

IoT-BASED MONITORING IN CARBON CAPTURE AND STORAGE SYSTEMS

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ABSTRACT

Carbon capture and storage (CCS) is critical for climate-change policies and strategies targeting global warming within the Paris Agreement. The overarching technological requirements are well described in the strategic plans, yet several barriers exist to the technology's widespread deployment, including improved cost-effectiveness and enhanced process integration. For the safe and reliable operation of large-scale CCS systems, the development of effective Internet of things (IoT)-based monitoring tools to ensure flow assurance of CO₂ throughout the CCS value chain is crucial. Further, reliable sensor measurements related to different transport parameters such as temperature, pressure, and flow across the process are essential to develop these methods. However, sensors are prone to errors due to inherent issues or environmental conditions which result in performance degradation of the overall monitoring system. Developing techniques for detecting anomalies in the measurements, identifying the faulty sensors and accommodating them with appropriately estimated data is one of the paramount requirements for the reliable operation of the CCS systems. In such context, the present article provides an overview of CCS's monitoring and control requirements, emphasizing data-fusion synergies. This work investigates the state-of-the-art methods for sensor validation and proposes a roadmap to further deploy metering technologies for industrial needs.

INTRODUCTION

Among the potential carbon emission reduction strategies, carbon capture and storage (CCS) serves as a promising technology to mitigate the anthropogenic effects of climate change and meet the goals of the Paris Agreement. The *Emission Scenarios*, which depict possible pathways that society might undertake to limit the emission of greenhouse gases, require widespread CCS deployment to help reduce direct emissions from the burning of fossil fuels or from industrial processes, and to create negative emissions, such as in combination with bioenergy (BECCS).

Several CCS projects are currently under development. The transport of CO₂ from industrial sources to storage in geological reservoirs is planned in Europe and elsewhere. The capture of CO₂ will expectedly arise from various industrial sources including cement, steel, petrochemicals, biofuel and waste incineration production, H₂ production from natural gas reforming, etc. Such industrial sources will not continuously operate at baseload conditions 24/7. Hence, temporal and spatial variations in pressure, temperature, flow, and composition are expected throughout the value chain.

The deployment of large-scale CCS requires a deep and reliable understanding of the physics and the thermodynamics of the processes involved [1] and accurate process monitoring and control to enable safe operation, reliable custody transfer, and auditing. Several research outputs have outlined how challenging achieving the above is and the potential impact on CCS's costs and the overall business [2, 3].

An efficient Internet of things (IoT)-based strategy is essential for the real-time monitoring of large-scale CCS to ensure

safe and reliable flow of CO₂ to the permanent storage sites. Recent advances in the design of IoT technologies are spurring the development of efficient strategies for industrial process monitoring based on industrial IoT (IIoT) and fault diagnosis using digital devices, sensors and accelerometers. By applying IIoT solutions, it is possible to realize effective monitoring methods for CO₂ to ensure environmental and public safety in implementing large-scale systems for CCS. Such accuracy, however, deteriorates during operation, and eventually, sensors become faulty and unreliable. The sensors are susceptible to faults due to (i) harsh environmental conditions; and (ii) hardware and inherited limitations, including low battery level, calibration issues, short life span, and poor connections [4]. Timely sensor fault detection and diagnosis play a crucial role in improving IIoT system safety, availability, and reliability as well as reducing the risks of catastrophic failures and maintenance costs [5].

Against this background, sensor validation through fault detection, isolation and accommodation (FDIA) methods serves as a promising solution for detecting anomalies in the CCS systems. FDIA techniques can broadly be classified into data-driven and model-based schemes. The data-driven approaches mainly rely on the huge volume of historical data to characterize the behavior of the system. The main advantage of these methods is that they do not require exact knowledge of the mathematical model of the system to be monitored. Hence, they are suitable for complex systems where explicit models are difficult to establish. They are easy to implement and can capture non-linear behavior by learning through historical data recorded by the sensors. Due to the merits stated above, several data-driven sensor fault detection, isolation and accommodation (SFDIA) approaches have been investigated for industrial process monitoring in [5]. Some of these approaches are based on artificial neural networks, convolution neural networks [6] and deep learning [7]. Further, a fault detection and diagnosis method for electric motors is presented in [8], where multiple features that indicate different faults are extracted by cross-correlation improved spectral kurtosis. The features are then combined to form a health index using principal component analysis (PCA) and a semisupervised K-nearest neighbor (KNN) distance measure, which is then evaluated for fault detection. However, the data-driven methods require a large amount of data especially

