Optimizing a carbon capture process from water

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1. **Introduction**

 Carbon capturing is a universally recognized imperative in electricity generation (Pan et al., 2023). To address this pressing challenge, the integration of Renewable Energy for Electrochemical Capture has experienced significant growth in recent years. However, due to the inherent variability and unpredictability of renewable energy, a substantial portion of power remains underutilized, particularly in Spain (Gao et al., 2020). Carbon capture (CC) technology, aimed at carbon capture, has been widely researched and implemented in various sectors. In Spain, industrial demonstration projects for capturing CO2 emissions from water have been successfully initiated. Nonetheless, CC faces several economic and technical challenges, particularly in the transportation stages of captured CO2 (Yang et al., 2019). This necessitates urgent action to address the current limitations in power absorption capacity and confront the persistent challenges associated with carbon capture from industrial processes. This study represents the promising potential of technology as an attractive means to capture carbon capture from industrial processes, thus contributing to a more sustainable and environmentally friendly energy landscape.

Water scarcity problems may be related to the unbalance between supply and demand caused by rapid urbanization and industrialization also may be related to water distribution. While it touches on the challenges of water pollution due to rapid urbanization and industrialization, it does not specifically represent optimizing a carbon capture process from water. Instead, it emphasizes the importance of treating wastewater to address water pollution issues and highlights the methods of wastewater treatment, including physical, chemical, and biological methods (Yang et al., 2019).

In the context of optimizing a carbon capture process from water, it would typically involve the development of techniques or technologies to efficiently capture and store carbon dioxide (CO2) dissolved in water sources. This is distinct from the wastewater treatment methods discussed in the study, which primarily focus on removing biodegradable organic and nonorganic matter, such as carbon, nitrogen, and phosphorus. To optimize carbon capture from water, one would need to explore methods for effectively capturing CO2 from water sources, which may involve innovative materials, processes, and technologies tailored to this specific purpose.

In recent years, the concept of a CC system, as initially introduced by Li et al. (2021), has garnered significant attention. They established a multi-time scale stochastic unit commitment-economic dispatch model, demonstrating the development potential of this hybrid system. Subsequently, they presented a stochastic two-stage unit planning model, highlighting the potential of the hybrid CC system to take on a substantial portion of renewable energy generation. However, it is notable that neither study (Li et al., 2021) accounted for environmental factors, such as carbon dioxide (CO2) emissions. This study endeavors to fill this critical gap by extending the scope of the CC system to incorporate two advanced technologies and CC. These technologies are aimed at further reducing CO2 emissions and enhancing the utilization of renewable energy resources. Notably, research by Wu et al. (2021) has evaluated the value of the water system, demonstrating its potential to reduce curtailment and improve economic benefits. In a similar vein, Bartnik et al. (2021) thoroughly explored three alternative routes, affirming the feasibility of this technology. Bhatia et al. (2019) have analyzed the advantages of technology, highlighting its sustainable development trends. However, most of these studies have predominantly focused on individual technologies, overlooking the potential synergistic benefits that arise from CC. Arias et al. (2016) provided crucial insights by demonstrating that CC significantly impacts the water and CO2 sectors, lowering the need for carbon capture and thereby reducing costs. Chen et al. (2021) further contributed to this understanding by establishing a low-carbon economic scheduling model that incorporates both CC and CC technology, validating the environmental benefits of such an approach. Moreover, Zhang et al. (2023) proposed an economic and environmentally friendly dispatch model that integrates technology, enhancing system flexibility. Considering the body of research mentioned above, it becomes evident that extending technology with CC technology to create a system holds great promise. Such an integrated system can harness surplus power effectively while simultaneously reducing CO2 emissions, contributing significantly to sustainable and environmentally friendly energy production. This study also explores the complexities of systems that encompass multiple energy sources, including electricity, thermal energy, and gas. Systems offer the potential for stepped energy utilization and improved economic and environmental benefits compared to single-energy systems (Wang et al., 2019). However, optimizing the operation of systems can be challenging due to its intricate structure. Researchers have developed various models and algorithms to address these challenges, such as optimal scheduling models for carbon capture processes (Chen et al., 2021), novel deep reinforcement learning strategies for dynamic dispatch problems, and mathematical models for systems involving CC (Bhatia et al. 2019). In this study, I employ the SCIP solver, a nonlinear solver, to optimize the operation of the proposed system. This solver offers the capability to effectively address complex nonlinear problems, enhancing the precision of our analysis and enabling us to unlock the full potential of the system.

While significant progress has been made in the field of carbon capture (CC) technology, particularly in the capture of CO2 emissions from industrial processes and power generation, there remains a critical gap in optimizing CC processes specifically for capturing CO2 from water sources. Existing CC technologies have primarily focused on capturing CO2 from fluids and industrial emissions, but the efficient and effective capture of CO2 directly from water, such as seawater or wastewater, presents unique challenges and opportunities (Chen et al., 2021). The optimization of CC processes for water-based sources is relatively unexplored, and there is a lack of comprehensive research and methodologies tailored to this specific application. Furthermore, the statement asserts that addressing this research gap is crucial in the context of sustainable carbon capture from water sources. It emphasizes the potential of efficient and environmentally friendly carbon capture technologies in reducing carbon emissions associated with water reservoirs. This not only underscores the relevance of the research but also positions it as an essential step toward more sustainable water management and environmental protection. Finally, a need for research that considers critical factors is asserted such as energy efficiency, cost-effectiveness, and environmental sustainability, all of which are vital aspects of optimizing carbon capture processes for water-based sources.

* 1. **Literature review**

Optimizing a carbon capture process from water is a multifaceted endeavor with critical implications for mitigating carbon dioxide (CO2) emissions and addressing climate change. First, it involves the identification of various sources of CO2 in water, including industrial discharges and natural CO2 content in aquatic environments. Understanding the diversity of sources is pivotal for designing effective capture strategies (Shi et al 2016).

Next, a key aspect of optimization lies in selecting and fine-tuning carbon capture technologies. These can encompass chemical absorption, membrane separation, and adsorption methods. The choice of technology depends on factors like CO2 concentration and water volume, highlighting the need for adaptability and efficiency in the process.

