A Womanium Quantum + AI Project

QAI - HEX

Quantum + AI for Hydrogen Excellence

‹ WOMANIUM | QUANTUM ›

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Introduction

Why This Project?

- **The production of blue hydrogen entails extracting hydrogen from natural gas via a method known as steam methane reforming (SMR). 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 CO2 capture.**

QAI-HEX UNDERTAKING

Objective

To improve the recovery rate of CO_2 in the inlet gas stream in an inexpensive and more efficient manner

Problem

In order to do this, there will be the need for column dimensions, which would lead to high costs

Solution

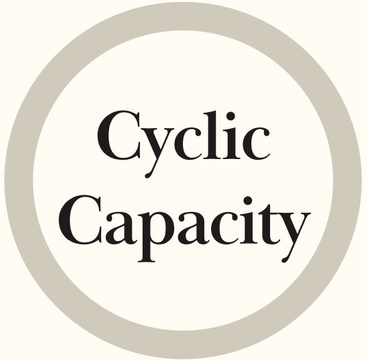
Utilise Quantum and Artificial Intelligence to improve the cyclic capacity of the solvent and to reduce solvent loss alongside reducing costs

01: OBJECTIVES

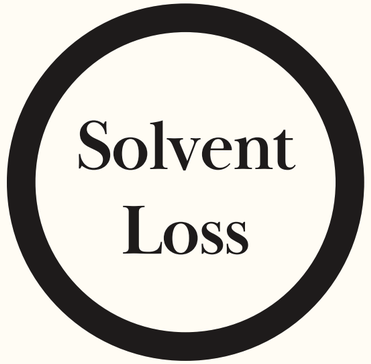
Two Stages	Absorption	Stripping
The CO2 chemical absorption process consists of two distinct stages: absorption and stripping.	Absorption: A chemical reaction occurs between the gas's CO2 and the absorbing medium, which is a mono-ethanol amine solvent (MEA)	Stripping (solvent regeneration): Removes the CO2 from the CO2-rich solvent to produce a lean solvent for reuse in the absorption step and captured CO2

02: PROBLEM - GENERAL

Challenges With Solvents in Blue Hydrogen Production



The solvent's capacity to absorb CO_2 diminishes over time due to factors such as chemical degradation, contamination, or a decline in effectiveness



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.

02: 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 dimensions and energy consumption would be necessary, which could result in significantly higher expenses.

Column Size

Enlarging the absorption and stripping columns is essential for boosting CO2 recovery rates, however, this can lead to high CAPEX & OPEX

Energy Usage

Achieving higher recovery rates demands additional energy for tasks such as solvent regeneration or CO2 desorption. This can lead to high OPEX that can affect the overall efficiency

03: Solutions

A. Improve Cyclic Capacity of Solvents

- **Variational Quantum Eigensolver (VQE): To model complex molecular interactions and identify optimal molecular structures and interactions that enhance the cyclic capacity of MEA.**

- **This enhances the performance and lifespan of solvents, therefore possibly leading to significant long-term savings, as it lowers operational expenses and decreases the need for frequent solvent replacements.**

B. Reduce Solvent Loss

- **Variational Quantum Eigensolver (VQE) & Artificial Intelligence (AI): To develop solvents with properties that minimize loss and predict when and where solvent loss is likely to occur**

- **This ability to predict can result in significant cost reductions by decreasing unforeseen maintenance and downtime. It can also enhance operational efficiency and lower energy usage, leading to reduced operational expenses in the long run.**

Step By Step Process - Solution

Select quantum simulation approach (VGE)	Integrate AI algorithm (Predictive Modelling)
Prepare the quantum simulation model	Molecular representation, Basis set selection
Perform quantum simulations	Set up the simulation (Qiskit Chemistry); Predictive modelling optimization
Optimize process parameters	Optimal conditions; Process parameters input; Iteration
Integrate with classical methods	Hybrid approaches; Reporting & analytics

FUTURE SCOPE

LIMITATIONS: The implementation of the code for the QAI-HEX, which can be seen in the notebook, was quite extensive, therefore, I was not able to run the code to its maximum potential

FUTURE PROSPECT: Most definitely, I will follow up with this project. The idea is one that can aid in the energy transition wherein the world is vying for more efficient, more integrated and more cost friendly technology implementations

THANK YOU

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