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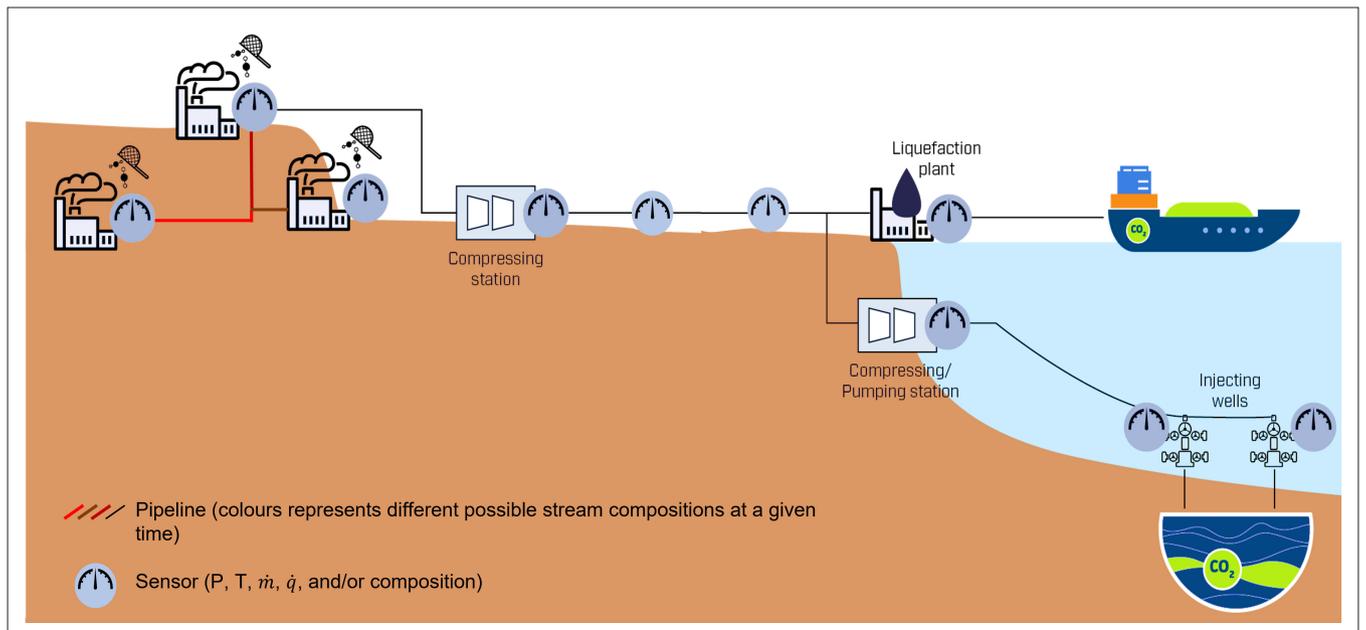


FIGURE 1. CCS value chain showing the main measuring points. Typical locations for sensors (pressure, temperature, mass/volume flowrates and compositions, or any combination of them) are indicated throughout. The different colors in the piping around CO₂ capture clusters and export pipelines illustrate different possible stream compositions at any given time.

for training, and can only be used if the given system can generate enough data from the sensors. Further, it is challenging to deal with incomplete data usually in terms of missing or erroneous data values and enormous computational effort makes these methods inappropriate for online implementation [5].