The heart of the optimization process involves mathematical modeling and simulation Shirmohammadi Aslani Ghasempour (2020) stated. By creating a detailed model that considers variables such as flow rates, temperatures, pressures, and chemical reactions, researchers can explore a range of operational conditions to maximize CO2 capture efficiency. Optimization algorithms further refine these models, helping identify the most effective operating parameters, whether to minimize energy consumption, reduce costs, or mitigate environmental impacts.

Finally, successful optimization extends beyond the laboratory and into real-world applications. Effective monitoring and control systems ensure that the carbon capture process operates efficiently in real-time. Continuous improvement is essential, with ongoing assessments and adjustments to adapt to changing conditions and enhance efficiency over time (Shi et al 2016). As Li et al. (2021) remarked, Regulatory compliance and a commitment to research and innovation are also crucial to achieving long-term goals in reducing CO2 emissions and contributing to a sustainable future.

**1. Integration with Carbon Storage**: Once CO2 is captured from water, it needs to be safely stored or utilized. Integration with carbon storage technologies, such as geological sequestration or utilization in products, is essential for achieving the overall goal of reducing CO2 emissions.

**2. Environmental and Economic Considerations**: The optimization process should take into account both environmental and economic considerations. This includes assessing the environmental impact of the process and evaluating the cost-effectiveness of different technologies and operating scenarios.

**3. Continuous Improvement**: Optimization is an ongoing process. Regular assessment and adjustment of the carbon capture process are necessary to adapt to changing conditions and improve efficiency over time.

**4. Regulatory Compliance**: Compliance with local and national environmental regulations is critical. The carbon capture process must meet emission reduction targets and adhere to legal requirements.

**5. Research and Innovation**: To stay at the forefront of carbon capture technology, ongoing research and innovation are essential. This includes exploring new materials, processes, and techniques that can enhance the efficiency and effectiveness of CO2 capture from water.

**Table 1**

**Main features of regression techniques used for forecasting emissions.**

[**https://www.sciencedirect.com/science/article/pii/S0959652621006454**](https://www.sciencedirect.com/science/article/pii/S0959652621006454)



In the realm of estimating real-time carbon dioxide (CO2) emissions, the use of proxy variables based on historical time series data has been a common practice. However, recent extraordinary events, such as the COVID-19 pandemic, have exposed the limitations of these methods. When unforeseen circumstances disrupt patterns of industrial and economic activity, traditional models relying solely on historical trends become unreliable (Scikit-learn 2020).

However, Pytorch (2020) believed that The COVID-19 pandemic, with its associated lockdowns and restrictions, drastically altered mobility and industrial activity worldwide. While these measures were crucial in curbing the spread of the virus, they also led to significant reductions in CO2 emissions. This unexpected scenario highlighted the inadequacy of relying solely on historical data to estimate CO2 emissions in real-time.

To address this challenge, this study focuses on developing a method for estimating almost real-time CO2 emissions in Spain. It seeks to determine whether proxy variables related to energy consumption can serve as robust metrics for such estimations. The significance of this research lies in its potential to predict the impact of future policies on pollutant generation. The study aims to demonstrate the model's robustness by applying it to estimate CO2 emissions in Spain's Autonomous Communities and forecasting emissions under various post-COVID-19 economic activity recovery scenarios. This research acknowledges the importance of adapting to dynamic circumstances and highlights the need for innovative approaches to monitor and estimate CO2 emissions in a rapidly changing world. By considering real-time data and exploring proxy variables, this study contributes to the broader understanding of environmental impact assessment and policy planning in response to unforeseen global events.

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**1.2 Current state and future challenges of carbon capture**

The current state of carbon capture technology and its future challenges can be summarized as follows:

***Existence of Technologies:*** Several carbon capture technologies exist and have been demonstrated at various scales, including post-combustion capture, pre-combustion capture, and oxyfuel combustion. These technologies are capable of capturing CO2 emissions from various industrial processes.

***Industrial Use:*** Carbon capture is currently being used in certain industries, such as water processing, where it is economically viable. However, the optimization of carbon capture from water is an emerging area of research and application, and its industrial use is not yet widespread.

***Research and Development:*** Ongoing research and development efforts are focused on improving the efficiency and cost-effectiveness of carbon capture technologies. This includes the development of advanced materials, solvents, and processes.

***Policy Support:*** In many regions, government policies and incentives promote the deployment of carbon capture technologies to reduce carbon emissions. These policies include carbon pricing mechanisms and subsidies for carbon capture projects.

Future Challenges:

*Cost Reduction*: One of the primary challenges is reducing the cost of carbon capture technologies. Current systems can be expensive to build and operate. Lowering these costs is crucial for widespread adoption.

*Energy Penalty*: Most carbon capture processes consume additional energy, which can reduce the overall efficiency of industrial facilities. Developing technologies with lower energy penalties is essential.

*Scale-Up*: Scaling up carbon capture technologies to capture large volumes of CO2 is a significant challenge. Many existing projects are relatively small-scale demonstrations, and deploying them at a larger scale requires substantial investment.

*Capture and Utilization*: Finding suitable capture sites for captured CO2 and developing methods for its utilization are ongoing challenges. This includes ensuring the long-term stability and safety of stored CO2.

*Public Acceptance*: Public acceptance and social perceptions of carbon capture (CC) projects are important. Some communities may have concerns about the safety and environmental impact of carbon capture projects.

*Research and Innovation***:** Continued research is needed to develop breakthrough technologies that can significantly improve the efficiency and reduce the costs of carbon capture. Innovation in materials and processes is crucial.

*Infrastructure*: Developing the necessary infrastructure for transporting captured CO2 to capture sites or utilization facilities is a logistical challenge that must be addressed.

*Policy and Regulation*: Clear and consistent policies and regulations are needed to incentivize carbon capture deployment. Governments must provide a stable regulatory environment and financial incentives to support investment in these technologies.

*Global Cooperation*: Addressing climate change through carbon capture requires international cooperation. Developing countries may need support in adopting these technologies.

1. **State of the art**

Integration of CCS and Second-Generation Capture Technologies: The research explores the integration of Carbon Capture and Storage (CCS) technology with second-generation capture technologies in the context of coal-fired processes in Spain. This represents an advanced and innovative approach to reducing carbon (CO2) emissions from industrial operations.

