

CARBON CAPTURE AND STORAGE USING AMINE ADSORPTION

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1 Overview and Background

1.1 Brief background

Questions to be answered: (1) What is carbon capture? (2) Why is it important? (3) What is Amine Adsorption? (4) What are the pros and cons? (5) Why is the Amine absorption method specifically good for carbon capture? (6) Research status of using Amine Adsorption for carbon capture.

(1) What is carbon capture? Carbon capture and storage (CCS) tackles global warming challenges by first capturing CO₂ from power generation and then storing it underground¹. (2) Why is it important? Coal is still the largest fuel source for power generation taking up to 38%. Although there is an urgent necessity to address the primary contributors to climate change, emissions from the power sector in 2019 were merely slightly lower than their record-setting peak in 2018, totaling 13.6 gigatons of carbon dioxide.² Presently, the CCS initiatives are annually sequestering close to 45 million tons of CO₂, approximately equivalent to the emissions generated by 10 million passenger cars. The capturing process is typically implemented at significant stationary CO₂ sources, such as power plants or industrial facilities involved in cement, steel, and chemical production.³ Leading companies in the energy sector like ExxonMobil have already laid out more than 1,500 miles of CO₂ pipeline owned and

¹Source from National Grid

²Source from IEA Reports.

³Source from MIT Climate Portal.

operated – the largest network in the U.S.⁴ (3) **What is amine adsorption?** Four primary technologies for CO₂ capture exist, namely chemical absorption, adsorption, membrane separation, and cryogenic distillation. Regarding chemical absorption, five major absorbent groups prevail amine-based absorbents, carbonate absorbents, hydroxide absorbents, ionic liquids (ILs), and amino acid salts. [5]

1.2 Benefits & challenges

(5) **Benefits?** Amine-based absorbents have garnered significant attention in research, primarily because of the early commercialization of monoethanolamine (MEA) for CO₂ capture in the 1970s. This early adoption popularized MEA as a promising absorbent, driving extensive studies in this domain. As of now, the primary amine system, specifically the use of monoethanolamine (MEA), remains the most widely employed CO₂ capture technology. [5] (6) **Challenges?** While primary amines present an effective CO₂ capture capability, they come with drawbacks, and the most common one is their susceptibility to degradation. Alkanol amines, including primary amines, can undergo two types of degradation: thermal degradation and oxidative degradation. [1, 5, 6] The deterioration of these materials can exacerbate additional issues, including solvent loss, fouling, heightened viscosity, and corrosion of downstream equipment. (6) **General Research Status:** In a review by Hamdy et al. [9], they reviewed the chemical reaction mechanism of amine absorption: The process begins with the initial creation of a C–N bond, resulting in the formation of carbamic acid. The amine proton of the carbamic acid is then transferred to a free base, such as a second amine or water, leading to the generation of the carbamate salt. In the work of computational modeling with molecular simulations by Bahamon et al. [2], they compared different solvents for absorbing CO₂. Their results show that non-aqueous amine solvents exhibit a 5–10% reduction in cyclic working capacity and a 10–30% decrease in the energy index compared to their aqueous counterparts, all while maintaining the same total amine mass concentration. They attribute the difference to the lower heat of vaporization and specific heat capacity of non-aqueous amine solvents. Danaci et al. [7] analyzed the amine absorption from the techno-economic perspective, and very interestingly, they state that reducing the cost of capital (i.e., interest rate) has a minor impact on the capture cost but it would be more beneficial to reduce steam requirements.

⁴Source from ExxonMobil Website

1.3 Chemical reactions or phase changes

Chemical reactions in Amine absorption:

- Absorption Reaction: The primary chemical reactions involve the absorption of acidic gases by the amine solution.
- Regeneration Reaction: After absorption, the rich amine solution containing absorbed gases undergoes a regeneration process to release the captured gases and regenerate the amine for reuse.

Phase changes in Amine absorption:

- Gas-Liquid Absorption: The absorption process involves the transfer of acidic gases from the gas phase into the liquid amine phase.
- Liquid-Gas Stripping: The regeneration process includes the removal of absorbed gases from the amine solution.

2 System Modeling with Molecular Dynamics

Inspired by Problem 2(E), the content covered in Prof. Zheng’s lecture, and the work by [2], we here conduct additional molecular dynamics simulation to demonstrate the CO_2 absorption system.

We used the standard 12-6 Lennard-Jones potential to model the gas mixtures for simplicity. Lennard-Jones potential is a mathematical model that describes the interaction between two neutral atoms or molecules. It combines the effect of attractive forces at long distances and repulsive forces at short distances. The equation writes:

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

where $V(r)$ is the potential energy as a function of the distance r between the interacting particles. ϵ is the depth of the potential energy well, representing the strength of the attractive forces. σ is the finite distance at which the inter-particle potential is zero, representing the size of the particles.

The first term $\left(\frac{\sigma}{r} \right)^{12}$ describes the long-range attractive forces, and the second term $\left(\frac{\sigma}{r} \right)^6$ describes the short-range repulsive forces. The combination of these terms results in a potential energy that has a minimum at a specific equilibrium distance.