On the other hand, model-based approaches have gained popularity because of their theoretical merits, higher accuracy, and effectiveness. These techniques serve as promising tools for anomaly detection and isolation, especially in scenarios where accurate mathematical model of the monitored industrial process and its associated parameters are precisely known. Generally, the model-based approaches perform fault diagnosis by computing residuals which represent a difference between the original output and its estimate obtained using an observer. The observers play an important role in model-based techniques and some of the model-based observers are Kalman filter (KF) for linear systems and cubature KF, extended KF (EKF), modal KF, and unscented KF (UKF) [9] for nonlinear systems, which are robust against model uncertainties and disturbances. Nevertheless, these methodologies are heavily dependent on the knowledge of system model/ parameters, which may not be always available and are difficult to implement in presence of nonlinearities. In conjunction with the model- and data-based techniques, multi-sensor data fusion techniques can be employed to minimize the computational burden and enhance the decision-making of the overall system [10].

Although SFDIA methods have been extensively developed for a wide selection of applications including combustion engines, electric motors, mining and several others, their applicability in CCS is not straightforward. It is challenging to perform fault diagnosis in CCS systems due to the need of a physical model that accurately replicates the dynamics of CO₂ transport between affected sensors over a broad range of operating conditions, including varying composition, phase changes, and transient phenomena, among others. To address the above-mentioned concerns, this article discusses the monitoring and control requirements of the CCS system and highlights the challenges associated with designing anomaly detection techniques for such systems.

The organization of the article is as follows. We provide an overview of the CCS systems and various challenges related to these systems. We investigate the existing state-of-the-art meth-

ods for sensor validation and their application in the context of CCS. We present a roadmap for IoT-based monitoring in CCS systems. The potentiality of a unique facility demonstration of flow assurance for CO₂ transport operations (DeFACTO), coupled with projects targeting monitoring and control networks for CCS (MACON CCS) and sensor validation for digital twins of safety-critical systems (SIGNIFY) are also outlined. Finally, we summarize the main conclusions of this study and suggests future research paths.

CHALLENGES IN MONITORING OF CCS STREAMS

CCS monitoring presents numerous challenges. Some of the main hindrances are related to the thermodynamic properties of CO₂, the presence of impurities in the CCS streams, and the transient character of the processes [11].

At the system level, the CCS conditions are intrinsically dynamic. The CO₂ capture plants are expected to asynchronously inject CO₂ to the downstream network and pipelines (Fig. 1), depending on the operational scheme of the CO₂-source processes. The downstream pipe networks and export pipelines, thus combine CCS streams of varied compositions from several CO₂ capture sites, as illustrated in Fig. 1. This setup leads to temporal and spatial variations in the compositions, mass flow rate, pressure, and temperature with distinct flow assurance challenges.

Even in small concentrations, impurities in the streams could drastically affect the phase behavior and can considerably deteriorate the accuracy of the measurement technologies, especially if a second phase arises. This is particularly relevant for composition tracking and for meters that are flow-pattern- or phase-sensitive, like fiscal meters. A second phase will typically be enriched with possibly flammable, corrosive, and/or toxic impurities. Two-phase liquid-gas conditions can occur in pipeline sections in a variety of scenarios, including after unintended shutdown sequences, due to terrain topography that favors liquid deposition in low points, from evaporated components from the CO₂ liquid stream, or when operational conditions are close to the saturation line, as is the case of CO₂ ship offloading.

The above challenges warrant monitoring solutions to ensure process control, inventory tracking, flow assurance, and swift leak detection. Continuous pressure and temperature monitoring and regular sampling are customary. This is however not the case with flow metering devices for long pipeline systems,

where relying on measurement layouts at short and regular intervals is impractical. Further, pipeline inspection can prove expensive, disruptive, and unfeasible. In this context, sensor validation and predictive knowledge of the CO₂ stream behavior are of the utmost relevance.

METERING

Under typical CCS operating conditions, CO₂-rich streams can be in gas, liquid, or dense phases throughout the value chain. The transport of large amounts of CO₂ is done via pipelines, with CO₂ being in a liquid or dense phase. At shorter distances, CO₂ streams may also be transported in a compressed gaseous phase. Depending on the operation conditions along the value chain, gas flow meters are needed in the outlet of capture plants and in onshore networks, and liquid-service meters in export pipelines, loading, and off-loading terminals, and injection wells (Fig. 1).

