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THE FUTURE OF CARBON CAPTURE AND STORAGE TECHNOLOGY: AN INNOVATIVE APPROACH WITH DIGITAL TWIN

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Abstract: In order to fight climate change, the EU has set a goal of achieving net-zero greenhouse gas emissions by 2050. To achieve carbon neutrality, greenhouse emissions from human activities should be at least 85% lower than in 1990. The remaining 15% can be achieved through additional measures such as increasing carbon capture and storage (CCS) and reducing emissions. CCS will facilitate the decarbonization of heavy industry, contribute to the emergence of a clean hydrogen economy, and aid in achieving net-zero emissions. As an emerging technology in the Industry 4.0, Digital Twin (DT) is gaining attention due to the possibilities arising from its application, such as precise process optimization in the design phase, quality control, monitoring, decision-making, and through comprehensive modeling of the physical world as a group of connected digital models. The introduction of digital technologies into the CCS sector has the potential to revolutionize the way CO_2 capture, transportation, and storage processes are carried out. This article aims to present the fundamental value of different modeling techniques, technologies enabling the creation of DT's uncertainty quantification methods commonly used in Digital Twins, as well as the application of Digital Twin in CCS technology and the potential benefits it can bring, including increases efficiency and cost minimization. Additionally, the possibilities of using DS's in improving process monitoring and forecasting were discussed which can contribute to better emission control and increases system effectiveness. Current research and projects utilizing this technology were also presented, including real-time modeling of fluid flow, CO_2 transport network optimization, and storage process improvement.

Keywords: CCS, Digital Twin, process simulation, CO_2 transport, risk analysis

1. Context and Overview: Exploring the Impact of Advanced Digital Technologies in the CCS sector

In recent years, digital technologies such as data analytics, artificial intelligence (AI), machine learning (ML) and computer modeling have found increasing application in numerous industries, including the energy sector. As industrial facilities become more intricate, it is vital to use advanced methods to track key performance measures and goals. The integration of state-of-the-art technologies is of great significance in the manufacturing sector for rapid and effective decision-making, leading to enhanced outcomes [1–3]. One of the areas showing a growing interest in advanced digital technologies is the CCS (Carbon Capture and Storage) sector. CCS technology, which aims to capture the carbon dioxide emitted by industry, transportation sector, or other sources and store it in deep geological formations in a supercritical state to reduce greenhouse gas emissions, is considered as one of the tools in the fight against the ongoing climate changes.

A Digital Twin can be described as a "coupled model of the real machine that operates in the cloud platform and simulates the health condition with an integrated knowledge from both data driven analytical algorithms as well as other available physical knowledge" [4]. A less complex definition describes DT as a digital representation of a human, device, system, or process, that mirrors the actual process and has full knowledge of its historical performance [1,5]. DT utilizes both assumed and real data that enable an efficient mapping of processes occurring in a particular system, and can be used for both optimization and predictive purposes.

In this context, DT is becoming an increasingly interesting approach to optimizing CCS processes. The potential applications of Digital Twins in the decarbonization sector are extensive. They can be employed to optimize CO_2 capture processes, facilitate efficient planning of CO_2 transport, assist in the selection of suitable geological storage locations, and enable comprehensive monitoring, forecasting, prevention, and management of risks and safety concerns at every stage of operation. The utilization of Digital Twins begins from the planning and design phase, supporting the development of robust and efficient CCS systems.

By leveraging the capabilities of Digital Twins, the decarbonization sector can unlock numerous benefits. Digital Twins provide a virtual environment where various scenarios and configurations can be simulated and evaluated, allowing for informed decision-making. These models enable the optimization of CO_2 capture processes, ensuring that the most effective strategies are implemented to achieve maximum efficiency. Digital Twins can also aid in the planning of CO_2 transport, optimizing routes and identifying potential challenges or bottlenecks.

This article explores the impact of advanced digital technologies, particularly Digital Twins, in the Carbon Capture and Storage sector. It highlights the increasing use of data analytics, AI, machine learning, and computer modeling in various industries, including energy. The integration of these technologies in the manufacturing sector has proven to be vital for effective decision-making and improved outcomes. The CCS sector, which aims to capture and store carbon dioxide to reduce greenhouse gas emissions, is showing a growing interest in advanced digital technologies.

