IN-DEPTH REPORT ON QAI-HEX (QUANTUM AND AI FOR HYDROGEN EFFICIENCY)

NAME: TEAM QAI-HEX (BY: JESSICA OMUNA ANABOR)

WOMANIUM GLOBAL QUANTUM + AI PROJECT

BACKGROUND

The production of blue hydrogen entails extracting hydrogen from natural gas via a method known as steam methane reforming (SMR). During this method, natural gas, primarily composed of methane, interacts with steam at elevated temperatures, resulting in the formation of hydrogen and carbon dioxide. To classify this process as "blue," the generated carbon dioxide is captured and stored through carbon capture and storage (CCS), preventing its release into the atmosphere.

In the context of SMR and CCS, a variety of solvents are used to improve the effectiveness of CO_2 capture. Frequently used solvents consist of amine-based solutions like Monoethanolamine (MEA). These solvents engage with CO_2 to create stable compounds, which are subsequently isolated and stored.

The CO_2 chemical absorption process consists of two distinct stages: absorption and stripping. During absorption, a chemical reaction occurs between the gas's CO_2 and the absorbing medium, which is a mono-ethanol amine solvent (MEA). Specifically, the CO_2 from the gas will dissolve in the solvent, resulting in a CO_2-rich solvent and a CO_2-depleted gas. Stripping, or solvent regeneration, then removes the CO_2 from the CO_2-rich solvent to produce a lean solvent for reuse in the absorption step and captured CO_2

Absorption: The process of absorption involves bringing a gas into contact with a solvent that contains MEA (R_1-NH_2) while circulating in a counter-current manner. Due to the viscous nature and ammonia-like odor of pure MEA, it is necessary to dilute it to a 30% weight concentration with water. The CO_2 present in the gas dissolves in the solvent, existing as carbonate anions (CO_3^{2-}), bicarbonate anions (HCO_3^-), dissolved carbon dioxide, or carbonic acid (H_2CO_3), following these equilibria:

CO_2 (dissolved) + $H_2O \leftrightharpoons H_2CO_3$

$H_2CO_3 + H_2O \leftrightharpoons HCO_3^- + H_3O^+$

$HCO_3^- + H_2O \leftrightharpoons CO_3^{2-} + H_3O^+$

The amine undergoes reaction with the weak acid (HCO_3^-) to have a carbamate anion produced:

$R_1\text{-}NH_2 + HCO_3^- \leftrightharpoons R_1\text{-}NHCOO^- + H_2O$

Typically, a packed column is used as the absorber, as this column contactor technology maximizes the surface area for interaction between the liquid and gas phases. The operation occurs at low temperatures, below 50°C, and at atmospheric pressure. The gas exiting the top of the absorber has a reduced CO_2 concentration, while the CO_2-rich solvent is pumped from the bottom and preheated from 50 to 100°C before entering the stripping column.

Stripping (Solvent Regeneration): Involves reversing the reactions and requires significant energy input. Increasing the temperature shifts the equilibrium of carbon species in the solution towards dissolved CO_2 and decreases CO_2 solubility, promoting its release into the gas phase.

Generally, steam is utilized to heat the liquid phase and facilitate the extraction of dissolved CO2 by lowering the partial pressure of CO2 in the gas phase.

PROBLEM - GENERAL

Challenges with Solvent in Blue Hydrogen Production:

Cyclic Capacity: The solvent's capacity to absorb CO_2 diminishes over time due to factors such as chemical degradation, contamination, or a decline in effectiveness. Cyclic capacity indicates the solvent's performance across multiple absorption and regeneration cycles. Enhancements in cyclic capacity are essential for maintaining effective CO_2 capture over longer durations.

Solvent Loss: Loss of solvent can happen through evaporation, degradation, or leaks. This not only hampers the efficiency of the CO_2 capture process but also raises operational expenses due to the necessity for solvent replacement and the disposal of degraded solvent.

PROBLEM - SPECIFIC

To be in the general range, 75 to 90% of the CO2 in the incoming gas stream is successfully captured. To enhance the recovery rate, modifications to the column size and energy usage would be necessary, which could result in significantly higher expenses. Let’s elaborate why that is:

1. Column Size: Enlarging the absorption and stripping columns is essential for boosting CO2 recovery rates. While bigger columns can enhance CO2 capture, the downside is the rise in capital and operational expenses.