In simpler terms, the Lennard-Jones potential captures the idea that particles are attracted to each other at long distances but repel each other at short distances

due to overlapping electron clouds. The parameters ϵ and σ are determined based on the specific properties of the interacting particles. Information about PBC can be accessed at Ref. [4]. Our parameters for the LJ potential implementation are obtained from Ref. [3]. The parameters for LJ potential are listed in Table 1:

	σ (LJ)	ϵ (LJ)	No. (S1)	No. (S2)	No. (S5)
H ₂	11	2.918	10	5	0
CO	50	2.9	50	29	0
CO ₂	50	3.3	40	22	200
N ₂	36	3.614	100	125	0
O ₂	51	3.297	0	19	0

Table 1: Parameters for fitting the Leonnard-Jones potential field and atomic numbers (No.) for different simulations of different states. The molecular dynamics simulations were run using the LAMMPS “**metal**” units setting. The parameters for the LJ potential are obtained via Ref. [3], where σ has the unit of Å and ϵ has the unit of K .

For simplicity and fast convergence, we used a Langevin dynamics thermostat. The Langevin thermostat maintains the temperature through a modification of Newton’s equations of motion

$$\dot{r}_i = p_i/m_i \quad \dot{p}_i = F_i - \gamma_i p_i + f_i \quad (2)$$

It is usually assumed that the strength of the noise is not affected by a time-dependent force and that it has a Gaussian probability distribution [8]⁵:

$$\sigma_i^2 = 2 m_i \gamma_i k_B T / \Delta t \quad (3)$$

Given this general formulation, we set up a simplified molecular dynamics simulation with no bond formulation (CO₂, CO are modeled as single particles), shown in Figure 1. The molecular ratio (or atomic numbers) are shown in Table 1, corresponding to our calculation in Cantera. The molecular dynamics simulations are run for 50 picoseconds. The potential energy change during the iteration of the simulation process is visualized in Figure 2. It can be deduced that the potential energy differences of the three states (S1, S2, & S5) agree with what we’ve learned in lecture — the more diverse the system is, the higher corresponding potential energy they have.

⁵We do not elaborate the parameters in details here to make the report more concise and focus on the thermodynamics calculation

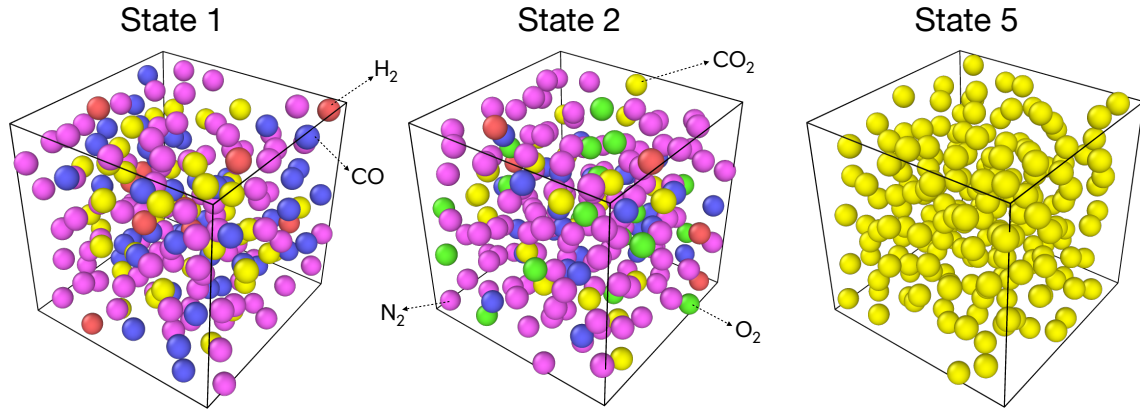


Figure 1: Molecular dynamics simulation schematic. The red particles stand for H₂. The blue particles stand for CO. The yellow particles stand for CO₂. The pink particles stand for N₂. The green particles stand for O₂.

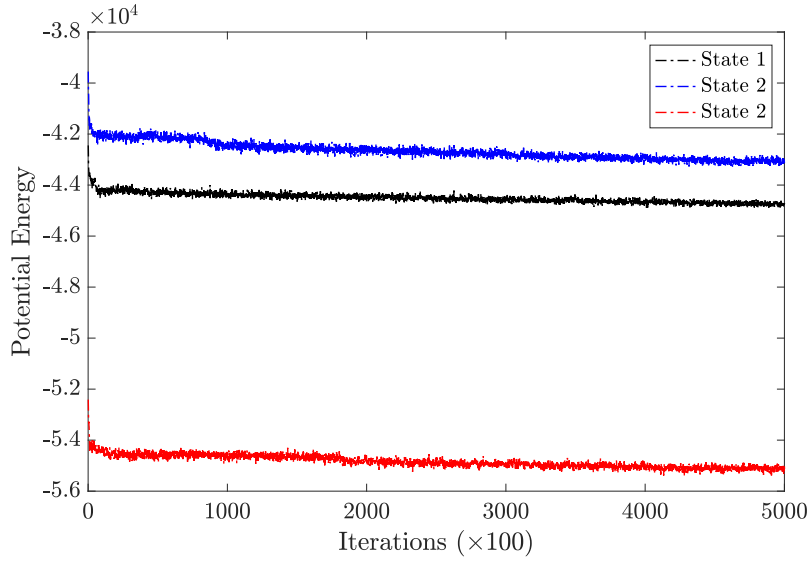


Figure 2: The potential energy evolution during the molecular dynamics simulation process for the three given states.

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