2. Digital Twin fundamentals

Digital Twin uses different techniques of learning and utilizes acquired data and knowledge in a flexible and integrated manner to simulate new and previously unencountered situations [6, 7]. There are many ways to classify DT's. Siemens divides them into three main groups [8]:

- *Digital Product Twin* – This type of Digital Twin is primarily used for design and simulation purposes. It enables engineers to create and test virtual prototypes of products, allowing for efficient product development and optimization.
- *Digital Production Twin* – The Digital Production Twin focuses on process simulation. It assists in simulating and optimizing manufacturing processes, enhancing production efficiency, and identifying potential bottlenecks or areas for improvement.
- *Digital Performance Twin* – The Digital Performance Twin is designed for continuous simulation throughout the product's lifetime in its current configuration. It enables real-time monitoring, performance analysis, and predictive maintenance to ensure optimal performance and longevity.

In addition to the previously mentioned classifications, the concept of a Digital Twin expands further when applied to the petrochemical and oil & gas industries. Within this context, a Digital Twin serves as a highly accurate 2D or 3D model representation of a facility, incorporating a comprehensive visualization system that encompasses individual unit operations expressed through advanced physics-based models [9].

This sophisticated representation captures the intricate details of the facility's components, ranging from pipelines and valves to columns and other essential elements. By integrating all relevant materials and systems into a cohesive and user-friendly format, the Digital Twin offers a powerful platform for visualizing and analyzing real-time and forecasted data derived from sensors, as well as simulation results. Graphical elements within the Digital Twin can display crucial information, such as current process parameters, performance indicators, and even predictive insights, allowing operators and engineers to have a holistic understanding of the facility's operations.

Furthermore, the Digital Twin can seamlessly reference and incorporate additional resources, such as unit P&ID's (Piping and Instrumentation Diagrams), technical documentation, maintenance records, and other relevant materials. This integration of data sources facilitates improved communication, collaboration, and decision-making within the facility. Operators, engineers, and other stakeholders can easily access and navigate through the Digital Twin's interactive interface, gaining valuable insights and leveraging the collective knowledge embedded within the system.

The benefits of an accurate and comprehensive Digital Twin are manifold. Firstly, it enables real-time monitoring and analysis of key performance metrics, facilitating proactive maintenance and efficient resource allocation. By visualizing sensor data within the Digital Twin, operators can quickly identify anomalies or deviations from expected operating conditions, enabling timely interventions and reducing the risk of unplanned downtime.

Moreover, the Digital Twin acts as a powerful tool for process optimization and improvement. Through the utilization of physics-based models, operators and engineers can simulate different operational scenarios, explore "what-if" analyses, and identify opportunities for enhancing efficiency, reducing energy consumption, or optimizing resource utilization [6, 7]. This capability to virtually test and evaluate changes before implementing them in the physical system significantly mitigates risks and costs associated with trial-and-error approaches.

Another crucial aspect of the Digital Twin's value proposition lies in its ability to support the planning and execution of complex tasks within the facility. By providing a centralized and easily accessible repository of information, including technical specifications, maintenance procedures, and historical data, the Digital Twin streamlines various processes, such as equipment inspections, maintenance activities, and safety assessments. This streamlined approach enhances collaboration among different teams and departments, promoting cross-functional coordination and knowledge sharing.

Furthermore, the Digital Twin's integration with data analytics and AI techniques enables advanced predictive capabilities. By continuously analyzing historical and real-time data, the Digital Twin can forecast equipment failures, detect performance degradation trends, and anticipate maintenance requirements. These predictive insights empower operators to take proactive measures, scheduling maintenance activities during planned shutdowns or low-demand periods, minimizing the impact on production schedules and optimizing the facility's overall operational efficiency.

3. Applications of Digital Twin in Carbon Capture and Storage

The European Commission actively supports CCS and Carbon Capture, Utilization and Storage (CCUS) projects, but the deployment of CCS on an industrial scale is contingent upon the justifiable demonstration of the duration and reliability of Carbon Capture and Storage technology [10]. Simulating CCS processes in a traditional manner is very time-consuming and computationally expensive; however, with the help of a DT, optimized simulation solutions can be provided and these costs can be reduced [11].

