monitoring method adopted in industry to provide real time assessment of micro-seismic events that may lead to possible cavern collapse events [13]. The micro-seismic data captured can enable early detection of cavern collapse failure and reduce the risks associated with it. The data can also be used to identify the position and nature of fractures that arise due to collapses that have taken place [13].

3. DIGITAL TWINS

The green hydrogen industry faces various challenges at the different stages, from the electrolyzers that are used to produce hydrogen to the transport and distribution of the gas. This paper addresses the challenges associated with hydrogen leakage from salt cavern storage and discusses what strategies could be employed for projects that are currently in the development phase, like SSE’s Aldbrough Hydrogen Pathfinder. It is essential to make hydrogen technologies and processes economically competitive and safe. For large scale hydrogen storage, this can be achieved through the implementation of enhanced monitoring and maintenance practices by using Industry 4.0 technologies, such as digital twins. This approach will allow the operators to leverage historical data to make data-driven decisions, thereby reducing uncertainties and risks related to the operations.

Digital twins have been a popular area of research for use in varying fields from healthcare to manufacturing. One of the key challenges has been the lack of a unified definition [5,17]. For this paper, a number of classifiers have been defined to create a framework where different definitions of digital twins can be compared. The descriptions of the different classifiers are below and a summary of comparison of various literature definitions are found in Table 4.

1. Scope – refers to the coverage of elements/entities covered by DT.
 - Narrow – DT focuses on specific devices within larger system.
 - Broad – DT covers entire processes and systems.
2. Resolution – refers to the level of detail that individual components are covered in the DT.
 - High resolution – detailed representation of individual components within system.
 - Low resolution – captures overall behaviour of system, high level overview.
3. Interactivity – refers to DT interaction with real time data.
 - Static – DT is a snapshot of a specific instance.
 - Dynamic – DT updates with real time data and responses.
4. Direction of data flow – describes how the data moves between the physical system and the DT.
 - Unidirectional
 - Bidirectional

Based on findings from Table 4, it is seen that the definitions of digital twins vary depending on the purpose and design objectives. The scope and resolution depend largely on the intended purpose of the digital twin. Using this, it is possible to outline a few characteristics that are needed to constitute as a digital twin. These are:

1. Representation of a physical entity
2. Bidirectional data flow
3. Real-time synchronisation and interaction

To determine which projects could benefit from a digital twin, various factors need to be taken into consideration. It is dependent on the nature of the project, the goals, the potential impacts – both benefits and disadvantages. The decision to implement a DT is dependent on a holistic evaluation of factors such as data availability, the criticality and impact on the process, the complexity of the process and resource intensity to name a few.

For the implementation of a digital twin for hydrogen storage in salt caverns, value can be seen in areas such as predictive maintenance due to the growing hydrogen market across the world and limited research and experience on hydrogen salt cavern storage.

TABLE 4: DIGITAL TWIN CLASSIFIERS

	Scope	Resolution	Interactivity	Data flow
Glaessgen et al. [18]	Broad	High	Dynamic	Bidirectional
Chen et al. [19]	Broad	Both	Dynamic	Bidirectional
Liu et al. [20]	Both	-	Dynamic	Unidirectional
Zheng et al. [5]	Both	Both	Dynamic	Bidirectional
Madni et al. [21]	Both	Both	Dynamic	Bidirectional
Meraghni et al. [22]	Narrow	High	Dynamic	Unidirectional
Shin et al. [23]	Narrow	Low	-	-

4. APPLICATION PROSPECTS OF DIGITAL TWINS TO GREEN HYDROGEN INDUSTRY

4.1. Digital Twins in the Context of Hydrogen

The data processing and visualisation capabilities of digital twins can be leveraged to aid in the maintenance and operation of salt caverns used in large scale hydrogen storage.