The overarching use of measurement technologies in the developing CCS value chains comprise

- Process monitoring, as redundancy measurements, or to complement other measurement methods in multimodal configurations as well as composition and flow-phase checks to ensure the accuracy of adjoining flow metering devices
- Flow assurance, including dry ice formation, pipeline integrity, and leak detection [11].

The CO₂ flow monitoring technology market is still in an early development stage with limited experimental data on two-phase flow or composition measurements for CO₂-rich mixture transport [2].

FLOW MODELING

The representation of pipeline transport conditions through mathematical models that predict the behavior of systems is beneficial for process design and control. The pressure drops along a pipe section can be estimated using density-energy formulations, given known process conditions, i.e., composition, pressure, and temperature from reliable sensor data. The value of flow modeling lies in the reduction of economic and physical risks as well as in the possibility of predicting flow behavior. The prediction of flow phenomena is relevant both under normal operating conditions where temporal and spatial variations of the CO₂ stream composition, phase distribution, and pressure are expected downstream of capture sites, as well as in the face of extraordinary events that escape normal operation schemes, such as leaks and rapid transients. The flow modeling provides accelerated estimates in the presence of changes in process variables, which minimizes control delays and operational costs.

The thermodynamic properties of pure CO₂ at equilibrium are described with high accuracy by the Span-Wagner reference equation of state (EoS) [3]. Even though multiparameter EoSs, currently developed for CCS have unparalleled accuracy in regions where experimental data are available, they have challenges related to robustness and limited extrapolative properties [12]. Also, EoSs are usually not written in a form suitable for fluid-dynamic simulations. The required density-energy formulations call for the development of fast and robust numerical algorithms to solve phase-equilibrium equations with the specification of energy and density. For CCS, in particular, the transport of CO₂-rich streams differs from that of other fluids such as pure CO₂ or natural gas in several ways. For CO₂ mixtures containing impurities, robust and time-efficient solutions of the phase equilibrium have proven to be challenging [13].

DIGITALIZATION COMPLEXITY

Safe and reliable large-scale CCS entails an effective health monitoring strategy to guarantee flow assurance and detect and minimize leakage throughout the value chain. The development of effective IoT-enabled monitoring tools for CO₂ relies on measurements from a sensor network, where sensors monitor

the temperature, pressure, and flow across the process. Various concerns exist regarding the performance and accuracy of flow meters at relevant CCS conditions and stream composition [2, 11], as well as the extraction of valuable data from high-frequency monitoring sensors to support real-time detections.

In this context, data fusion could prove effective to capture reliable and accurate information from different sources along the CCS value chain and combine information about spatial locations. However, data fusion techniques require a physical model of the CCS system that reveals the dynamics of CO₂ transport and decreases the uncertainty of CO₂ handling [14]. The capabilities of modeling tools for the predictive assessment of CO₂ are key. The complexity of transient computation for CCS transport processes could benefit from a step-wise approach based on simple geometries and fully developed flows. It is crucial that high-quality and highly accurate experimental data is used to provide a certain measure of the degree to which a given flow simulation model is accurately representing the physical phenomena governing the transport process. The reference experimental data must necessarily be representative of the relevant thermophysical properties of CO₂ to target flow assurance and be able to replicate the issues of concern at relevant process conditions.

Once the flow model is successfully validated, the simulation outputs can be used for the design of optimal sensor numbers and distribution along with a pipeline network and for control operations based on the detection and the replacement of measurements from faulty or unreliable sensors with the estimates corresponding to virtual sensors.

Unreliable sensor data can arise from hardware/software failures or other process-driven reasons, e.g., phase transitions. The erroneous measurements from the sensors may hamper the secure and reliable functioning of the system and can even cause severe damage to the whole system. Dependable sensor measurements are of paramount importance to ensure safe operation, comply with regulations, and enable fair trading of 5 Gt of CO₂ per year by 2050, ultimately warranting the CCS business model. To ensure measurement reliability, addressing sensor faults is key. Sensor validation, in turn, requires efficient fault diagnosis techniques, which are discussed in detail in the subsequent section.