2. Energy Usage: Achieving higher recovery rates demands additional energy for tasks such as solvent regeneration or CO2 desorption. This uptick in operational costs can hamper the overall efficiency of the process.

It is essential to optimize CO2 capture and manage costs in blue hydrogen production. Increasing CO2 recovery rates without overspending on column size and energy usage is a significant challenge. Enhancing the cyclic capacity of the solvent and minimizing solvent loss are effective approaches. The integration of advanced technologies such as the Variational Quantum Eigensolver (VQE) and AI (in this case, predictive modeling) can boost these strategies, whilst reducing long term costs

SOLUTION

1. Improving the Cyclic Capacity of the Solvent

Significance of Cyclic Capacity:

Boosted Efficiency: A solvent with elevated cyclic capacity can effectively absorb and release CO_2 across numerous cycles without substantial degradation. This leads to improved solvent utilization, resulting in higher CO_2 recovery rates while minimizing the need for frequent solvent changes or additional processing steps.

Cost Savings: A high cyclic capacity decreases the necessity for solvent replacements, which in turn reduces the expenses associated with acquiring fresh solvent and lessens maintenance downtime. This approach aids in more efficient management of operational costs.

The Role of VQE and AI:

VQE in Molecular Modeling:

- **Comprehending Interactions:** The Variational Quantum Eigensolver (VQE) is a quantum computing method utilized to model intricate molecular interactions. By employing VQE, researchers can obtain valuable insights into the interactions between CO_2 and Monoethanolamine (MEA), a widely used solvent in CO_2 capture.

- **Enhancing Solvent Performance:** VQE can assist in identifying the most effective molecular structures and interactions that improve the cyclic capacity of MEA. By accurately simulating these interactions, VQE plays a crucial role in developing solvents with superior performance traits, such as increased CO_2 absorption capacity and enhanced stability over multiple cycles.

AI for Data Analysis and Enhancement:

- **Predictive Analysis:** AI can evaluate data produced from VQE simulations and experimental findings to forecast how variations in solvent composition or processing conditions influence cyclic capacity.

- **Optimization Suggestions:** AI can propose adjustments to the solvent formulation or processing parameters that optimize cyclic capacity. For instance, AI can recommend ideal concentrations of additives or processing conditions that bolster solvent stability and overall performance.

2. Reducing Solvent Loss

Significance of Reducing Solvent Loss:

Cost Efficiency: Reducing solvent loss decreases the requirement for additional solvents, thereby cutting down expenses related to solvent replenishment and disposal. This is vital for ensuring the economic viability of large-scale CO2 capture initiatives.

Environmental Considerations: Lower solvent loss contributes to less environmental pollution and supports sustainability objectives.

Role of VQE and AI:

VQE in Molecular Dynamics:

- **Analyzing Loss Mechanisms:** VQE can assist in modeling the molecular dynamics of solvent interactions, revealing potential routes for solvent loss. By comprehending these mechanisms, researchers can formulate solvents that are less prone to loss or degradation.

- **Material Enhancements**: Findings from VQE can facilitate the creation of solvents with characteristics that reduce loss, such as decreased volatility or improved resistance to degradation.

AI for Oversight and Management:

- **Instantaneous Analysis:** AI can be used to track solvent consumption and loss in real-time, processing data from sensors and operational controls to detect trends and origins of solvent loss.

- **Predictive Maintenance:** AI systems can forecast when and where solvent loss may happen, enabling preemptive actions to address it. For instance, AI can recommend modifications to operational parameters or maintenance timelines to minimize loss.

STEP BY STEP PROCESS - INTEGRATION OF QUANTUM AND AI

1. Identify the Challenge

For instance: We will refine a method that employs amine-based solvents to extract CO_2 from industrial emissions. Our aim is to enhance CO_2 capture efficiency and cyclic capacity while reducing both solvent consumption and expenses.

Essential Elements: Amine solvent (such as Monoethanolamine, MEA), CO_2.