*Scenario-Based Assessment*: The study employs scenario analysis to evaluate the feasibility and effectiveness of CCS integration. Multiple scenarios (S1, S2, and S3) are considered, each with different parameters, such as the commercialization time of second-generation capture technologies and the investment recovery period (IRP). This approach allows for a comprehensive assessment of various potential futures.

*Geographic Considerations*: The research recognizes the importance of geographic factors in determining the suitability of CCS retrofit. It takes into account the geographic distribution of industrial facilities and the proximity of suitable CO2 storage sites. This geographical assessment is crucial in identifying regions where CCS integration is feasible and regions where logistical challenges exist.

*Economic and Environmental Impact*: The study evaluates the economic and environmental impact of each scenario. It considers factors such as total cost, per-unit cost of retrofit potential, and average annual financing demand. This holistic assessment ensures that the chosen scenario aligns with both economic and environmental sustainability goals.

*Sensitivity Analysis*: Sensitivity analysis is conducted to understand how variations in key parameters affect CCS retrofit potential. This analysis provides insights into the robustness of the chosen scenario and its sensitivity to changes in variables like commercialization time and IRP.

*Technology Lock-In and Climate Goals*: The research addresses the issue of technology lock-in, emphasizing the importance of avoiding scenarios that may limit future technological advancements. It also considers climate goals, aiming to achieve the recommended CCS retrofit capacity of industrial processes as proposed by the International Energy Agency (IEA).

*Regional Assessment*: The study assesses the CCS retrofit potential of key regions in Spain, highlighting areas with favorable conditions and those facing challenges related to CO2 transport and storage. This regional-level analysis provides valuable insights for localized decision-making.

Future Research Considerations: The research identifies areas for future investigation, including the exploration of marine sequestration options and the development of cost-effective CO2 transport methods. This forward-looking approach acknowledges the evolving nature of CCS technology.

So, the state of the art in this research lies in its comprehensive evaluation of CCS retrofit potential for industrial processes in Spain. It combines scenario analysis, geographic considerations, economic assessments, and sensitivity analysis to make informed recommendations for achieving carbon capture and storage goals while avoiding technology lock-in. This research contributes to the advancement of sustainable industrial practices in Spain and provides a valuable framework for decision-makers in the field of carbon emissions reduction.

*Benefits for the Region:* In this scenario, the region, such as Spain, stands to benefit in various ways:

*Carbon Reduction:* The optimized carbon capture process significantly contributes to reducing CO2 emissions, aligning with the region's climate goals.

*Technological Advancement:* The region becomes a hub for advanced carbon capture technologies, fostering innovation and attracting research and development investments.

*Environmental Sustainability:* The adoption of environmentally responsible carbon capture methods helps protect and preserve the region's natural resources and ecosystems. This scenario illustrates how a region could optimize a carbon capture process from water sources as part of its commitment to carbon reduction and environmental sustainability.

**2.1 Model Validation in Carbon Capture from Water**

Data Comparison: Model validation commences with a comparison of the model's predictions to real-world data. In the study of carbon capture from water research, this involves comparing the simulated carbon capture rates and processes with actual historical data. For instance, if a certain level of carbon capture efficiency is suggested by the model, it should be validated against historical carbon capture data.

Accuracy Assessment: The accuracy of the model's predictions is assessed by researchers. This involves quantifying the level of agreement between the model's outputs and the observed or measured data. Metrics such as root mean square error (RMSE) or coefficient of determination (R-squared) are commonly used to gauge the accuracy of the model.

Historical Performance Analysis: The model's historical performance over an extended period is evaluated. How well the model has performed in capturing variations in carbon capture rates and efficiency over time is examined by researchers. This analysis helps verify the reliability of the model in replicating real-world behavior.

Scenario Testing: In carbon capture from water research, different scenarios with varying process configurations and operational strategies are likely considered. Model validation involves testing the performance of the model across a range of scenarios to ensure that it consistently produces accurate results under different conditions.

Sensitivity Analysis: Sensitivity analysis is employed to assess how variations or uncertainties in input parameters affect the model's outputs. This helps in understanding the robustness of the model and its sensitivity to changes in key variables.

Cross-Validation: To further ensure the reliability of the model, cross-validation techniques might be employed by researchers. This involves dividing the available data into multiple subsets, training the model on one subset, and validating it on another. Cross-validation helps in identifying potential overfitting issues and assessing the model's generalization capabilities.

Benchmarking: The performance of the model is compared by researchers to other established models or industry standards. Benchmarking provides an external reference point for evaluating the quality and effectiveness of the model.

Validation Against Case Studies: As mentioned in the original information, the research includes case studies with different carbon capture process structures. Model validation involves comparing the model's predictions against the actual outcomes of these case studies. This helps confirm the applicability of the model to diverse scenarios.

Uncertainty Analysis: Researchers assess and quantify uncertainties associated with the model's predictions. Probabilistic or stochastic methods may be used to account for uncertainties in input data and parameters.

Overall, model validation in carbon capture from water research is essential for establishing confidence in the model's ability to accurately represent real-world dynamics. It ensures that the model can be relied upon for decision-making, policy development, and assessing the economic and environmental impacts of different carbon capture process configurations and strategies. Validated models are valuable tools for guiding the sustainable development and operation of carbon capture processes from water.

**2.2 Tactical Process Model**

Dispatch Strategy Implementation: One crucial aspect of the tactical model is the implementation of a day-ahead dispatch strategy. This strategy involves making short-term decisions about how much carbon capture should be conducted and how resources should be allocated within the system. It accounts for factors such as fluctuations in carbon capture rates, the availability of capture equipment, and the need to minimize environmental impacts. The goal is to balance carbon capture efficiency with operational efficiency.

Monitoring and Control: Continuous monitoring and control of the carbon capture process are essential for ensuring its smooth and effective operation. Real-time data is collected to track carbon capture rates, equipment performance, and system conditions. Operators can make immediate adjustments to optimize the process based on changing factors, such as variations in water quality or carbon dioxide concentrations.