SENSOR VALIDATION

CO₂ monitoring is highly dependent on reliable sensor measurements. Yet, sensors are susceptible to faults and, consequently, the accuracy, the stability, and the reliability of CCS systems get affected by sensor faults. Sensor faults may exhibit different characteristics depending on the type of sensors and the operating scenario, however, they are usually represented through analytical models for statistical analysis.

The most common models for sensor faults are:

- Bias/offset fault, where sensor values deviate by an additive constant bias
- Drift fault, where sensor values drift with a small slope from the original values
- Freeze/stuck at fault, where sensor value gets stuck at a constant value
- Noise fault, where sensor values experience large noise levels.

To efficiently exploit the CCS, an early sensor fault diagnosis is crucial for risk management, while assuring the reliability and safety of the overall system. Generally, the SFDIA comprises of following tasks:

- *Detection*, i.e., determination of the presence of an anomaly within the network
- *Isolation*, i.e., identification of the faulty sensor(s)
- *Accommodation*, i.e., replacement of the faulty sensor measurements with reliable measurements.

Therefore, by employing the SFDIA architecture, the processing of corrupted sensor data and the associated consequences ranging from performance degradation to risk of danger and

lack of security can be avoided. Based on the above framework, the data-driven and model-based architectures for SFDIA in CCS systems are discussed next.

DATA-DRIVEN SFDIA APPROACH

A data-driven SFDIA architecture that exploits the temporal correlation of faulty and non-faulty sensor measurements is developed for digital twins in [4]. The goal of the proposed SFDIA is to detect anomalies in the sensor measurements, identify the faulty sensors, and replace them with fault-free estimated data, thus facilitating reliable digital twins. The proposed framework is a three-stage SFDIA architecture, as demonstrated in Fig. 2. The first stage entitles a bank of virtual sensors which allows to accommodate for unreliable sensors by estimating measurements of the faulty sensors. This stage effectively models the nonlinear behavior of estimators through a multilayer perceptron (MLP) architecture. The second stage is the residual computation unit, which computes a measure of dissimilarity between the sensor measurement and its corresponding estimate obtained from the virtual sensor. Finally, the last stage represents the sensor-fault classifier, which classifies a sensor as faulty or reliable based on the residual measures from the unreliable sensors and also replaces the faulty measurements with the estimate obtained through its corresponding virtual sensor.

The performance of the architecture has been validated for three distinct real-world data sets corrupted with synthetically-generated soft and hard sensor faults. Results published in [4] demonstrated that, for the data sets used, the proposed approach can achieve high detection probability and correct classification with a low probability of false alarm in the presence of weak drift and bias faults, which are difficult to detect. Further, the proposed machine-learning-based SFDIA framework has also been validated for the emerging CCS technology. A preliminary set of results are provided in Fig. 3 and Fig. 4, which demonstrate the efficacy of the proposed architecture in detecting the synthetically-generated bias faults. The results are performed using the real measurements from the temperature sensors installed on the surface of the CO₂ pipeline DeFacto (described next) with simulated faults. Figure 3 shows encouraging performance in terms of probabilities of detection (P_d), classification (P_c), and false alarm (P_f), however these results are to be considered preliminary as more critical operational conditions need to be explored. Moreover, Fig. 4 demonstrates the training phase evolution of the classifier (per-sensor) binary cross-entropy (BCE) loss function versus the number of epochs on both training (solid lines) and validation (dashed lines) sets under bias faults.

MODEL-BASED SFDIA APPROACH

Among the model-based techniques, the KF-based FDIA approach is widely employed because of its theoretical merits and effectiveness. The quickest change detection methods can also be employed for the real-time detection of abrupt changes in the behavior of the observed signal from a single sensor or a group of sensors [15]. Recently, fault and state estimation in nonlinear systems have gained research interest, which has led to the development of various FDI approaches based on EKF, UKF, and particle filter. A systematic three-step fusing UKF based approach for fault diagnosis in nonlinear DC microgrids is proposed in [9]. The method offers a low computation burden, especially in the case of multiple sensors and multiple faults. Such compelling advantages could be leveraged to detect single and multiple sensor faults in the CCS systems. A similar model-based SFDIA framework that employs UKF, EKF, or particle filter targeting CCS systems can be designed as follows. All sensor measurements are initially grouped into locals, which are utilized by the local UKFs to estimate the nonlinear system states. Then, the state residuals are evaluated to detect the faulty sensors. Lastly, the faulty sensors and their