Goals: Boost CO_2 capture efficiency, minimize solvent degradation, and improve CO_2 recovery during the stripping process, all the while reducing capital and operational expense in the long run

2. Select the Quantum Simulation Method

For instance: We can opt for the Variational Quantum Eigensolver (VQE) to simulate the interactions between CO_2 and MEA. Alongside quantum simulation, incorporate AI techniques, such as predictive modeling to evaluate the data and propose enhancements in solvent cyclic capacity and reduction of solvent loss.

3. Develop the Quantum Simulation Framework

For instance:

Molecular Representation: Transform CO_2 and MEA molecules into a quantum mechanical framework.

Basis Set Choice: Select a basis set such as 6-31G**.**

Predictive Modeling Integration: Employ this machine learning model to forecast potential improvements in solvent performance based on historical simulation data.

4. Execute Quantum Simulations

For instance:

Simulation Setup: Make use of Qiskit Chemistry for the quantum simulation. Execute VQE to determine the ground state energy of the CO2-MEA complex.

Predictive Modeling Optimization: Interpret simulation outcomes and anticipate improvements in cyclic capacity and solvent utilization. This may involve training models on simulation data to recommend optimal conditions.

5. Analyze Outcomes

For Instance:

Evaluate Energy Levels: Assess the binding energies and stability of the CO2-MEA complex.

Predictive Modeling Insights: Leverage predictive modeling to detect trends or irregularities in the data, propose enhancements in solvent formulations or operational conditions to boost cyclic capacity and reduce solvent loss.

Data Visualization Interface: Develop a dashboard to showcase essential metrics such as binding energy, solvent capacity, and CO2 capture efficiency.

Please Note: The two remaining steps below focuses on the QAI-HEX application interface

6. Refine Process Parameters

For Instance:

Informed by AI recommendations and quantum simulation findings:

Ideal Conditions: Identify the optimal MEA concentration and settings for peak CO2 absorption and minimized solvent loss.

Parameter Input Tool: Enable users to enter various parameters (such as temperature, pressure, and solvent concentration) into a simulation tool to explore different scenarios.

Iterate as Necessary: Adjust the parameters based on AI guidance and further simulations to enhance performance.

7. Merge with Classical Methods

For Instance:

Integrated Approaches: Fuse quantum simulation and AI findings with classical optimization techniques to formulate the comprehensive process.

Reporting and Analysis: Produce in-depth reports on simulation outcomes, solvent effectiveness, and process efficiency. These reports can feature visual data from the dashboard and insights from AI models.

INTEGRATION BENEFITS

Enhanced Accuracy: VQE delivers accurate models of molecular interactions, facilitating a deeper comprehension of how to enhance solvent performance. AI further supports this by examining extensive datasets to refine solvent formulations and processing conditions.

Cost-Effectiveness: The integration of VQE and AI fosters the development of economical solutions by offering comprehensive insights into solvent behavior and streamlining processes to lower operational expenses.

Sustainability Improvements: By boosting solvent cyclic capacity and minimizing losses, these technologies play a vital role in creating a more sustainable CO2 capture process, adhering to environmental standards and decreasing the overall carbon footprint associated with blue hydrogen production.

Long-Term Savings (VQE):

Refined Molecular Structures: VQE aids in crafting more effective solvents with increased cyclic capacity and reduced solvent loss. This advancement can yield long-term savings by enhancing solvent performance and durability, thereby lowering operational costs and the frequency of solvent replacements.

Increased Efficiency: Through the optimization of solvent characteristics and capture processes, VQE can enhance overall efficiency, potentially diminishing the necessity for larger and more costly capture equipment.

Long-Term Savings (AI - Predictive Modeling):

Proactive Maintenance and Optimization: AI can forecast when and where solvent loss may occur, enabling preemptive actions that can curtail waste and operational interruptions. This foresight can result in cost savings by reducing unexpected maintenance and downtime.

Efficiency Enhancements: AI can fine-tune various elements of the CO2 capture process, such as energy consumption and solvent efficacy. This optimization can lead to more efficient operations and decreased energy use, ultimately lowering operational costs over time.