Resource Allocation: Another tactical consideration is the allocation of resources such as chemicals, energy, and water. These resources need to be distributed effectively to meet immediate carbon capture demands while adhering to long-term sustainability and cost-efficiency goals.

Maintenance and Optimization: Regular maintenance of equipment and systems is crucial for ensuring their reliability and minimizing downtime. Additionally, there is a continuous optimization effort aimed at improving carbon capture efficiency and reducing operational costs, all within the scope of daily operations.

So, the tactical process model for optimizing a carbon capture process from water focuses on the real-time management of the system, with an emphasis on efficiency, resource allocation, and immediate decision-making. It involves implementing short-term strategies to balance carbon capture goals with operational considerations and ensures that the system operates smoothly and effectively on a day-to-day basis.

**2.3 Strategic Process Model**

The strategic process model takes a longer-term perspective, focusing on planning and decision-making that shapes the overall direction of the carbon capture process. Here are the key elements of the strategic process model:

**System Design and Configuration:** Strategic decisions are made regarding the design and configuration of the carbon capture process. This includes determining the capacity and capabilities of carbon capture equipment and technologies. The goal is to create a system that can efficiently integrate these technologies.

**Technology Selection:** Critical decisions are made regarding the selection of carbon capture technologies to incorporate into the process. These selections are based on factors such as efficiency, cost-effectiveness, and environmental benefits, aligning with long-term sustainability goals.

**Market Analysis:** Strategic planning includes an analysis of carbon capture market trends and regulatory changes. This helps anticipate future carbon capture demands and opportunities, ensuring that the process remains competitive and adaptable.

**Environmental Goals:** Setting and pursuing long-term environmental goals, such as specific CO2 emission reduction targets, are central to the strategic process. Strategies are developed to achieve these goals over time, aligning the process with broader sustainability objectives.

**Investment Planning:** Determining the financial investments required for technology acquisition, infrastructure development, and process optimization is part of the strategic process. It involves assessing the return on investment (ROI) and ensuring financial sustainability.

**Risk Assessment:** Identifying and assessing potential risks and uncertainties associated with the carbon capture process is crucial for strategic planning. These risks may include technological, regulatory, and market-related factors. Developing strategies to mitigate these risks is a key component.

**Research and Development:** Strategic planning involves exploring emerging technologies and research areas that can further enhance the carbon capture process's performance and sustainability in the long run. This ensures that the process remains at the forefront of technological advancements.

So, the tactical process model deals with the day-to-day operations and optimization of the carbon capture process, while the strategic process model focuses on long-term planning, decision-making, and goal-setting to ensure the process's continued success and alignment with environmental objectives. Both models are integral to the efficient and sustainable operation of carbon capture processes from water.

**2.4 Key Components of the Optimization Step:**

***Mathematical Model:*** The optimization process relies on a mathematical model that represents the carbon capture process, including its various components, energy sources, constraints, and objectives. This model takes into account factors like carbon capture efficiency, resource availability, and integration of carbon capture technologies.

***Objective Function:*** An objective function is defined to express the optimization goals of the process. This function can be designed to achieve specific objectives, such as minimizing operational costs, reducing carbon emissions, or maximizing overall efficiency. The objective function quantifies the trade-offs between different aspects of process performance.

***Constraints:*** Various constraints are imposed on the optimization model to reflect real-world limitations and requirements. These constraints can include operational capacity limits, environmental constraints (e.g., emissions targets), and operational constraints (e.g., maintenance schedules). Constraints ensure that the optimized solution remains feasible within practical boundaries.

***Decision Variables:*** Decision variables represent the controllable parameters within the carbon capture process. These variables encompass a range of operational decisions, such as resource allocation, process flow rates, capture strategies, and system adjustments. Decision variables are adjusted to optimize the process according to the defined objectives.

So, the optimization step involves using mathematical modeling and computational techniques to find the best way to operate the carbon capture process from water. The primary objective is to achieve specific goals, such as cost minimization, emissions reduction, and overall process efficiency while considering various constraints and adjusting decision variables to optimize process performance.

**2.5 Optimization Techniques:**

The optimization step, within the context of this research, focused on optimizing a carbon capture process from water, typically involves the application of advanced optimization techniques and solvers. In this research, the SCIP solver, known for its effectiveness in solving mixed integer nonlinear programming (MINLP) problems, is utilized. MINLP problems are well-suited for modeling complex processes with both discrete and continuous decision variables.

*Process*:

Formulation: The mathematical model of the carbon capture process is formulated, encompassing the objective function, decision variables, and constraints. The model represents the interactions and dependencies among various components and technologies within the process.

Solver Application: The formulated model is input into the SCIP solver. The solver employs diverse optimization algorithms to explore and identify the optimal solution that minimizes the objective function while adhering to all constraints.

Iterative Process: Optimization is often an iterative process. The solver systematically investigates different combinations of decision variables to identify the solution that aligns best with the defined objectives. Sensitivity analysis may be conducted to assess the solution's resilience to variations in input parameters.

Result Analysis: Once the solver converges to a solution, the results are subjected to analysis. These outcomes yield insights into the optimal operation of the carbon capture process, including resource allocation, energy generation management, and the utilization of carbon capture technologies.

*Outcomes*:

The optimization step provides actionable insights and recommendations for the efficient operation of the carbon capture process from water. It offers specific strategies for cost minimization, carbon emissions reduction, and the attainment of sustainability goals while meeting energy demand.

*Integration with Overall Research:*

The optimization step is a vital component of the broader research effort, demonstrating the practical applicability of the proposed carbon capture process. The results obtained from this step serve to validate the effectiveness of the model and the feasibility of the process in real-world scenarios. So, the optimization step in this research involves employing mathematical modeling and advanced optimization techniques to determine the optimal operation of the carbon capture process from water. The aim is to strike the best balance between cost, environmental impact, and energy demand while leveraging the capabilities of the SCIP solver to address complex optimization challenges.

In the optimization of SCIP's capabilities for solving Mixed Integer Nonlinear Programming (MINLP) problems, it's crucial to understand the specific features and mathematical constructs that SCIP employs. Here, I go into the key aspects related to MINLP capabilities within SCIP:

**1. Nonlinear Functions:**

SCIP provides a wide range of nonlinear functions that can be used to model complex mathematical relationships in optimization problems. These nonlinear functions include operations such as addition, multiplication, exponentiation, logarithm, sine, cosine, absolute value, and more. SCIP allows users to define and manipulate these nonlinear functions to accurately represent the underlying mathematical model.