Another problem with adequate geological sequestration is not only dependent on price of emissions allowances (EU Carbon Permits) but also the proper selection of the underground rock formation. The rock layers must create a suitable barrier that ensures the safe storage of CO_2; otherwise, it could pose a serious risk. Simulations of such a process are characterized by complex thermodynamics and a high level of complexity – this is an ideal application for machine learning, which can utilize batch simulation data and subsequent measurements and data collected from all sensors to correct the model and make accurate predictions about the process. Input parameters can include reservoir parameters, such as temperature, hydrostatic and surface pressure, depth, injection schemes, injection rates etc. [11].

The use of numerical models in CCS technologies is a continuous subject of research, development, and presentation in various scientific articles. In the paper of *Accelerating Carbon Capture and Storage Modeling Using Fourier Neural Operators* [12], the authors utilized a set of input data for machine learning and neural network, allowing them to obtain a geological model for CO_2 storage and the changes occurring in reservoir over time. This allowed for the presentation of pressure buildup and gas saturation predictions, which is a very complex and time-consuming process that is difficult to represent without the use of appropriate numerical models and machine learning.

A research paper written by Wen at all. presents the development of a neural network focused on machine learning model of multiphase flow in porous media [13]. The authors obtained a trained model that can be an alternative numerical solution to the simulation of CO_2 injection and related problems, with a very short simulation time. This work perfectly illustrates the methodology of applying advanced neural network architectures. A Neural Network is a network of many interconnected artificial neurons that gather input signals, process then, and send them further [14, 15]. Neurons are arranged in layers. The output of the first neuron sends a signal to the input of the next one, which processes the signal and sends it to the next one (Fig. 1).

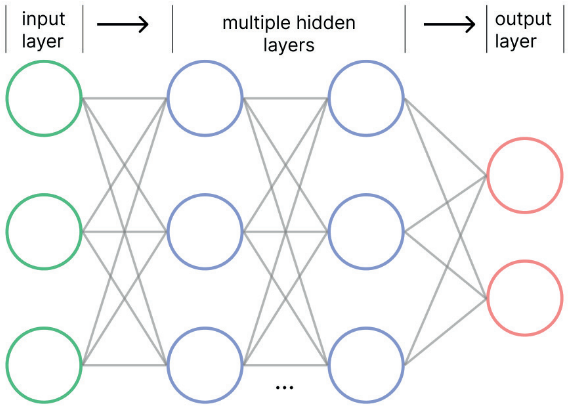

Fig. 1. A simplified typical neural network diagram

The first layer is the input layer, which registers external signal (data), and subsequent layers are called hidden layers, which process information obtained from previous layers, and through the output layer, a decision result is obtained. In a neural network, each neuron has an associated weight and threshold. If the output of any given node exceeds the specified threshold value, that node becomes activated, and data is sent to the next layer of the network. If the output does not exceed the threshold, data is not passed along to the next layer. The neural network created by the authors of the previously mentioned publication allowed for the optimization of multiphase CO_2 flow while maintaining the required accuracy, resulting in high performance of the forecasts conducted over a 30-year simulation period [12].

In conclusion, the integration of neural networks and machine learning in the field of Carbon Capture and Storage (CCS) holds tremendous promise as it presents a wide array of opportunities for optimizing various processes, effectively reducing operational costs, and significantly enhancing the accuracy of predictions. By harnessing the power of neural networks and machine learning algorithms, CCS technologies can undergo substantial advancements, playing a pivotal role in facilitating the global transition towards a sustainable and low-carbon future.

4. Advantages and challenges of using Digital Twin in CCS

Digital Twin solutions have gained widespread commercial adoption in the field of CCS (Carbon Capture and Storage) globally. A notable example is the Shell QUEST CCS project in Canada, where Digital Twins were successfully implemented to address the challenge of pressure change and compressor performance matching. After identifying low performance in the relief valve, the Digital Twin of the unit enabled uninterrupted compressor operation, leading to the storage of over 5 million tons of CO_2 [16, 17].

