Modeling of CO_2 capture via chemical absorption processes – An extensive literature review

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ABSTRACT

Climate change mainly due to the release of greenhouse gases into the atmosphere is getting alarming dimensions. CO_2 capture from point source emissions is a promising solution, lately receiving significant attention. In particular, chemical absorption of CO_2 from flue gases using aqueous solvents (mainly alkanolamines) is a well-known process, studied in detail. Modern research aims to optimize this process, maximizing the absorption rates and minimizing the parasitic but not negligible energy requirements for solvent regeneration. This type of analysis requires considering the coupling of the absorption with the power plant operation or other source of CO_2. The operation fluctuations and disturbances, such as load variations or start-up mode have to be reflected in the process modeling, justifying the emerging need for dynamic modeling. However, dynamic analysis is not always realizable as dynamic experimental data are scarce in order to enable accurate model validation. Thus, steady state models are still convenient for certain cases. The current work provides a short description of the main modeling approaches followed and enlists representative steady state and dynamic models found in literature. Finally, a primary comparison is performed for some comparable models that used the same set of experimental data for model validation.

Contents

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1. Introduction

Facing climatic change as a detrimental result of the increasing global energy demand, various policies have been adopted aiming to mitigate the consequences, mainly to the reduction of greenhouse emissions. During the last years, the penetration of renewable sources of energy has been mainly promoted as a promising solution. However, it seems that fossil fuels will still be a predominant component of the global energy mix, posing the need for more direct ways of response. At the same time, EU and its member states are committed to an emission reduction target of 20% by 2020, compared with 1990 levels. This target could be increased to 30% under conditions set out by the European Council [1]

Carbon Capture and Storage (CCS) is a promising technique gaining increasing interest among researchers and policymakers. In specific, CCS is a process where CO_2 is separated from industrial production or energy conversion, is transported to the storage site under high pressure and finally geologically stored, aiming to realize zero emissions in the process of fossil energy extraction, conversion and usage [2]. CCS refers to the capture of CO_2 emissions either before the combustion of the fuel or directly from the flue gas. Post combustion methods are more applicable as they have no retrofitting requirements for the existing equipment. The most applied and efficient post combustion method is chemical absorption. In comparison with other post-combustion CO_2 absorption processes, chemical absorbents ensure higher absorption efficiency and selectivity, and lower energy [3].

In order to enable a wider scale implementation of CCS, detailed and efficient modeling of the process is a prerequisite. This is because the study of reactive absorption is mainly based on simulations, as experimental data are limited and not always reliable. Chemical absorption of CO_2 by aqueous solvents, mainly amines, has been studied for decades by numerous researchers with satisfying results. The developed models include both kinetic and thermodynamic aspects and are aiming to optimize the absorption. It is only recently though, that these attempts include dynamic characteristics and more realistic representations of the process.

The current work objective is to outline briefly the common modeling approaches in the field of post-combustion CO_2 absorption and also attempt to list a wide spectrum of specific models, steady and dynamic, encompassing their assumptions, modeling and validations tools and main outcome. Finally, the paper aims to conclude on the prediction efficiency of several models, comparing, to the point it is possible, results of different researchers which are based on the same experimental data.

2. Structure

The article is structured in 5 Sections. Section 1 is the introductory section providing information about the CO_2 emissions problem and the necessity to confront this. In following, Section 2 outlines the chemical absorption process and certain commercially used solvents. Section 3 provides the fundamentals, assumptions and requirements of the reactive absorption

modeling. Different mass transfer models, thermodynamic and kinetic models are listed. At the end an introduction to dynamic modeling is included. Section 4 includes the analysis of representative models from literature. Different sub-sections for steady state and dynamic models are encompassed, providing information for the assumptions made, equations applied and main outcome. In following in the same Section, three absorption units are presented that have provided very useful and widely used experimental results. Based on these data, certain rough comparisons are performed between models. Summarizing, Section 5 outlines the conclusions made by this literature research and suggest fields for future work.

3. Chemical absorption process and solvents

Chemical absorption (or reactive absorption) is the process where a gas is absorbed by a liquid phase with combination of reaction and absorptive mass transport. Amine-based systems, carbonate-based systems, aqueous ammonia and ionic liquids–based systems are typical systems for chemical absorption.

In specific for CO_2 capture, chemical absorption involves the reaction of CO_2 with a chemical solvent forming a weakly bonded intermediate compound, a process that can be reversed applying heat and resulting to the original solvent and a CO_2 stream [3]. The regeneration process is the most demanding by means of energy, as it may cost up to 14% of the power plant efficiency [4]. During chemical absorption the flue gas enters usually an absorption tower where it contacts countercurrent the solvent under low temperature (40–60 °C). The rich in CO_2 solvent is compressed, heated in an exchanger and inserted in the desorption column (stripper) where it is regenerated under low pressure (close to ambient) and high temperatures (100–140 °C). The regenerated (lean) solvent exits the column and re-enters the absorber after dissipating its heat in the rich solvent through the above mentioned exchanger.

The chemical absorption process was initially performed using amine aqueous solvents. The most mature and commercially applied amine is Monoethanolamine (MEA) due to its high absorptive capacity. MEA is considered an attractive solvent at low partial pressures of CO_2 in the flue gas due to its fast reaction rates compared to that of secondary and tertiary amines [5]. Other common amines are Diethanolamine (DEA), Methyl diethanolamine (MDEA), Diglycolamine (DGA), and Diisopropanolamine (DIPA) and Piperazine (PZ) or mixtures of amines that are characterized by satisfactory reaction rates and lower regeneration energy than MEA. Piperazine is usually added as a promoter as it has been found to have faster reaction rates than MEA. Due to its high volatility though, its application in CO_2 absorption is more expensive and is still under development [6]. A special category of amines are sterically hindered amines (SHA) that e.g. 2-Amino-2-methyl-1-propanol (AMP). SHA form more unstable carbamates in comparison with other amines. Thus, they are more efficient during regeneration, as the unstable carbamates are easier to be reversed, leading therefore to quicker desorption and less energy