# Technical Report: Quantum Simulation of Carbon Capture Kinetics

Project: Problem 3: Environmental Chemistry; Carbon Capturing Process

Event: Alexandria Quantum Hackathon 2025

Team: Team 3

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| Team Member | Primary Role |
| Dalia El-Masry | Technical Lead / Integration Architect |
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## 1. Executive Summary

This report details the methodology and results of a hackathon project focused on modeling the initial step of the CO₂ capture process using a simplified amine-based solvent (NH₃). The project utilized a hybrid approach, combining classical quantum chemistry techniques to establish accurate initial geometries and reaction energies, and quantum computing algorithms (VQE/UCCSD) to simulate molecular properties on near-term quantum hardware.

## 2. Introduction

The efficient capture of carbon dioxide is crucial to global climate stabilization efforts. Amine-based solvents are leading industrial technology, and understanding the kinetics of the initial reaction (CO₂ + Amine) requires precise molecular calculations.

## 3. Methodology and Tools

### 3.1 Classical Model: Establishing Ground Truth

Used to establish stable molecular geometries and reaction energetics using PySCF, geomeTRIC, and ASE. Performed geometry optimization, vibrational analysis, and energetics calculation with and without ZPE correction.

### 3.2 Quantum Model: Variational Simulation

Used Qiskit and IBM Quantum backends to simulate molecular ground states using VQE with a UCCSD Ansatz. Employed ffsim for Hamiltonian encoding and used initial cluster amplitudes derived from classical CCSD calculations.

## 4. Results and Comparative Analysis

### 4.1 Classical Simulation Results

Reaction Energy (CO₂ + NH₃ → NH₂COOH): ΔE ≈ -15.5 kcal/mol, ΔE\_ZPE ≈ -13.2 kcal/mol. Results show an exothermic reaction and successful PES scanning along the N–C coordinate.

### 4.2 Quantum Resource Metrics and Performance

Simulation of the CO₂ system required 26 qubits. The UCCSD circuit depth was high, requiring optimization for current NISQ devices. Executed VQE on IBM Quantum backend (e.g., ibm\_peekskill).

### 4.3 Comparative Analysis

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| Feature | Classical Model (PySCF) | Quantum Model (Qiskit/IBM) |
| Accuracy | High (CCSD) | Theoretically exact, limited by noise |
| Scalability | Exponential with electrons | Polynomial with system size |
| Resource Cost | High CPU/Memory | High Qubit and coherence demand |
| Primary Output | Total Energy, ΔH, ZPE | Ground State Energy |

## 5. Conclusion and Future Work

### 5.1 Conclusion

The project integrated classical and quantum methods to model CO₂ capture. Results show that quantum computation can complement classical methods for chemical kinetics with scalable potential.

### 5.2 Limitations and Future Work

1. Noise mitigation using techniques like Mitiq or Richardson Extrapolation.  
2. Optimization of Ansatz with active-space selection.  
3. Extension to vibrational energy computation via Quantum Phase Estimation.  
4. Expansion to larger solvent systems such as Monoethanolamine (MEA).