Process simulation-based performance analysis for large-scale CO_2 sequestration via indirect carbonation of coal fly ash

K.R. Senadeera, A.M.P.D. Adikari, M. Rathnayake*
Department of Chemical and Process Engineering, University of Moratuwa, Moratuwa, Sri Lanka
*Corresponding Email: mratnayake@uom.lk

ABSTRACT - Mineral carbonation of CO_2 using coal fly ash (CFA) is identified as a promising way of mitigating carbon emissions safely and permanently with a low material cost. However, the available literature has been limited to laboratory scale studies. Thus, a process simulation-based analysis was conducted using the Aspen plus process simulation software for a large-scale CO_2 sequestration process from CFA. Carbonation performance was analyzed against variation of several process conditions while validating the developed simulations with published experimental results. Regarding multiple column arrangements for the scaled-up process, the simulation results showed that a parallel arrangement would be more effective in both CO_2 sequestration performance and economic aspects.

Keywords: Carbon capture; Coal fly ash; Mineral carbonation

INTRODUCTION

Anthropogenic emissions of CO_2 is considered as the main cause of accelerated increments in global temperature levels within the past 60 years, and thus climate change (Jaschik, Jaschik, & Warmuzinski, 2016; Ji et al., 2019; Ukwattage, Ranjith, Yellishetty, Bui, & Xu, 2015). Carbon capture and storage (CCS) is considered as the most economically viable and feasible solution regarding this issue (Ma et al., 2017). CO_2 capture methods can be categorized into chemical or physical absorption, adsorption, membrane separation, cryogenic fractionation, and mineral carbonation (Nyambura, Mugera, Felicia, & Gathura, 2011). Chemical absorption is the most matured and widely applied carbon capture method (Lillia, Bonalumi, Grande, & Manzolini, 2018), with other processes, such as alcohol-amine, amino-acid salt, Benfied, and ammonia washing. These methods have high CO_2 absorption and high selectivity, but substantial energy consumption in solvent regeneration. Physical absorption, including Rectisol, Flour, Selexol, and Purisol methods are incorporated with strong CO_2 solubilities but substantial solvent costs (Li et al., 2018). CO_2 capture cost accounts for nearly 2/3 of total CCS cost (Li et al., 2018). The expensiveness of the mainstream amine absorption process has resulted in applying only for selling CO_2 as a product to applications, such as enhanced oil recovery and urea manufacturing (Dindi, Quang, Vega, Nashef, & Abu-Zahra, 2019). The demand in those fields is much less than the capture requirements to meet the climate targets (Dindi et al., 2019). Thus, finding cheaper methods of CO_2 capture and storage has become a pinnacle of interest in the field of carbon capture research.

Mineral carbonation (MC) of CO_2 is an emerging post-combustion carbon capture method to rival the conventional techniques (Tamilselvi Dananjayan, Kandasamy, & Andimuthu, 2016), which is the transformation of CO_2 into calcium, magnesium and other forms of stable carbonates (Ukwattage et al., 2015). Using industrial solid waste or by-products containing CaO and MgO for MC has been identified to be more promising than using raw minerals, with higher reactivity and dissolution capacities (Jo, Kim, Lee, Lee, & Choh, 2012). Coal fly ash (CFA) has shown a great potential for MC due to its rich production and close proximity to the site of utilization. Calcium and Magnesium content has been the main reason for the underutilization of CFA, which has created environmental impacts, such as turning groundwater turbid and non-potable and reducing the quality of air. Thus, CO_2 sequestration using CFA is not only an attractive method of greenhouse gas control but also a way to reduce the environmental impacts of CFA, by expanding its utilization potential.

Despite extensive lab-scale studies, studies regarding the implantation of CFA-based CO_2 sequestration in the large scale have not been performed in the present context. Thus, in this study, an Aspen plus supported process simulation-based analysis was conducted for large scale CO_2 sequestration using CFA.

METHODOLOGY

Composition of flue gas, including the CO_2 content which is required to be sequestrated was obtained from calculations conducted for the stoichiometric combustion of coal. Steady state process simulations were conducted for two scenarios of fly ash mineral carbonation: 1. Using pure water and 2. Using seawater as fly ash solvents, respectively. The process simulations were performed using the Aspen plus V10 chemical process simulation software, applying the ENRTL-RK thermodynamic method. RadFrac distillation column model in Aspen plus software was used to model the reactive absorption column for CO_2 sequestration.