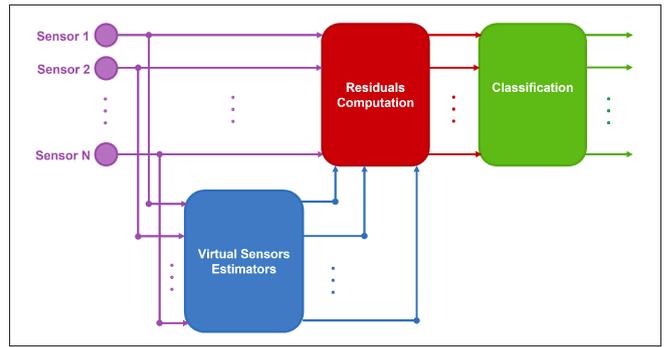


FIGURE 2. Block diagram of the SFDIA system.

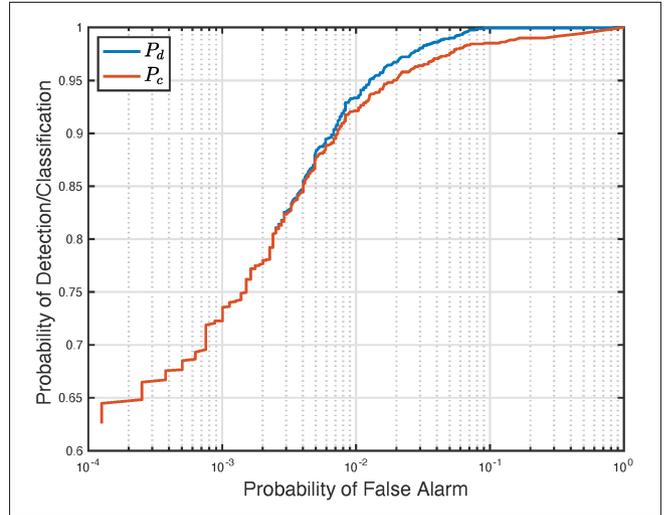


FIGURE 3. Detection and classification performance of the data-driven SFDIA scheme.

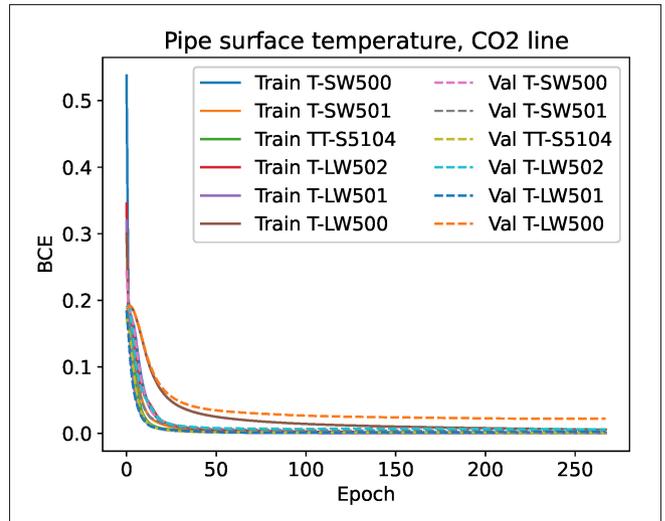


FIGURE 4. Training/validation loss of the data-driven SFDIA scheme.

corresponding state estimations are isolated and replaced by fault-free measurements, which are used to compute accurate global estimates.

Further, data fusion methods, which focus on combining information from multiple sensors, can also be integrated with both model- and data-driven approaches to facilitate the fault diagnosis in the CCS systems. The implementation of these methodologies will help in reducing the computational burden and eventually enhance the decision-making of the overall system.