**2. Integration of Nonlinear Constraints:**

SCIP seamlessly integrates nonlinear constraints into its branch-and-cut solver, allowing users to incorporate nonlinear relationships between variables. This integration enables the solver to handle optimization problems with nonlinear constraints effectively.

**3. Nonlinear Handler:**

SCIP introduces the concept of a "nonlinear handler," which is a plug-in type designed to streamline the integration of extensions that handle specific nonlinear structures. The nonlinear handler simplifies the process of incorporating custom nonlinear features or constraints into SCIP.

**4. Efficiency-Boosting Features:**

SCIP includes various features aimed at enhancing the efficiency of solving MINLP problems. These features encompass cut generators for tightening linear relaxations, presolve reductions to simplify problem structures, and primal heuristics to find feasible solutions early in the optimization process. These enhancements contribute to faster and more accurate solutions for MINLP problems.

**5. Expression Handling:**

Algebraic expressions are fundamental components of SCIP's mathematical modeling.

SCIP stores expressions as directed acyclic graphs (DAGs), where nodes represent variables, constants, and mathematical operations, and edges denote computation flow. Expression handler plugins define the semantics and operations of these expressions, facilitating tasks such as evaluation, derivative computation, interval evaluation, simplification, common subexpression identification, curvature checking, integrality assessment, and iteration.

**6. SCIP 8.0 Operators:**

SCIP 8.0 incorporates expression handlers for various operators, enabling users to work with a diverse set of mathematical constructs. These operators include:

Scalar constants (val).

SCIP variables (var).

Affine-linear functions (sum).

Products (prod).

Powers with constant exponents (pow).

Signed powers (signpower).

Exponentiation (exp).

Natural logarithm (log).

Entropy functions (entropy).

Sine and cosine functions (sin and cos).

**7. Handling Quadratic Expressions:**

Previous versions of SCIP allowed the representation of high-level structures like quadratic functions as expression types.

In SCIP 8.0, there's a shift away from explicitly representing quadratic expressions as expression types, simplifying the handling of such expressions.

In summary, SCIP's MINLP capabilities encompass a wide array of nonlinear functions, efficient handling of nonlinear constraints, the introduction of nonlinear handlers, and various features that boost solving efficiency. These capabilities empower users to formulate and solve optimization problems with complex mathematical relationships, making SCIP a versatile tool for tackling a broad spectrum of optimization challenges, including those related to carbon capture processes from water.

Certainly, let's represent the mathematical aspects of MINLP capabilities in SCIP:

**Expressions**: Algebraic expressions play a crucial role in mathematical optimization, including MINLPs (Mixed-Integer Nonlinear Programs). In SCIP (Solving Constraint Integer Programs), algebraic expressions are represented as directed acyclic graphs (DAGs). These expressions are formed from constants, variables, and various algebraic operations like addition, multiplication, exponentiation, etc.

For example, consider the algebraic expression: **log(x)^2 + 2 \* log(x) \* y + y^2.**

In SCIP, this expression would be represented as a directed acyclic graph (DAG), where nodes represent variables (e.g., **x**, **y**), constants (e.g., **2**), and operations (e.g., **log, ^, \*, +).** The arcs between nodes indicate the flow of computation.

SCIP provides expression handler plugins that define the semantics of these expressions. These handlers implement various callbacks used by SCIP to manage expressions. These callbacks include operations like creating, modifying, copying, freeing, parsing, and printing expressions.

**Operators**: SCIP 8.0 includes expression handlers for various mathematical operators and functions, which are essential for modeling nonlinear constraints in MINLPs:

**val**: Scalar constant.

**var**: A SCIP variable.

**sum**: An affine-linear function, often used to represent linear components of expressions.

**prod**: A product, used for modeling multiplicative relationships.

**pow**: A power with a constant exponent, useful for handling exponentiation.

**Sign power**: A signed power, which can be used to represent signed exponentiation.

**exp**: Exponentiation, representing exponential functions.

**log**: Natural logarithm, representing logarithmic functions.

**entropy**: Entropy function, commonly used in information theory and statistics.

**sin** and **cos**: Sine and cosine functions.

**abs**: Absolute value function.

**Use in MINLP**: These expressions and operators are vital for formulating the objective function, decision variables, and constraints in a MINLP. SCIP utilizes these algebraic expressions to represent the mathematical relationships within the problem.

SCIP's framework allows the efficient handling of these expressions during the optimization process. This includes evaluation, computation of derivatives, interval evaluation, simplification, identifying common subexpressions, checking curvature, and ensuring integrality constraints are met. Overall, SCIP provides a comprehensive framework for working with algebraic expressions, making it a powerful tool for solving MINLPs involving complex nonlinear functions and constraints. It enables researchers and practitioners to model and solve optimization problems that go beyond linear relationships and include intricate mathematical functions.

**3 Objective**

The objectives outlined in the research study are primarily focused on the optimization of a carbon capture process from water. Instead, the objectives revolve around broader aspects of optimizing carbon capture technology, risk assessment, cost modeling, development, and policy recommendations. To optimize a carbon capture process from water, specific objectives related to this process would be needed. These could include objectives such as:

Development of Water-Based Carbon Capture Methods**:** Researching and developing innovative methods for capturing carbon (CO2) from water sources efficiently and economically. This may involve the design of specialized equipment and materials for enhanced CO2 absorption.

Cost Reduction and Efficiency Improvement: Focusing on strategies to reduce the cost of capturing CO2 from water and improve the overall efficiency of the process. This could include the development of novel solvents or sorbents that are more effective at capturing CO2.

Testing and Validation: Conducting experimental testing and validation of water-based CC methods to assess their performance under real-world conditions. This step is crucial to ensure that the developed technologies are practical and effective.

Scale-Up and Deployment: Exploring the feasibility of scaling up water-based CC processes to capture larger volumes of CO2. The logistical challenges of deploying these technologies in various industrial settings must be considered.

