Modeling and Simulation of catalyst-aided low temperature CO$_2$ desorption from blended Monoethanolamine (MEA) – N-methyl-diethanolamine (MDEA) solution

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Introduction

Post combustion CO$_2$ capture using chemical solvents is the most mature CO$_2$ capture technology for removing CO$_2$ from low pressure flue gases emanating from coal-fired electrical power plants. Most often, 5 M aqueous Monoethanolamine (MEA) solution is used as a reference or base case to evaluate new developments or technologies for capturing CO$_2$. At present, the solvent technology suffers a major drawback of high heat requirement for desorption of the absorbed CO$_2$. Numerous researchers have shown that using amine blends/mixtures can reduce the heat required for desorption to some extent, but it is still too high. The incorporation of a solid acid catalyst (such as $\gamma$ Alumina and HZSM-5) into the desorber by Idem et al (2011) has shown to significantly decrease the heat requirement for CO$_2$ desorption using single or blended amines. This research was conducted as a batch process. It is therefore essential to perform this catalyst-aided process in a continuous system to determine the performance. In this work, catalyst-aided CO$_2$ desorption experiments were performed using a blended solution of MEA and MDEA in a small scale CO$_2$ capture plant with modified desorber configuration. Then, a 1 dimensional rate-based model for regeneration of CO$_2$ in the blended solution of MEA and MDEA was developed in Aspen Custom Modeler and validated against experimental results. The model was used to extensively study the behavior and performance of the system.

Model Development

The model uses the Electrolyte Non-Random Two Liquids (eNRTL) thermodynamic model to calculate the phase behaviour and the physical properties of the gas and liquid states. The Maxwell-Stefan generalized mass transfer equation was used to model the transport of components in the liquid and gas phases while the dusty fluid model was used to model the transport of chemical species in and out of the solid phase. In all these cases, the film theory was used to describe the interface behaviour. The model takes into account the presence of electrolytes, column hydrodynamics, both catalytic and non-catalytic reactions as well as heat and mass transfer limitations.

Experimental Setup
Two experimental setups were used in this work. A low (85 °C) temperature setup in which the reboiler is removed because the temperature is too low to produce enough vapour for heat and mass transfer. The high temperature (above 85 °C) process follows the conventional desorption process with reboiler. The setups are shown in Figure 1. Both setups are operated as full cycle CO₂ capture plant; thus, each desorber is operated alongside an absorber.

**Model Simulation and Validation**

Due to the complexity of the model equations, simpler models (equilibrium and effective diffusivity models) were developed first to serve as model initialization as well as to test for the simplification of the model. The column was discretized into stages while the liquid, gas and solid mass transfer films were discretized using the forward finite difference method. Multidimensional Newton Raphson method was used to solve the model equations. The experimental results of the high temperature process were validated using RadFrac in Aspen Plus. The results are shown in Figure 2. In this case RadFrac is able to sufficiently model the conventional system. The low temperature process however cannot be modeled with RadFrac because of the absence of the reboiler. Consequently, the developed model was used. There are three stages of model development. These are: the simple model (assumes no film resistance during mass transfer and every stage to be in phase equilibrium), the intermediate model (considers film resistance but uses effective diffusivity in the constitutive relation) and the complete model (also considers film resistance but uses Maxwell Stefan Generalized Mass Transfer equation). The validation of the temperature profile with the simplest model (equilibrium model) is shown Figure 3.

**Conclusions**

The developed model was able to sufficiently predict the composition and temperature profiles in both the liquid and the gas phases as well as predict the heat requirements for desorption. The developed model was as able to predict the lean loading given a rich loading and catalyst weight. Major process parameters that influence the catalytic process were investigated in this work. The developed model provides a range of capabilities for design/scale up, optimization and control of the catalytic process.

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**References**

Figure 1 - Process configuration of the desorption process. Left: Low temperature catalytic process. Right: Conventional desorption (High temperature) process with reboiler.

Figure 2 - Validation of Aspen Radfrac with experimental “high temperature” (average bed temperature of 105°C) data at 0g catalyst.
Figure 3 - Validation of equilibrium model (simplest model) with experimental data for low temperature (average bed temperature of 85 °C) at 0g catalyst.