In the context of salt caverns, a digital twin can be utilised for enhanced monitoring and data visualisation. The internal conditions of the cavern can be monitored to get an understanding of the operating conditions. These include collecting data on environmental conditions like temperature, pressure. Conclusions can also be made about the cavern integrity and deformation present based on data such as the hydrogen concentration levels. These can help identify what chemical reactions may be dominating in the cavern. Real time monitoring of the gas condition allows site operators to have instant understanding of any anomalies that may be present which may have immediate consequences or lead to potential issues if left undetected. This can be used to implement condition-based maintenance on the salt cavern, saving money for the cavern operators as it can reduce overall downtime. Other

parameters that can be monitored include vibrations and the mechanical strain on cavern infrastructure.

A digital twin can be used in predictive modelling and performance optimisation [24]. Historical data that is collected on site on the cavern performance can be analysed using advanced methods which utilise machine learning and artificial intelligence; and operational decisions can be made based on the results. Furthermore, due to the advanced data analysis capabilities, scenario analyses can be conducted to understand and prepare for changes in external factors [24]. Examples of these include varying amounts of renewable energy in the grid, or reduced hydrogen production due to the degradation of electrolyser components such as the membrane.

From an operational perspective, data collected on possible gas leaks can also be used to improve safety and the emergency alertness by using the digital twin interface to trigger emergency response protocols that can be managed by those who have access to the DT. This is also important to manage any environmental risks associated with gas leakage from the cavern. The visual interface of the DT can be used by the operators from various backgrounds to manage the incidents using automation enabled by (Internet of Things) IoT sensors. An example of this may be the automation of valve positions; reducing the need for routine maintenance to be carried out by operators.

The dynamic and responsive digital twin can also be utilised from a management perspective to improve energy efficiency and overall facility output. The data integration of energy consumption and operational costs can allow the identification of critical points in the process where energy consumption or operational costs may be particularly high. This can allow for better cost modelling and budget optimisations during the project lifetime [24].

Due to the dynamic nature of the green hydrogen industry, accurate emission tracking is of interest to ensure regulatory compliance with standards that are updated frequently as the industry matures. A digital twin can be used to generate reports for regulatory authorities based on the real-life data that is collected and collated. It can also be utilised as a tool in the Lifecycle Assessments (LCA) that are conducted at specified intervals, depending on the nature of the project.

Overall, the aim of implementing a digital twin into a green hydrogen production facility is to have a responsive tool that can enhance efficiency and safety in addition to extending the lifespan of equipment and infrastructure to maximise profits over the years.

4.2. Advanced Monitoring

To facilitate the development of a digital twin, it is favourable to introduce advanced monitoring techniques into the standard monitoring methods. This is because on-line/in-situ monitoring systems are required to make the digital twin a dynamic system.

These include downhole monitoring of temperature and pressure, using Distributed Temperature Sensing (DTS) and Distributed Acoustic Sensing (DAS) [12].

Downhole monitoring of temperature and pressure provides real time data collection of these parameters in the cavern. Directly measuring these parameters reduces uncertainties associated with the prediction of downhole environment and increase the accuracy of the capacity calculations [12].

DTS utilises fibre optic fibres to record temperatures along the cable allowing a continuous temperature profile to be developed. Temperature profiles and their temporal variations are sensitive to vertical migration of fluids during injections and withdrawal. Therefore, the use of DTS enables continuous recordings of temperature profiles allowing insight into the behaviour of the flow. Similarly, DAS uses fibre optic cables to record acoustic field data along the borehole. After establishing a normal sound baseline, acoustic anomalies, due to leaks for example, can be identified and located [12].

4.3. Challenges of Industrial Digital Twins

Whilst the realisation of digital twins provides ample opportunity for ‘futureproofing’ new process, there are various challenges that need to be addressed in process. A key barrier to the wider DT implementation is due to the availability of consistent, good quality data [24]. To effectively build a DT tool to aid in operation and maintenance of salt caverns to prevent gas loss, it is essential that there is an automated integration of consistent data between the physical salt cavern and the digital representation. However, with pre-existing sites and older projects, it may be difficult to integrate the current systems and devices in place into the digital twin due to a gap in the operability [24]. Furthermore, there is also an additional cost associated with the retrofitting caverns with new sensors and smart devices that may be required to facilitate the digital transition. As a result, the cost of implementation, including upskilling staff to train them on changing job descriptions, can be a deterring factor for industrial leaders to take on digital twins and other digital strategies.