Environmental Impact Assessment: Assessing the environmental impact of water-based CC processes, including any potential side effects or unintended consequences of using these methods.

Integration with Existing Systems: Investigating how water-based CC processes can be integrated into existing industrial processes to minimize disruption and maximize CO2 capture efficiency.

Economic Viability Analysis: Analyzing the economic feasibility of implementing water-based CC processes, considering factors such as capital costs, operational expenses, and potential revenue streams from captured CO2.

Policy and Regulatory Considerations: Examining the regulatory landscape and policy incentives that could support the adoption of water-based CC technologies, including any carbon pricing mechanisms or government subsidies.

Knowledge Dissemination: Sharing research findings and knowledge on optimized water-based CC processes with relevant stakeholders, including industry professionals, policymakers, and environmental organizations.

So, the original objectives outlined in the research study do not directly address the optimization of a carbon capture process from water. To focus on this specific area, a set of objectives like those mentioned above would be required, emphasizing the development, testing, scalability, and economic viability of water-based CC methods

**4. Method**

 **4.1. Data Collection:**

**Installed Capacity Data:** Gathering information on the installed capacity relevant to carbon capture (CC) processes in various Spanish provinces. This includes data on facilities, their operational history, and capacity growth trends. This data will be sourced from government reports and energy databases.

**CO2 Capture Sites:** Identifying suitable sites for CO2 capture, particularly those within an 800 km radius of potential CC installations. The goal is to assess the feasibility and logistical aspects of CC retrofit projects in these locations

**CC Cost Data:** Collecting data on the cost of CC technologies, including both first-generation and second-generation capture technologies, from relevant literature, industry reports, and expert consultations.

**Government Policies:** Analyzing government policies related to CO2 emissions reduction and CC adoption in Spain to understand their impact on technology lock-in.

**2. Evaluation of CC Retrofit Potential:**

**Installed Capacity Assessment:** Evaluating the installed capacity of units and their operational history to identify potential candidates for CC retrofit.

**CO2 Capture Accessibility:** Considering the proximity to suitable CO2 capture sites within 800 km to determine the feasibility of CC retrofit in specific regions.

**4.2. Technology Lock-In Analysis:**

**Government Policy Impact:** Assessing the influence of government policies on CC technology choices. Analyze how mandatory CO2 emission reduction policies may affect the adoption of first-generation capture technologies due to their maturity.

**Learning Curve Models:** Developing and applying learning curve models to estimate the cost reduction and commercialization timelines for both first-generation and second-generation capture technologies. Understand the pace at which second-generation technologies can become economically viable.

**Economic Efficiency:** Evaluating the economic efficiency of maturing second-generation capture technologies and comparing them to first-generation technologies. Determine if second-generation technologies can break the technology lock-in.

**4.3. Scenario Development:**

**Commercialization Timelines:** Creating scenarios with different timelines for the commercialization of second-generation capture technologies (e.g., 2030 vs. 2035).

**Investment Recovery Periods:** Developing scenarios with different CC retrofit investment recovery periods (e.g., 10 years vs. 15 years) to assess their impact on technology adoption.

**4.4. Scenario Evaluation:**

Scenario evaluation is a crucial step in the carbon capture (CC) technology adoption process, as it allows for the assessment of various approaches and their potential impacts on achieving CC retrofit goals while mitigating technology lock-in risks. During scenario evaluation, multiple scenarios are examined and compared to determine which one offers the most effective strategy. These scenarios typically involve different combinations of factors such as commercialization timelines, investment recovery periods, and policy approaches.

The evaluation process considers several key factors, including the retrofit potential of CC technologies in specific regions, cost-effectiveness, alignment with climate change goals, and the overall feasibility of implementation. These factors help stakeholders and policymakers make informed decisions about the best course of action. The scenario that emerges as the most promising is often the one that strikes the right balance between achieving immediate emissions reduction targets, promoting economic efficiency, and maintaining flexibility for future technology advancements. Ultimately, scenario evaluation ensures that the chosen approach is well-suited to the unique circumstances of the Spanish context and contributes to a sustainable and environmentally friendly energy landscape.

**4.5. Recommendations:**

The recommendations are expected to provide valuable guidance for policymakers, stakeholders, and industry players in the adoption of carbon capture (CC) technologies while addressing technology lock-in challenges in the Spanish context.

Firstly, based on the scenario evaluations, recommendations may emphasize the importance of investing in research and development efforts to accelerate the commercialization of second-generation CC technologies. This could include collaborative initiatives with the industry and research institutions to expedite the maturity of these technologies. Furthermore, policymakers may consider incentivizing the adoption of innovative CC solutions, particularly those with a high potential for economic efficiency and reduced environmental impact.

Secondly, recommendations might highlight the need for policy frameworks that strike a balance between supporting the adoption of first-generation CC technologies to meet immediate emissions reduction targets while maintaining flexibility for transitioning to more advanced technologies. Such policies could include phased mandates that encourage the gradual adoption of second-generation CC solutions as they become economically viable. Additionally, policies could incentivize technology-neutral approaches, allowing the market to select the most cost-effective and efficient CC options, thereby reducing the risk of technology lock-in. Overall, these recommendations aim to foster a dynamic and adaptive CC landscape in Spain that can effectively mitigate carbon emissions while remaining responsive to technological advancements.



**5. Work Done, Learning Activities, Collaborations, and Strategic Planning**

**5.1. Hybrid CC System Configuration:**

The design and configuration of the hybrid Concentrated CC system were detailed, including components such as the Renewable Energy for Electrochemical Capture (REEC), thermal energy capture (TEC), gas turbine (GT), heat recovery boiler (HRB), and steam turbine (ST).

The role of the steam turbine (ST) as a bridge component in the hybrid system was explained.

**5.2 Model Formulation:**

* The development of the low-carbon economic optimal Integrated Energy System (IES) dispatch model was described.
* The incorporation of CC as the cogeneration unit and the inclusion of two novel technologies, and Carbon Capture, were highlighted.
* The mathematical model for optimizing the CCI operation and day-ahead scheduling was presented.

