Selective CO_2 Absorption in Bioreactors based on Molecular Modelling, Thermodynamics, Kinetics and Experiments

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Abstract

Biogas, a renewable energy source composed of CO_2-CH_4 mixtures, offers an eco-friendly alternative to natural gas but requires effective CO_2 separation to enhance its heating value and reduce greenhouse gas emissions. Various techniques, including absorption, membrane, cryogenic separation, and adsorption, have been explored for CO_2-CH_4 separation. Among these, adsorption stands out for its simplicity, low cost, and operational flexibility. However, the economic viability of methods like photosynthetic bacteria systems is challenged by cultivation complexities. The study focuses on MgO-$Mg(OH)_2$ composites for their superior CO_2 adsorption capacity, despite the challenges posed by $MgCO_3$ shell formation that limits CO_2 diffusion. Inspired by the Namib Desert beetles' water-harvesting strategies, this research investigates structured combinations of MgO and $Mg(OH)_2$ to enhance CO_2 adsorption while minimizing CH_4 adsorption, due to the latter's weak interaction with $Mg(OH)_2$ surfaces. Employing both bulk thermodynamic and surface Density Functional Theory (DFT) modelling, the study initially simulates selective CO_2 absorption over CH_4, laying the groundwork for experimental validation. The experiments utilize biological (PNSB) and chemical (MgO-$Mg(OH)_2$ solutions and solid MgO powder) absorption agents in a pig farm's anaerobic fermentation bioreactor. By comparing biological and chemical methods against model predictions, the research validates the effectiveness of MgO-$Mg(OH)_2$ composites in CO_2-CH_4 separation and proposes a synergistic approach that combines the rapid CO_2 removal of MgO-$Mg(OH)_2$ solutions with the bioresource recovery capabilities of PNSB.

Early Career Scientist

NO, I am not an early career scientist.

IGAC Activities

CCMi: Chemistry Climate Model Initiative