Womanium AI + Quantum
Final Project

Carbon Capture, Storage And Transportation

By Three Entangled Qubits

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Background

We all know that the Earth is heating up, and global warming is the culprit. The 10 warmest years in the historical record have all occurred in the past decade (2014-2023) [1], and there is a pressing need for action.

To give a brief description, global warming is caused by the excessive accumulation of greenhouse gasses in the Earth's atmosphere. These gasses, including carbon dioxide (CO_2) from human activities like burning fossil fuels and deforestation, trap heat and contribute to a rise in average global temperatures. This phenomenon poses significant threats to ecosystems, weather patterns, and human well-being.

When people talk about reducing climate change, they often focus on carbon dioxide (CO_2) emissions, and for good reason. CO_2 is the primary driver of climate change. It remains in the atmosphere for hundreds of years, meaning that once in the atmosphere, it can continue to affect the climate over a long timeframe [2]. But a lot of damage has already been done, and a lot of damage is being done today. All of the damage done is still in the air.

Hence, we arrived at the problem statement.

The Problem: Improving the process of carbon reduction, from capture to storage.

The problem we have chosen can be divided into three parts:

1. Carbon capture

The problem here is simulating large complex molecules for carbon capture, which is a significant challenge in the fight against climate change. Simulating these molecules is crucial for discovering new catalysts that are more efficient and cost-effective for carbon capture than current models.

To date, scientists have not found a viable method to simulate large complex molecules using conventional computers. The problem grows exponentially with the size and complexity of the molecules being simulated. This exponential growth makes it impractical to simulate large complex molecules using current computing capabilities. According to The World Economic Forum, “This exponential scaling quickly renders a traditional computer useless: simulating a molecule with just 70 atoms would take longer than the lifetime of the universe (13 billion years).” [3].

2. Transporting the captured carbon

The transportation of captured carbon involves logistical challenges, including selecting the appropriate mode of transport (pipelines, ships, or trucks) and ensuring safe handling and storage during transit. Factors such as quantity, source, and injection locations need to be considered.

Moreover, the costs associated with compressing, liquefying, and transporting CO_2 can be significant. These costs include infrastructure development, maintenance, and compliance with safety regulations. There are other risks like leaks associated with the transportation of the captured carbon.

3. Storing the transported carbon

If CO_2 leaks into the surrounding environment, it can have negative effects on ecosystems, including acidification of water bodies and harm to plant and animal life. Therefore, ensuring the long-term integrity of storage sites is crucial. Over time, there is a possibility of geological shifts or changes that could compromise the stability of the storage site and potentially lead to CO_2 leakage.

Literature review

Paper 1 [4]

The paper titled "Recent developments on carbon capture and storage: An overview" by J.C.M. Pires et al. (2011) provides a comprehensive overview of the advancements in Carbon Capture and Storage (CCS) technology. CCS is a strategy for mitigating climate change by capturing carbon dioxide (CO2) emissions from sources like power plants and storing them underground in geological formations.

The authors discuss various capture technologies, including pre-combustion, post-combustion, and oxy-fuel combustion methods. They also delve into transportation methods for captured CO2, highlighting pipelines and ships as the primary options. The paper explores potential geological storage sites like depleted oil and gas reservoirs and deep saline formations.

The summary emphasizes that CCS is a promising approach for reducing CO2 emissions, but it faces several challenges.These challenges include high costs, technical limitations, and public perception concerns. The authors conclude by highlighting the need for further research and development to make CCS a more viable and cost-effective solution for climate change mitigation.

Paper 2 [5]

The paper titled "Uncertain storage prospects create a conundrum for carbon capture and storage ambitions" by Lane et al. (2021), discusses a potential roadblock for a major climate change mitigation strategy: carbon capture and storage (CCS).

According to the paper:

- CCS aims to capture CO2 emissions from sources like power plants and store them permanently underground. It's seen as a crucial technology for achieving ambitious decarbonization goals.
- The authors argue that a key assumption about CCS – the abundance of suitable storage locations – might be overly optimistic.