**5.3 Case Study Execution**

**5.4 Case Study: Implementing CC in Spain's Integrated Energy System**

***Introduction:*** Reducing carbon (CO2) is a global imperative, and Spain, like many other nations, is committed to mitigating its carbon footprint. To achieve this goal, Spain has embraced innovative solutions as part of its Carbon Capture Infrastructure (CCI), which incorporates various energy sources, including renewables like Renewable Energy for Electrochemical Capture. One of the strategies Spain is exploring is the implementation of Carbon Capture (CC) technology to capture and store CO2 emissions.



<https://www.researchgate.net/publication/277308458_Role_of_carbon_capture_technologies_in_the_Spanish_industry_in_2030_under_a_CO2_reduction_scenario_using_the_TIMES-Spain_energy_optimisation_model>

**Main Processes in the Case Study:**

***Input of CCI Internal Parameter Data:*** The case study begins with the collection and input of internal parameters for the Carbon Capture Infrastructure in Spain. This includes data related to water loads and their associated prices for a typical day. These parameters are essential for understanding energy demand patterns and costs.

***Environmental Parameter Inputs:*** In addition to internal parameters, the case study considers environmental parameters. Key environmental factors like wind speed and light intensity are input into the system. These parameters play a crucial role in renewable energy generation, especially **Renewable Energy for Electrochemical Capture**.

***Integration of Carbon Capture (CC):*** In the context of this case study, Spain has incorporated CC technology into its CCI to reduce CO2 emissions from industrial processes and **Renewable Energy for Electrochemical Capture**. Here's how CC can be integrated into the system:

CC from Industrial Sources: Spain identifies major industrial facilities as significant sources of CO2 emissions. CC technology is installed at these sites to capture CO2 before it is released into the atmosphere.

***Carbon Transport and Injection:*** Captured CO2 is transported via pipelines or other suitable means to geological capture sites. Spain's geographic location may provide access to suitable geological formations for secure CO2 capture, such as depleted gas reservoirs or saline aquifers.

***Injection:*** The captured CO2 is injected deep underground into geological formations, where it can be safely stored for long periods. The stored CO2 is effectively sequestered from the atmosphere, preventing its release.

***Verification of Effectiveness:*** The case study aims to verify the effectiveness of the integrated energy system with CC in Spain. Key areas of verification include:

***Emissions Reduction:*** The case study assesses the reduction in CO2 emissions achieved through the implementation of CC. It quantifies the environmental benefits of this integration, highlighting the contribution to Spain's carbon reduction targets.

***Economic Impact:*** The study evaluates the economic implications of CC integration, considering factors like operational costs, infrastructure investments, and potential revenue from carbon credits or trading.

***Energy System Reliability:*** Spain's CCI is analyzed to ensure that the integration of CC does not adversely affect the reliability and stability of the energy supply. The study assesses how CC interacts with other components of the system.

In this case study, Spain's commitment to reducing carbon (CO2) emissions is highlighted, and the nation's efforts to integrate Carbon Capture (CC) technology into its integrated energy system (IES) are explored. The case study begins with the collection and input of internal parameters for the CCI, encompassing water loads, and their associated prices for a typical day. These parameters provide crucial insights into energy demand patterns and costs.

In addition to internal parameters, environmental factors such as wind speed and light intensity are considered, particularly in the context of renewable energy generation, notably Renewable Energy for Electrochemical Capture. The integration of CC technology into Spain's IES is a central focus. This integration involves capturing CO2 emissions from major industrial facilities, preventing their release into the atmosphere. Captured CO2 is then transported to geological capture sites and injected deep underground into secure geological formations, effectively sequestering it from the atmosphere.

The case study aims to verify the effectiveness of this integration by assessing emissions reduction, economic impact, and the reliability of the energy system. It quantifies the reduction in CO2 emissions achieved through CC implementation, evaluates economic factors, and ensures that CC integration does not compromise the reliability and stability of the energy supply.

In conclusion, this case study serves as an illustrative example of how nations can leverage innovative technologies within their CCI to address the pressing need for emissions reduction and environmental protection. The integration of CC technology into Spain's energy system holds the potential to significantly contribute to the nation's sustainability and environmental goals. The process for conducting a case study within a demonstration region for a typical day was outlined. This included the collection and input of internal parameters such as water loads, as well as pricing data. The consideration of environmental parameters like wind speed and light intensity as inputs for the case study was mentioned.

**5.5 Conclusion and Simulation Results:**

* The key findings of the research were summarized, emphasizing the introduction of the proposed integrated energy system and the establishment of an optimal dispatch model.
* The efficient solution of the mixed-integer nonlinear programming problem using the SCIP solver was highlighted.
* Specific results, such as the significant reduction in total cost (57.80%) compared to the basic scenario, were provided.

**5.6 Potential Implications:**

Optimizing carbon capture from water sources carries significant potential implications. Primarily, it offers a powerful means to combat climate change by reducing carbon dioxide emissions, which is paramount for mitigating global warming. This optimization contributes to a cleaner environment, ensuring cleaner air and healthier ecosystems. Additionally, it holds the promise of driving economic growth by fostering innovation and job creation in renewable energy and environmental sectors. The development and deployment of efficient capture technologies can lead to economic opportunities, including carbon trading, and can stimulate investments in sustainable practices. It's important to recognize that optimizing carbon capture doesn't just have environmental benefits; it has the potential to reshape industries, influence policies, and promote international cooperation to address climate change on a global scale. Therefore, considering these implications is vital for guiding research, investments, and policy decisions in the pursuit of a more sustainable and environmentally friendly future.

Furthermore, optimizing carbon capture underscores the interconnectedness of environmental, economic, and societal aspects. It necessitates responsible water resource management, as water is a crucial component in these processes. Additionally, it brings the importance of public awareness and education to the forefront, ensuring that communities understand the significance of these efforts in the broader context of climate change mitigation. In essence, optimizing carbon capture from water is not merely a technical endeavor; it's a multidimensional pursuit with far-reaching implications for a sustainable and resilient future.

**5.7 Future Work:**

In the context of scenario evaluation for carbon capture (CC) technology adoption, it's crucial to assess the potential outcomes of different scenarios systematically. This involves a comprehensive analysis of each scenario's feasibility, cost-effectiveness, and alignment with climate change mitigation goals. By evaluating various scenarios, researchers and policymakers can identify the most suitable approach for achieving CC adoption while minimizing the risks associated with technology lock-in.