Comparative Costs:

Initial Investment vs. Long-Term Gains: Both VQE and AI require considerable initial investments in technology and development. Nevertheless, their capacity to optimize processes and enhance efficiency can result in significant long-term benefits (i.e, benefits mentioned above)

WHERE IN THE BLUE HYDROGEN PRODUCTION PROCESS WILL THESE TECHNOLOGIES BE MOST BENEFICIAL?

1. Solvent Design and Selection

Where: Prior to the absorption phase.

Reason: Employing quantum mechanical simulations, such as VQE will aid to analyze and forecast the performance of various solvents (such as MEA) regarding their efficiency in CO_2 absorption and cyclic stability. This approach leads to the identification of the most effective solvent or formulation that boosts CO_2 capture while reducing energy demands.

2. Absorption Process Optimization

Where: During the absorption phase.

Reason: Investigating the molecular interactions between CO_2 and the solvent will aid in enhancing the absorption reaction's efficiency. Quantum simulations, such as VQE can assist in fine-tuning reaction conditions and solvent concentrations to optimize CO_2 uptake.

3. Improvement of Stripping (Regeneration) Efficiency

Where: During the stripping phase.

Reason: Examining the molecular interactions and energy requirements involved in CO_2 release from the solvent can lead to the optimization of temperature and pressure conditions for regeneration, potentially lowering energy consumption and enhancing CO_2 recovery.

4. Forecasting Solvent Performance Across Multiple Cycles

Where: Following the stripping phase, before the solvent is reused in the absorption phase.

Reason: Using a combination of quantum and AI can help us anticipate how the solvent may degrade or alter over several cycles of absorption and stripping. This information can guide the creation of more durable solvents or methods to reduce degradation.

5. Integration into the Hydrogen Production Framework

Where: Throughout the entire CO_2 capture process.

Reason: Integrating findings from both quantum and AI research into the comprehensive hydrogen production framework can drastically improve efficiency and cost reduction. This includes refining the design of CO_2 capture systems, adjusting operational parameters, and enhancing the overall efficiency of the hydrogen production process by ensuring that CO_2 capture and stripping operations are optimally effective.

SUMMARY

By leveraging VQE for detailed molecular modeling and AI (predictive modeling) for data analysis and optimization can significantly enhance the effectiveness of improving cyclic capacity and reducing solvent loss in CO_2 capture processes. This approach helps in balancing the need for higher CO_2 recovery rates with the constraints of capital and operational costs, leading to more efficient and sustainable blue hydrogen production.

REFERENCES

- Benjamin, Lokku Henry & B N, Mithun & Bc, Santhrupth & P C, Chaitra. (2024). Exploring Quantum Simulation: Leveraging VQE and QAOA Algorithms for modeling of Natural Systems.

- Banerjee, Tanumoy, and Ganesh Balasubramanian. 2023. "Predictive Modeling of Molecular Mechanisms in Hydrogen Production and Storage Materials" Materials 16, no. 17: 6050. https://doi.org/10.3390/ma16176050

- DOI: 10.1039/D1SE01508G (Perspective) Sustainable Energy Fuels, 2022, 6, 66-75

- George, Jan & Müller, Viktor & Winkler, Jenny & Ragwitz, Mario. (2022). Is blue hydrogen a bridging technology? - The limits of a CO2 price and the role of state-induced price components for green hydrogen production in Germany. Energy Policy. 167. 113072. 10.1016/j.enpol.2022.113072.

- Panagiotis Alexandros Argyris, Jared Wong, Andrew Wright, Luis M.C. Pereira, Vincenzo Spallina,
Reducing the cost of low-carbon hydrogen production via emerging chemical looping process,
Energy Conversion and Management,
Volume 277,
2023,
116581,
ISSN 0196-8904,
https://doi.org/10.1016/j.enconman.2022.116581.

- Xiang Yun Debbie Soo, Johnathan Joo Cheng Lee, Wen-Ya Wu, Longgang Tao, Cun Wang, Qiang Zhu, Jie Bu,
Advancements in CO2 capture by absorption and adsorption: A comprehensive review,
Journal of CO2 Utilization,
Volume 81,
2024,
102727,
ISSN 2212-9820,
https://doi.org/10.1016/j.jcou.2024.102727