- There is a challenge of accurately determining how much CO_2 can be safely injected and stored in a particular location at a sustainable rate. This uncertainty creates a "chicken and egg" problem.
- Investors in capture projects hesitate to build without confidence in sufficient storage capacity. Conversely, storage developers are cautious to invest without confirmation of capture projects going ahead.
- The authors suggest this uncertainty could particularly affect major developing Asian economies aiming to decarbonize.
- There is a need for immediate action to reduce uncertainty surrounding CO_2 storage potential. This includes better evaluation of storage sites, planning for future needs, and strategies to mitigate the risks associated with limited injection rates.
- The authors argue that while CCS holds great promise for mitigating climate change, addressing the uncertainty around storage capacity is crucial for its successful implementation, especially in developing economies.

Paper 3 [6]

Note: We chose this paper because this article is relevant not only for the logistics industry but also to any industries transporting important articles like the hazardous CO_2 which can cause asphyxiation if leaked. This article is just one of the many that show promising results when using AI for real-time route optimization.

This research paper focuses on developing an efficient route planning system for logistics vehicles using artificial intelligence. The authors recognized the limitations of traditional route planning methods which primarily consider time and distance, ignoring other crucial factors like traffic conditions.

To address this, they proposed a system that incorporates:

- Using a multilayer perceptron model to forecast traffic conditions based on historical data.
- Considering multiple delivery points simultaneously for optimal route optimization.

- Employed to calculate the shortest path considering predicted traffic conditions and vehicle speed.

By combining these elements, the system aims to minimize idle driving time, enhance transportation efficiency, and provide logistics operators with real-time vehicle tracking.

The proposed system demonstrated improved performance compared to traditional methods, indicating its potential for practical application in the logistics industry.

Current Stage in Carbon Capturing- The Criticisms

Even though the concept of decarbonization straight from the air seems promising, a lot of people are not convinced, for the right reasons. The following are the main criticisms I could find for Carbon Capture Plants in their current stage.

1. If the energy used to power the carbon capture process comes from fossil fuels, the overall environmental benefit is reduced.
2. Large-scale CCS projects require significant land for infrastructure, potentially impacting ecosystems and communities.
3. The carbon capture process can be water-intensive, raising concerns about water scarcity in certain regions [6].
4. Many argue that investing in renewable energy sources is a more direct and effective way to reduce greenhouse gas emissions.
5. The process of capturing carbon dioxide requires significant energy input, reducing the overall efficiency of the power plant or industrial process. [7]

Proposing Solutions

Here us out - Quantum Computing for problems defined for carbon capture and Artificial Intelligence for problems identified with transportation and storage!

Our solution is divided into three parts.

Part 1

Quantum computing has the potential to revolutionize the simulation of large complex molecules and significantly improve our ability to tackle climate change. Quantum computers leverage the principles of quantum mechanics to perform calculations that are exponentially faster than classical computers for certain types of problems, including simulating complex molecules .

Quantum algorithms can create multidimensional computational spaces or run calculations that mimic the behavior of molecules themselves, making them more efficient for solving complex problems like chemical simulations . Quantum computers could potentially simulate large complex molecules and accelerate the discovery of new catalysts for carbon capture, leading to more effective and sustainable solutions for mitigating climate change .

The following are the different precise ways through which we can improve the carbon capture processes using Quantum Computation:

Simulation

Quantum computers can model the behavior of molecules involved in carbon capture reactions with unprecedented accuracy. This could lead to the discovery of novel materials and catalysts with superior carbon capture properties [8].

By simulating various reaction environments, quantum computers can pinpoint the ideal conditions for maximizing carbon capture efficiency.

What can we focus on

1. Developing highly efficient catalysts for carbon capture reactions. [3]
2. Identifying optimal solvents for carbon dioxide absorption.
3. Designing advanced membranes for carbon dioxide separation.