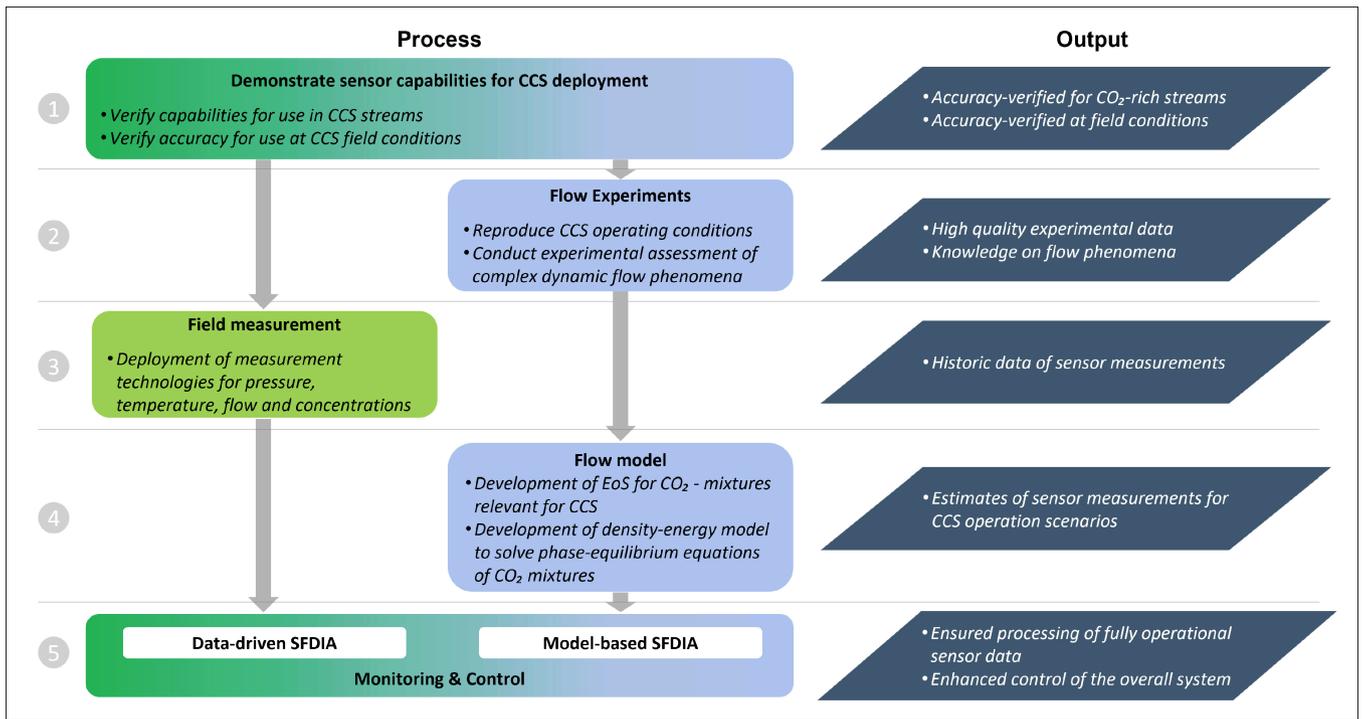


FIGURE 5. Roadmap to develop monitoring & control capabilities for CCS with the output from each development stage.

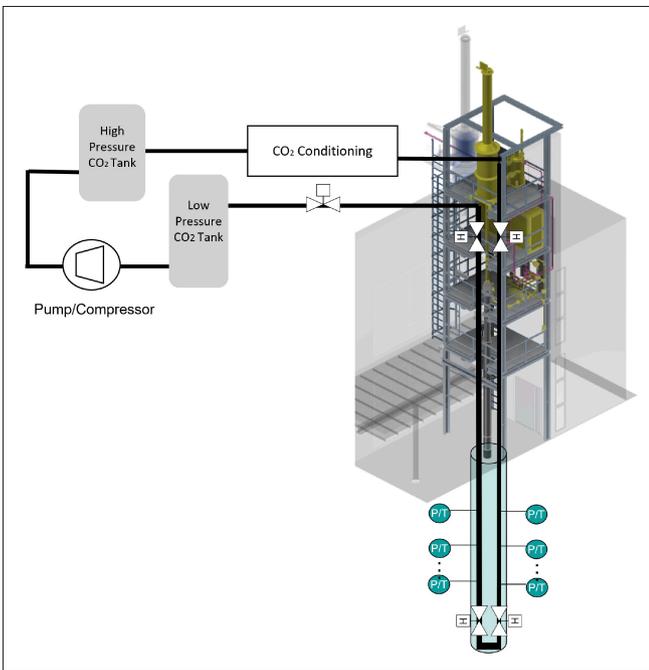


FIGURE 6. Illustration of the DeFACTO experimental facility.