Another significant application of Digital Twins in the CCS domain is observed in SaskPower's Boundary Dam Carbon Capture Project, which captures CO_2 from a coal-fired power plant in Estevan, Canada [18]. The captured CO_2 is utilized for enhanced oil recovery and stored in the Aquistore project for long-term geological storage. However, the project encountered challenges due to damage to the storage formations resulting from previous water injection. To overcome this, a detailed analysis of subsurface flow and behavior was necessary. By leveraging a wide range of dynamic operational data such as pressure, temperature, and saturation estimates, a calibrated model was developed to simulate the temporal evolution of CO_2 behavior [19]. Schlumberger, a key player in the energy sector, successfully integrated this data into simulators to accurately map changes over time. Furthermore, monthly history matching and cloud simulations were provided to SaskPower to meet regulatory requirements.

The Carbon Dioxide Capture and Storage Project, led by The Midwest Geological Sequestration Consortium (MGSC), involved the injection of CO_2 captured from an ethanol plant using Alstom's amine process [20]. The Digital Twin of the unit played a crucial role in accurately predicting the dynamic flow behavior during CO_2 injection. By developing a transient model for the existing equipment, process optimization was achieved, leading to increased unit safety and performance.

These examples demonstrate the practical application and effectiveness of Digital Twins in addressing complex challenges within the CCS sector. By harnessing the power of advanced data analytics, simulation capabilities, and real-time monitoring, Digital Twins enable enhanced operational efficiency, optimized performance, and improved safety in CCS projects.

5. Conclusion

Industry 4.0 technologies are becoming increasingly accessible and are being implemented in many industries, taking into account the evolutionary changes in production management systems and the need for cybersecurity. Digital Twin solutions are widely used globally in the field of CCS. The technology has been successfully implemented in various projects and enabled uninterrupted operation, optimized processes, and increased safety of the units. In the case of CCS, Digital Twins can be used to model carbon capture and storage processes and to analyze the impact of parameter changes on their efficiency. Thanks to DT, CCS operators can conduct virtual tests and simulations before implementing changes in real systems. They can also monitor and control CCS processes in real-time, allowing for quick detection and the resolution of issues.

In summary, the utilization of Digital Twins in CCS brings a range of benefits. It enables more precise, effective, and economical carbon capture and storage practices, which are paramount in combating the challenges posed by climate change. By providing a virtual platform for modeling, analysis, and real-time monitoring, Digital Twins empower CCS operators to optimize their processes, ensure operational reliability, and make data-driven decisions. The insights gained from Digital Twins enhance our understanding of CCS mechanisms and pave the way for enhanced sustainability in carbon capture and storage initiatives.

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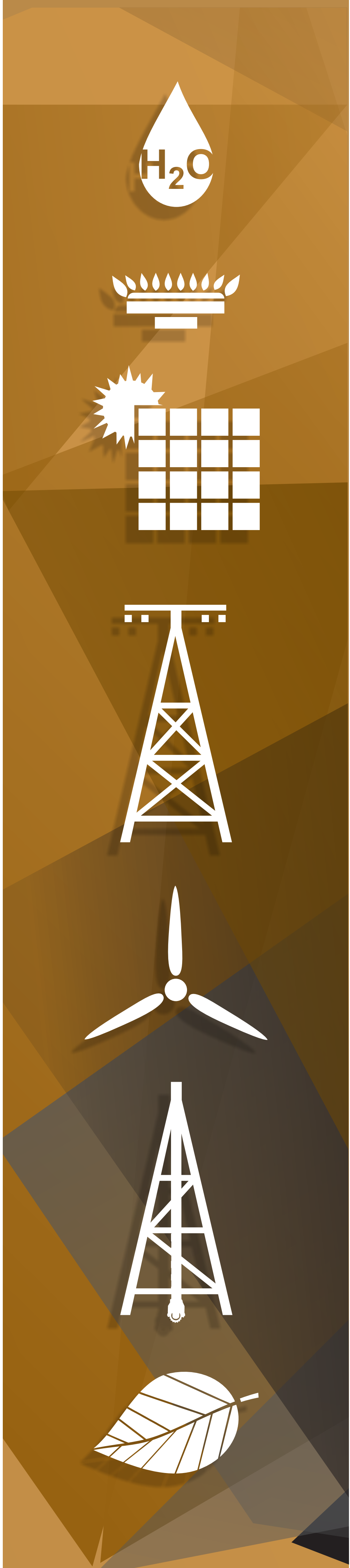
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