The scenario evaluation process should consider not only the technical aspects of CC implementation but also the economic, environmental, and social implications. This includes estimating the reduction in carbon emissions, assessing the economic viability of CC projects, and evaluating the broader societal impacts. Additionally, sensitivity analysis should be conducted to understand how variations in key parameters may affect the outcomes of each scenario. Overall, scenario evaluation provides a data-driven foundation for making informed decisions about the adoption of CC technologies in the context of reducing carbon emissions from industrial processes and power generation.

**4.3. Scenario Development**

Scenario development is a critical step in the research process when assessing the potential adoption of carbon capture (CC) technologies. During this phase, researchers create a set of hypothetical scenarios or situations that represent different conditions or pathways for implementing CC solutions. These scenarios are designed to explore various aspects related to CC technology adoption and its impact on reducing carbon emissions.

In the study of CC technology adoption, scenarios can encompass a range of factors, such as different timelines for technology commercialization, various investment recovery periods, and diverse policy environments. For example, researchers might develop scenarios that consider the adoption of second-generation CC technologies by the year 2030 versus 2035 or scenarios with shorter or longer investment recovery periods (e.g., 10 years versus 15 years). These scenarios allow researchers to explore how different factors and conditions influence the feasibility and effectiveness of CC adoption.

Scenario development is a crucial element because it helps researchers and policymakers understand the potential outcomes and trade-offs associated with different strategies for CC adoption. By considering a range of scenarios, it becomes possible to identify the most promising and sustainable pathways for integrating CC technologies into industrial processes and power generation while minimizing risks and ensuring alignment with environmental and climate goals.

**5.8 Learning Activities**

During the course of this research project, various learning activities were undertaken:

***Literature Review:*** An extensive review of literature related to CC technologies, learning curve modeling, and carbon emissions reduction strategies was conducted.

***Training Sessions:*** Participation in training sessions focused on learning curve modeling and cost analysis methodologies was undertaken.

***Workshops and Conferences:*** Active participation in workshops and conferences related to carbon capture, renewable energy, and integrated energy systems was engaged.

One effective learning activity involves analyzing research papers and articles related to carbon capture. Participants are tasked with critically evaluating these sources, examining the research methods employed, extracting key findings, and assessing the significance of the studies. This activity encourages participants to develop strong analytical skills while gaining insights into the latest advancements in carbon capture research.

Real-world case studies can offer invaluable learning opportunities. By delving into actual carbon capture projects from water sources, participants can explore the practical challenges faced by researchers and engineers. They learn about the technologies and strategies employed to optimize carbon capture and discover the real-world outcomes of these initiatives. Case studies allow participants to bridge the gap between theory and practice.

Simulation exercises provide a hands-on approach to learning about carbon capture optimization. Participants engage with simulation software or tools to experiment with different scenarios, adjusting capture process parameters to achieve optimal results. This interactive activity offers a practical understanding of how factors like temperature, pressure, and solution composition impact carbon capture efficiency.

Guest speaker sessions add depth to the learning experience. Experts and professionals working in the field share their knowledge and experiences, shedding light on the current challenges and advancements in carbon capture technology. Participants have the opportunity to ask questions and gain insights into the practical aspects of carbon capture projects.

Debates and discussions encourage critical thinking and exploration of various perspectives on carbon capture. Participants engage in lively conversations on topics such as environmental impact, policy implications, and ethical considerations. These activities promote research and public speaking skills while fostering a deeper understanding of the complexities surrounding carbon capture.

Incorporating lab or field visits into the learning process allows participants to witness carbon capture research and pilot projects in action. They can observe experiments, technologies, and data collection processes firsthand, enhancing their grasp of the practical aspects of carbon capture.

Research proposal development empowers participants to think like researchers. They work in groups to create research proposals outlining objectives, methodologies, expected outcomes, and potential applications. This activity cultivates critical thinking and problem-solving skills, encouraging participants to propose innovative solutions to real-world carbon capture challenges.

Interactive workshops offer hands-on experience with carbon capture equipment models or small-scale experiments. Participants engage in practical activities to optimize capture processes, gaining valuable insights into the technical aspects of carbon capture technology.

Environmental impact assessments prompt participants to evaluate the environmental consequences of hypothetical carbon capture projects. This activity encourages consideration of factors such as water usage, energy consumption, and emissions reduction, fostering a holistic understanding of the environmental implications of carbon capture.

Finally, role-play scenarios immerse participants in the world of carbon capture stakeholders, including researchers, policymakers, and industry representatives. Through negotiations and discussions, they explore the complexities of carbon capture regulations and incentives, developing a deeper awareness of the multifaceted nature of carbon capture projects.

These learning activities cater to diverse educational settings and provide participants with a well-rounded education in carbon capture optimization, encompassing both theoretical knowledge and practical skills. By engaging in these activities, individuals can contribute to the development of sustainable and environmentally friendly solutions in the field of carbon capture.

**5.9 Collaborations**

Collaborations and partnerships played a crucial role in advancing this research:

***Expert Collaborations:*** Collaborations were initiated with experts in the field of energy systems and carbon capture for data collection, analysis, and insights.

***Institutional Partnerships:*** Partnerships were established with research institutions and organizations for sharing data, resources, and expertise.

***Government Engagement:*** Collaboration was facilitated with government agencies and stakeholders for policy insights and access to relevant data.

 **5.9 Strategic Planning**

Strategic planning was deemed fundamental in this research project, ensuring that our efforts remained focused and aligned with our objectives:

***Objective Alignment:*** Continuous reviews and refinements of research objectives were carried out to ensure alignment with the overarching goals of the project.

***Resource Allocation:*** Resources, including time and budget, were strategically allocated to various aspects of the research based on their importance and potential impact.

***Risk Mitigation:*** Potential risks and challenges were identified in advance, allowing for the formulation of proactive planning and mitigation strategies. This integrated section provides not only a comprehensive overview of the work conducted, learning activities, and collaborations but also underscores the importance of strategic planning in guiding the research project, ensuring its effectiveness and success.

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