In addition to technological and physical limitations, there are cybersecurity, ethical and legal concerns associated with increased connectivity throughout complex gas storage sites [25]. With increased data generation and output, there is more emphasis on sensitive data protection, ownership, and usage. A contributing factor to the complexity of this is the lack of standards and industry guidelines available. Early adopters of DT technologies will be among the bodies forming these industry guidelines, making it challenging at the conception stage.

Another key challenge in the wider uptake of DT among wider gas storage operators is due to resistance to technological innovation because of factors such as organisational structure. It is evident that there are efforts for wider employment of digital

strategies within companies. However, organisations and their employees are largely accustomed to their current practices. A wider perceived value of digital twins is required for successful implementation. This requires a shift in workplace culture which can be difficult to implement and quantify results.

4.4. Future Work

Going forward, to facilitate the broader implementation of DT technologies in gas storage operations to enhance storage efficiency, comprehensive guidelines could be outlined. These guidelines could advise on various aspects of DT implementation, including the establishment of a metric or method to compare the cost and benefits gained from a DT, allowing companies to make more informed investment decisions. Furthermore, protocols to ensure data quality and consistency should be included; accounting for issues that may arise such as data gaps and anomalies in the collected data. To address concerns regarding data security, the guidelines could outline details on measures such as data encryption requirements and backup frequencies.

Moreover, new projects could be designed with the potential to implement DT's from the initial stages. This approach can help avoid challenges associated with the implementation of DT's into legacy systems, as previously discussed. It can also be a motivator to further standardise documentation and reporting processes within companies and industries. This not only aids in collaboration within a company but it could also enable more effective cross industry collaboration, which is essential in a joint effort to achieve net zero.

In the context of the Aldbrough Hydrogen Pathfinder, the project aims to demonstrate hydrogen dispatchable power. Therefore, the stored hydrogen will act as a buffer to balance the energy supply and demand. Consequently, work is to be done to analyse the impact of different operational characteristics to the gas storage operations. This can be done by using a digital twin as a tool. As the project is currently in the development phase, efforts are being made to anticipate the end use requirements in terms of a digital strategy. Considerations are given to build in the capacity and capability to integrate a DT into the project if it is deemed beneficial later in the project development. A parallel approach to project and digital development could also help overcome some challenges like the resistance to technological innovation within companies.

5. CONCLUSION

This paper has reviewed a range of hydrogen loss and system degradation mechanisms for large scale salt cavern storage of hydrogen in addition to current cavern monitoring practices used in industry.

The geochemical and microbial interactions between the geological salt cavern environment and the stored hydrogen are documented from previous gas storage applications. The

physical losses are also evaluated based on existing projects and understanding of hydrogen leakage pathways. These mechanisms must be evaluated in the specific context for each hydrogen storage project due to varying geologies. It was identified that the greatest point of hydrogen loss is the physical leakage from the wellhead.

To facilitate the development of digital twins for use in salt cavern hydrogen storage, advanced monitoring methods would be required. These methods include using in-situ DTS and DAS to monitor downhole conditions to better identify any hydrogen losses occurring from the cavern.

Moving forward, the impact of the operational characteristics in green hydrogen storage applications are to be evaluated if hydrogen storage is used to balance the energy supply/demand as buffer system as there will be an increased storage cycling. These increased cycling regimes, i.e., loading/unloading of hydrogen storage will cause increased mechanical demands on all components of the system. Work should also be done to outline industrial guidelines on digital twin implementation, as one of the key challenges is the lack of a standard procedure to follow. Key aspects of these guidelines include the establishment of a metric or a process to assess the digital twin cost-to-benefit ratio, enabling companies to make more informed investment decisions.

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