ROADMAP FOR IOT-BASED MONITORING IN CCS SYSTEMS

Various ongoing initiatives are underway to advance the current state of the art of CCS monitoring, in correspondence with the roadmap proposed in Fig. 5. The project MACON CCS focuses on the first two development stages, namely demonstration of sensor capabilities for CCS and flow experiments, to advance the development of dynamic simulation models targeting the transport of CO₂-rich mixtures at relevant operational conditions. Emphasis is on advancing in development and integration of novel EoS into a modeling software solution enduring fast and robust numerical solution phase-equilibrium equations of

CO₂ mixtures containing impurities. MACON CCS will also provide an overview of measurement principles and existing commercially available technologies that could potentially be used for flow and concentration measurement scenarios in ongoing and future CCS projects, i.e. field measurement – stage 3.

SIGNIFY is another complimentary project that covers processes 2, 4 and 5 of the roadmap (Fig. 5). SIGNIFY works to develop IoT-based fault diagnosis methods, especially, data-driven and model-based approaches to prevent the processing of corrupted sensor data by digital twins in real-time, especially in safety-critical applications, and avoid erroneous action planning. Further, the project aims to develop a physical model for CCS systems, yet the model's capability to reproduce complex operating conditions and obtain sound results depends on the reliability of the experimental data and on the accuracy of the sensors.

For stage 2, both projects above exploit the experimental capabilities of SINTEF's DeFACTO infrastructure. DeFACTO is a highly instrumented experimental facility that includes a 139 meters long horizontal loop and a 90 meters deep vertical U-tube, enabling the study of both horizontal and vertical flow phenomena relevant to transport phenomenon for CCS (Fig. 6). The CO₂ loops operate at up to 160 bar, the vertical section has a tight heat transfer system that allows operation at temperature between 5°C and 35°C. The experimental studies within MACON CCS and SIGNIFY comprise steady-state liquid or gas flow and transient phenomena, including rapid depressurization and cavitation. The gathered data will allow the validation of simulation tools to reduce model error's effects and improve the understanding of CO₂ transport phenomena and the associated flow assurance problems. Further, the integration of IoT-based monitoring systems will enable timely detection and identification of process anomalies and sensor anomalies in real time.

CONCLUSIONS

This manuscript presented an overview of the monitoring and control requirements of the CCS system, with particular attention on the challenges associated with metering, flow modeling, and digitalization. Further, the state-of-the-art methods for sensor validation specifically model-based and data-driven approaches in conjunction with the data fusion strategies and their application in the context of CCS systems were investigated.

A roadmap for monitoring and control of CCS processes was proposed. Ongoing work focus is on tackling the intrinsically challenging thermodynamic properties of CO₂-rich streams, the extrapolation constraints of existing multiparameter EoSs, and the lack of readily available fast and robust numerical algorithms for flow modeling of CCS conditions. The validation of flow simulation tools for IoT-based monitoring is also being addressed through acquisition of high-quality and highly accurate experimental data at relevant transport conditions. This is done within the MACON CCS and SIGNIFY projects by exploiting the capabilities of the unique DeFACTO facility. The experimental data is to be used for EoS formulation, flow model tuning, and sensor validation.

Future areas of research could include the development of traceable measurement methods and equipment to verify the accuracy of meters under real CCS operation conditions, the development of model-based and hybrid analytic solutions for facilitating fault detection in the CCS systems, followed by validation of the proposed solutions for synthetic data and real-sensor measurements. In addition, the proposed framework can be extended to support real-time fault diagnosis for multiple sensor failures.

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