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Validation of a CESAR1 solvent model with a focus on water wash conditions

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Abstract

The most prominent method of post-combustion carbon capture is reaction with aqueous amines in an absorber-regenerator loop. Historically, the benchmark solvent for this process has been 30 wt% monoethanolamine (MEA). However, one notable disadvantage of MEA is a high regeneration energy demand of around 3.7 MJ/kg_{CO2}[1]. Since a large part of the process energy requirement is related to the solvent's heat of absorption, research has long been concentrated in developing solvents with low energy requirements. One such solvent that has captured the attention of researchers is CESAR1, which is an aqueous blend of 1.5 M piperazine (PZ), and 3.0 M 2-amino-2-methyl-1-propanol (AMP). Studies have shown that CESAR1 is capable of reducing the process energy requirement to below 3 MJ/kg_{CO2}. While there is much less literature about CESAR1 than there is for MEA, plant and VLE results so far have increased confidence that CESAR1 could replace MEA as the benchmark carbon capture solvent1[2]. In order to evaluate whether this is the case, accurate calculation of the energy requirement, proper design of the process, and quantification of volatile emissions are necessary. Therefore, an accurate process model is highly important.

Amine gas treating models have two distinguishing characteristics. First, absorbers consist of a high level of non-ideal behaviour that gives rate-based methods an advantage over equilibrium-stage methods. Second, the regenerator operates close to equilibrium, which causes accurate representation of vapor-liquid equilibria (VLE) data to be one of the most important features of the process model. Currently, literature VLE data is available only at absorber/desorber conditions and severely lacking at lower concentrations that would be found in the water wash section for a CO_2 capture plant. Under the Sustainable Operation of Post-Combustion Capture Plants (SCOPE) project, novel experimental data under water wash conditions presenting low amine concentrations were generated for the CESAR1 solvent. This new data was then used to update the proprietary thermodynamic model of ProTreat®, a mass-transfer rate-based simulator developed by Optimized Gas Treating, inc.

In this work, validation is performed on the most updated ProTreat® CESAR1 model. In ProTreat®, the activity coefficients are calculated using the Deshmukh-Mather model[3] while the gas phase is corrected using a fugacity coefficient calculated from the Peng-Robinson equation of state. To tune the model, over 1800 VLE data points from

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18 different sources were used in parameter fitting. These data came from various experimental methods including ebulliometry, reaction calorimetry, and fourier-transform infrared spectroscopy, and contained both unloaded and CO_2-loaded solutions. Literature VLE data was compared with initial results from the ProTreat® model to show a high level of agreement as observed in figure 1a and figure 1b. Since the ProTreat® model is rate-based, physical property calculation is also essential for accurate plant simulation. Validation and refitting of the physical properties for the CESAR1 system was carried out for this purpose. These results will be discussed, too. Currently, plant validation is being performed to show that the predictions of the ProTreat® model extend to operational results using data obtained from various proprietary sources. Comprehensive comparison between plant and model results will be covered with emphasis on the implications of CESAR1 for future post-combustion carbon capture plant design.

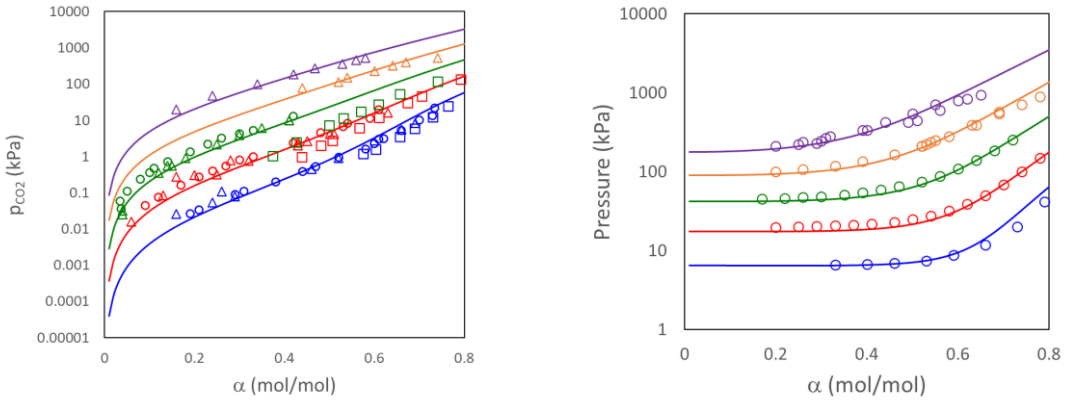

Figure 1: Experimental and calculated equilibrium pressures as function of the loading (α) for 27 wt.% AMP + 13 wt.% PZ aqueous solutions. (a) Partial pressure of CO_2, p_{CO2}; and (b) Total pressure, p_{total}. Temperatures: 40˚C (blue), 60˚C (red), 80˚C (green), 100˚C (orange), and 120˚C (purple). Experimental points: (o)[4], (Δ)[5], (□)[6].

References

[1]Knudsen, Jacob N., et al. "Evaluation of process upgrades and novel solvents for the post combustion CO2 capture process in pilot-scale." *Energy Procedia* 4 (2011): 1558-1565.

[2]Feron, Paul HM, et al. "An update of the benchmark post-combustion CO2-capture technology." *Fuel* 273 (2020): 117776

[3]Deshmukh, R. D., and Alan E. Mather. "A mathematical model for equilibrium solubility of hydrogen sulfide and carbon dioxide in aqueous alkanolamine solutions." *Chemical engineering science* 36.2 (1981): 355-362.

[4]Hartono, Ardi, et al. "New solubility and heat of absorption data for CO2 in blends of 2-amino-2-methyl-1-propanol (AMP) and Piperazine (PZ) and a new eNRTL model representation." *Fluid Phase Equilibria* 550 (2021): 113235.

[5]Brúder, Peter, et al. "CO2 capture into aqueous solutions of piperazine activated 2-amino-2-methyl-1-propanol." *Chemical Engineering Science* 66.23 (2011): 6193-6198.

[6]Yang, Zih-Yi, et al. "Equilibrium solubility of carbon dioxide in (2-amino-2-methyl-1-propanol+ piperazine+ water)." *The Journal of Chemical Thermodynamics* 42.5 (2010): 659-665.

Acknowledgements

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