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Model calibration for the carbon dioxide-amine absorption system

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HIGHLIGHTS

- A steady state simulation for CO_2 removal by amine absorption is considered.
- The Peclet number was evaluated for the absorber column.
- The high Peclet numbers obtained proved the plug-flow behavior of the column.
- Composition and temperature profiles were examined for different number of segments.
- It was proved that the number of segment has a paramount importance in modeling.

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ABSTRACT

Carbon dioxide absorption by monoethanolamine (MEA) is a very extensively studied process and its modeling represents an open issue in the specialized literature. In the present work, the key parameters necessary to set the absorber model are discussed and evaluated based on rigorous analysis. The experimental data from two different absorption plants size were considered to validate the model. The material and the thermal Peclet number were evaluated for both plants in order to quantify the influence of the axial diffusion/dispersion. The results obtained from the Peclet number evaluation were used to correctly define the number of segments required in the rate-based model. Moreover, the uncertainty in the kinetic parameters associated to the reaction between MEA and CO_2 reaction was examined to define a new set of values that minimize the standard error between the experimental and predicted temperature and composition values. The model proposed describes correctly the experimental data and particularly the bulge in the temperature profile, independently on its location. This result is particularly significant when it is required to examine the dynamic behavior of the column or when it is necessary to set an appropriate control system.

1. Introduction

The dualism carbon dioxide emission – climate change is nowadays a topic able to influence and to drive agreements between nations, to set global targets to be achieved and to define single plants sustainable programs. According to the Climate Change 2014: Mitigation of Climate Change, carbon dioxide contributes for 76% of the total greenhouse gases emitted and the energy production and transportation are the main responsible sectors [1]. The high impact of the topic to the public opinion, together with the strict emission limits imposed by the Governments, influences also the industrial production for both retrofit of existing plants or design of new ones [2].

Although the promotion and the utilization of renewable sources has a constant positive trend, fossil fuels power plants still represent the main contributors to satisfy the global energy demand and post combustion carbon dioxide capture is the most important technology suitable for the emission reduction. Carbon dioxide Capture and Storage (CCS) has been defined in the IPCC 2005 report: "Carbon dioxide capture and storage is a process consisting of the separation of CO_2 from industrial and energy-related sources, transport to a storage location and long-term isolation from the atmosphere [...]. The CO_2 would be compressed and transported for storage in geological formations, in the ocean, in mineral carbonates, or for use in industrial processes" [3].

As discussed by Rackley [4], three main types of CCS are recognized:

1. post-combustion capture: based on the CO_2 separation from the exhausted combustion gases;

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Nomenclature

C	molar concentration (kmol m^{-3})
c_p	specific heat at constant pressure (kJ $kmol^{-1}$ K^{-1})
$\mathcal{D}$	diffusion coefficient (m^2 s^{-1})
d_{eq}	packing equivalent diameter (m)
d_k	thickness of the k-th segment in the liquid film (m)
FDR	film discretization ratio (–)
G	gas molar flow (kmol s^{-1})
H	column height (m)
h	hold-up (m^3 m^{-3})
K	equilibrium constant (–)
k_T	thermal conductivity (kW m^{-1} K^{-1})
L	liquid molar flow (kmol s^{-1})
MSE	mean squared error (–)
Pe	Peclet number (–)
RCF	reaction condition factor (–)
S	column cross sectional area (m^2)
SE	standard error (–)
T	temperature (K)
x	molar fraction (–)

Greek letters

ε	void fraction (m^3 m^{-3})
ΔG^0	standard Gibbs free-energy change (cal/mol)

Subscripts

d_{eq}	characteristic length
i-th	component in the mixture
k-th	segment in the liquid film
H	characteristic length
M	material
mix	mixture
T	thermal

Superscripts

G	gas
L	liquid

2. pre-combustion capture: the CO_2 is removed from the syngas before the combustion;
3. oxy-combustion: oxygen rather than air is used as combustive agent, no separation is needed for the exhausted gas.

The post-combustion approach is usually preferred to the other two options since it is a mature and cost effective technology that can be easily integrated in existing plants [5,6]. Different separation alternatives such as adsorption, physical absorption, cryogenics separation, membrane absorption, chemical absorption or algal systems have been reported [7,8], however chemical absorption is undoubtedly the most used method. On this regard many research works are available in literature and they can be grouped into four main categories: (i) identification of the best solvent for the carbon dioxide absorption; (ii) kinetic studies; (iii) synthesis of new process configurations; and (iv) process modeling.

In the first group, solvents are compared for their efficacy in carbon dioxide absorption, foam tendency, degradation, corrosion properties, regeneration easiness and many other physical properties [9,10]. The proposal of a reaction mechanism and the evaluation of the kinetic parameters characterizes the scope of the second group [11,12]. In the third group different process configurations are proposed in order to decrease the energy consumption of the plant. Absorber intercooling, stripper interheating, split of the stripper feed are some of the possible alternatives discussed and compared in the work of Jung et al. [13].

Finally, the studies focused on modeling can be further divided into steady state and dynamic analysis. Steady state analysis has been mainly used for comparative assessment of different power plant technologies and to study how the CO_2 removal section affects the overall performance of a defined power plant flowsheet [14,15]. Moreover, steady state models are successfully applied in the optimization of key process operating parameters, to predict the composition and temperature profiles, for data validation and to optimize the energy consumption [16–20]. Dynamic models are mainly used to study different transient operational scenarios [21,22] or to optimize operating conditions to maximize for example the CO_2 capture rate [23]. Since the reactive absorption includes the combination of complex thermodynamic and kinetics, the presence of ionic species, complex mass transfer-reaction coupling; its behavior is not fully understood [24] and the process modeling still represents an open topic attracting the interest of both academia and industry.

The present work is focused on the study of the influence of different parameters required for the modeling of the CCS absorption section in steady state conditions. Two different experimental absorption setups were considered for the model validation. Among all the parameters examined, a special emphasis was given to the number of segments used to divide the packing height in the rate based model. Very often this parameter is too easily defined and in the literature its influence on the absorber model was not appropriately discussed. For example, Mores et al. [25], Kucka et al. [26] and Mac Dowell et al. [27] focused their research on the mathematical modeling of the CO_2-monoethanolamine (MEA) absorption system, validating their models using the experimental data reported by Tontiwachwuthikul et al. [28]. They all considered the same absorber with a packing height of 6.55 m. The first research group modeled the packing height using 10 segments, the second one 15 and the third 25.

The same incongruity was observed in the works of Lawal et al. [29], Zhang et al. [30] and Kvamsdal and Rochelle [31], who modeled the experimental 6.1 m packed absorber studied by Dugas [32]. Even in this case, with the same plant, the first authors used 15 segments, the second one 20 and the third 30. This variation in the number of segments used to model the same absorber height indicates how its importance in the model results was not extensively studied. The number of the segments used to discretize the spatial domain for the absorber is here considered with particular emphasis on the resulting column temperature and composition profiles.

2. Process description

In the classical absorption process for CO_2 capture, the flue gas enters the bottom of the absorption column where it flows countercurrent with the lean amine aqueous solution. The CO_2 contained in the flue gas reacts with the amine solution and the purified gas exits from the top of the absorber and is sent to the stack. The rich amine exits from the absorber's bottom and is then sent to solvent regeneration section.

In this work, experimental data obtained from two different plants with different peculiarities, have been chosen to study the influence of the model parameters and to validate the proposed model.

The first case considered is the pilot-scale absorption system assembled by Tontiwachwuthikul et al. [28]. The absorber is