4. Improving the overall efficiency of carbon capture plants.

Quantum Algorithms we can consider

- **Variational Quantum Eigensolver (VQE):** For calculating the energy of molecular systems and finding optimal configurations [9].
- **Quantum Phase Estimation:** For determining the properties of molecular systems and simulating chemical reactions.
- **Quantum Approximate Optimization Algorithm (QAOA):** For solving optimization problems related to carbon capture processes.

Note: We acknowledge that our knowledge about these algorithms is not really vast, so we apologize if there are any errors in the following methods. The following is what we understood by just reading about the algorithms and we don't have any substantial practical experience in implementing these.

Variational Quantum Eigensolver

VQE is a hybrid quantum-classical algorithm designed to find the ground state energy of a quantum system. In the context of molecular simulation, this translates to finding the lowest energy configuration of a molecule.

How to use it:

1. Create a parameterized quantum circuit to represent the molecular system.
2. Use a classical optimizer to find the optimal parameters for the ansatz that minimize the energy.
3. Measure the energy of the quantum system using the optimized parameters.
4. Repeat steps 2 and 3 until convergence to the ground state energy is achieved.

Quantum Phase Estimation

QPE is a quantum algorithm for estimating the eigenvalue of a unitary operator. In molecular simulation, it can be used to determine the energy levels of a molecule.

How to use it:

1. Create a quantum state representing the molecular system.

2. Apply controlled-U operations to the quantum state, where U is a unitary operator representing the molecular Hamiltonian.

3. Apply the inverse Quantum Fourier Transform to extract the phase information, which corresponds to the energy level.

Quantum Approximate Optimization Algorithm

QAOA is a variational algorithm for solving optimization problems. In the context of molecular simulation, it can be used to find optimal configurations for molecules or materials.

How to use it:

1. Represent the optimization problem as a quantum circuit.

2. Use a classical optimizer to find the optimal parameters for the quantum circuit that maximize the objective function.

3. Measure the objective function to evaluate the solution quality.

4. Repeat steps 2 and 3 until convergence to a satisfactory solution is achieved.

Part 2

There are numerous ways AI can significantly enhance the safety and efficiency of transporting captured carbon dioxide. We will only list a few of them for the sake of brevity.

- AI can analyze sensor data from transportation equipment (pipelines, ships, trucks) to predict potential failures, allowing for proactive maintenance and reducing the risk of leaks or accidents.

- It can determine the safest and most efficient routes for transporting carbon dioxide, considering factors such as weather conditions, traffic, and pipeline integrity.

- AI can analyze environmental and geographical data to identify potential hazards along transportation routes, such as seismic activity, soil instability, or proximity to populated areas.

Note: Training these models demands massive amounts of data, powerful computers (GPUs, TPUs), and ample storage. Specialized sensors might also be required but they are usually not that expensive.

1. Predictive Maintenance

- To analyze historical equipment data and predict failures. Algos like ARIMA can be used.
- To identify unusual patterns in sensor data that might indicate potential issues. Isolation Forest, or Autoencoders can be used.
- To predict the remaining useful life of equipment components. Cox proportional hazards model might be used.

2. Route Optimization

- Dijkstra's algorithm can be used to find the shortest path between origin and destination (as we saw in the third paper of the Literature review).
- For problems with overlapping subproblems, such as considering multiple factors like traffic, weather, and road conditions, we can use Dynamic Programming.

3. Hazard Identification

- To classify geographical areas based on risk factors, Random Forest, Support Vector Machines, or Gradient Boosting can be used.
- To analyze spatial patterns of hazards, techniques like Geospatial Data Mining can be used.

Part 3

For storage, AI can be used for the selection of the site, and risk monitoring (like above). The resource consumption will be as stated in Part 2 as well.

Site Selection:

- To identify suitable geological formations for storage based on various parameters (porosity, permeability, pressure, temperature, etc.). Algorithms like Random Forest, Support Vector Machines, or Gradient Boosting can be used.
- To analyze spatial distribution of geological properties and identify potential storage sites. Kriging and co-kriging techniques can be utilized.
- To optimize the location of monitoring wells for effective surveillance. Spatial optimization techniques can be used.

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