The mechanism of carbonation reaction between dissolved CO_2 and Ca^{2+} in the aqueous medium was reported by Li et al. as follows (Li et al., 2018).

$$CO_{2(g)} + H_2O_{(l)} \leftrightarrow H^+_{(aq)} + HCO^-_{3(aq)} \quad (1)$$

$$HCO^-_{3(aq)} \leftrightarrow H^+_{(aq)} + CO^{2-}_{3(aq)} \quad (2)$$

$$Ca^{2+}_{(aq)} + CO^{2-}_{3(aq)} \leftrightarrow CaCO_{3(s)} \quad (3)$$

If the standard state free energy change (ΔG^0), is known for a chemical process at some temperature (T), the equilibrium constant (K) for the process can be calculated at that temperature, using the relationship between ΔG^0 and K.

$$K_{eq} = e^{-\Delta G^0 / RT} \quad (4)$$

The considered performance parameters were CO_2 sequestration and CO_2 sequestration percentage. Varied parameters were temperature, pressure, flow rate and CO_2 mass fraction of flue gas, and liquid to solid ratio of fly ash and water. Furthermore, the most optimum multiple column arrangement was assessed for sequestration performance and relevant costs.

RESULTS AND DISCUSSION

The most significant variations from the obtained results are as follows.

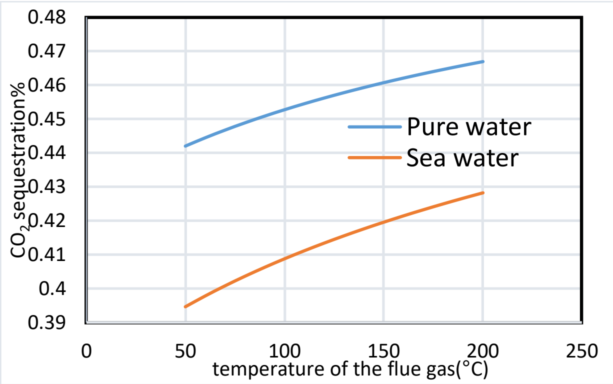

Figure 1. CO_2 sequestration% vs temperature of the flue gas

Sequestration percentage showed to rise with the rising temperature, which was also the observation in published laboratory-scale studies.

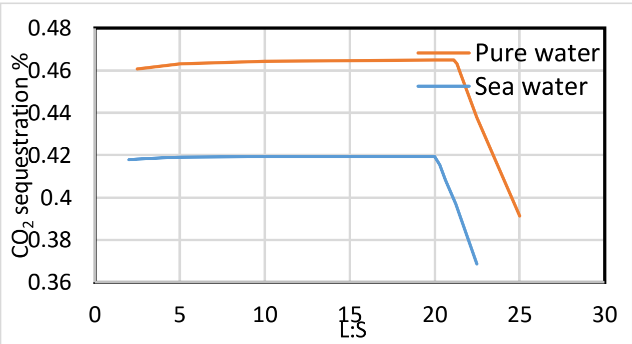

Figure 2. CO_2 sequestration% vs L:S

Sequestration percentage showed a slow rise to hit a peak with the lowering L:S temperature, which then decreased rapidly. This was also observed in published lab-scale studies, which validates the developed simulation model.

As another interesting observation, CO_2 sequestration showed a decrease with increasing mass fraction of CO_2 in flue gas, despite the increment of a reactant.

Regarding multiple column arrangements, sequestration percentage was found to be 1.17% for series arrangement and the approximate capital cost and total annual operating cost for this setup was calculated by Aspen process economic analyzer tool, to be nearly 22.7 million USD and 2.58 million USD/year.

For the parallel arrangement, CO_2 sequestration percentage was 1.18% , and the approximate capital and total operating costs were 9.9 million USD, and 1.7 million USD/year, respectively.

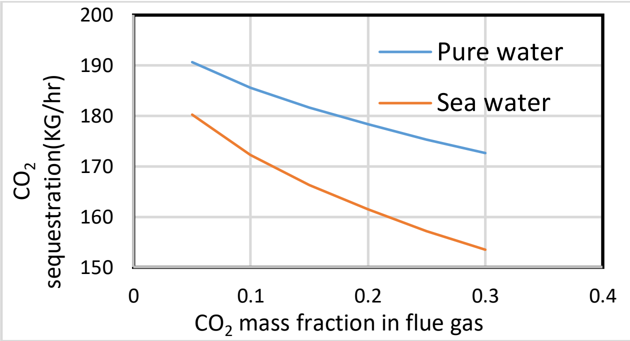

Figure 3. CO_2 sequestration vs CO_2 mass fraction in flue gas

These results showed that the parallel arrangement is superior over the series arrangement in terms of performance as well as economics.

CONCLUSION

A process simulation-based study was conducted for the industrial-scale indirect mineral carbonation of coal fly ash, for CO_2 sequestration from coal power plant flue gas. Two process simulation models were developed using the Aspen Plus simulation software, using pure water and seawater as the fly ash solvent, respectively. Results were comparable with the previous lab-scale studies, which validated the developed simulations, while some novel observations were also obtained. In the case of multiple column arrangements, the parallel arrangement was shown to be superior over the series arrangement in terms of performance as well as economics.

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