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Modelling CO_2 chemical absorption using the CESAR1 solvent

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Abstract

Reducing carbon dioxide (CO_2) emissions is a significant global challenge in combating climate change. Chemical absorption using aqueous amine solution is the most mature technology for post-combustion carbon capture [1]. An aqueous blend of 3 M 2-amino-2-methyl-1-propanol (AMP) + 1.5 M piperazine (PZ), also known as CESAR1, is considered the current benchmark of this technology [2]. However, experimental gaps in thermodynamics, kinetics and physical properties have been detected in the open literature [3]. In previous works, we filled some of these experimental gaps to accurately characterize the properties of the CESAR1 blend [4, 5].

Accurate data are needed to develop robust and reliable models that can be used for the design of CO_2 capture absorption process units. In this conference, we want to present the results of our modelling work of the CESAR1 blend. We developed an e-NRTL (electrolyte Non-Random Two-Liquid) thermodynamic framework for aqueous AMP/PZ/CO_2 solution in Aspen Plus. The model has been fitted on existing literature data and the new experimental results collected in our previous work [4]. Preliminary results of the thermodynamic modelling work are shown in Figure 1. The model developed in this work accurately predicts the CO_2 solubility for the CESAR1 blend over a broad range of temperatures, up to 150 °C. Furthermore, the model predicts well the liquid speciation of the CESAR1 blend, an important thermodynamic property that impacts the CO_2 absorption kinetics performance, by affecting the reaction reversibility, and all the thermodynamic properties calculated from the liquid speciation, i.e. solvent volatility.

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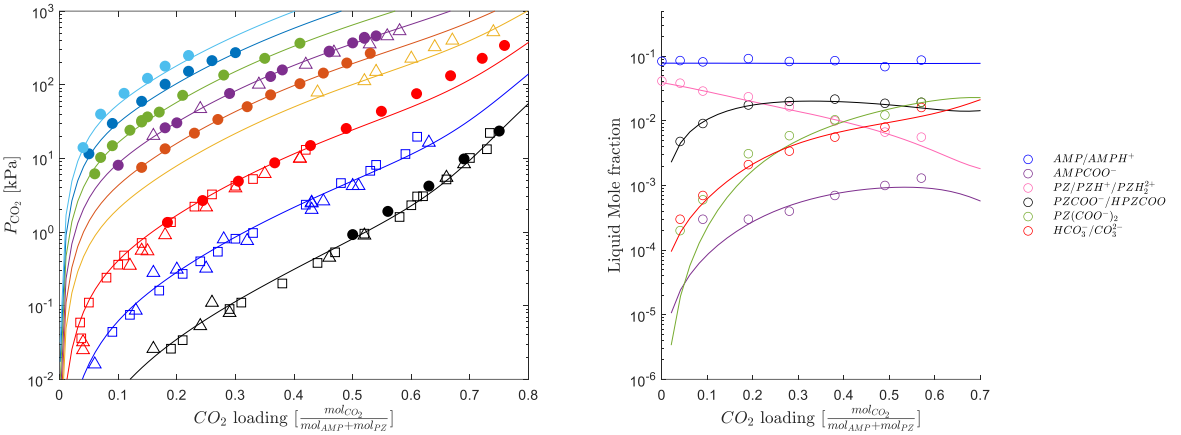

Figure 1: (a) CO_2 solubility of the CESAR1 blend (● [4], □ [6], Δ [7]),(Black 40 °C, Blue 60 °C, Red 80 °C, Yellow 100°C, Orange 110 °C, Purple 120°C, Green 130°C, Dark Blue 140 °C, Cyan 150°C), (b) Liquid speciation of the CESAR1 blend at 25°C.

The thermodynamic model developed has been then used, in combination with mass transfer and kinetics modelling, to build a rate-based model that has been validated on two pilot plant campaigns, one performed at the University of Kaiserslautern [8] and one at the Technology Center of Mongstad (TCM) [9]. These two pilot campaigns are independent datasets used to validate the performance of the model developed starting from lab-scale data. Figure *2* shows the rich loading model predictions for the two experimental campaigns studied. The model predicts the rich loading within an absolute average relative deviation (AARD) of 1.8 % and 3.6% for the Kaiserslautern campaign and TCM campaign, respectively.

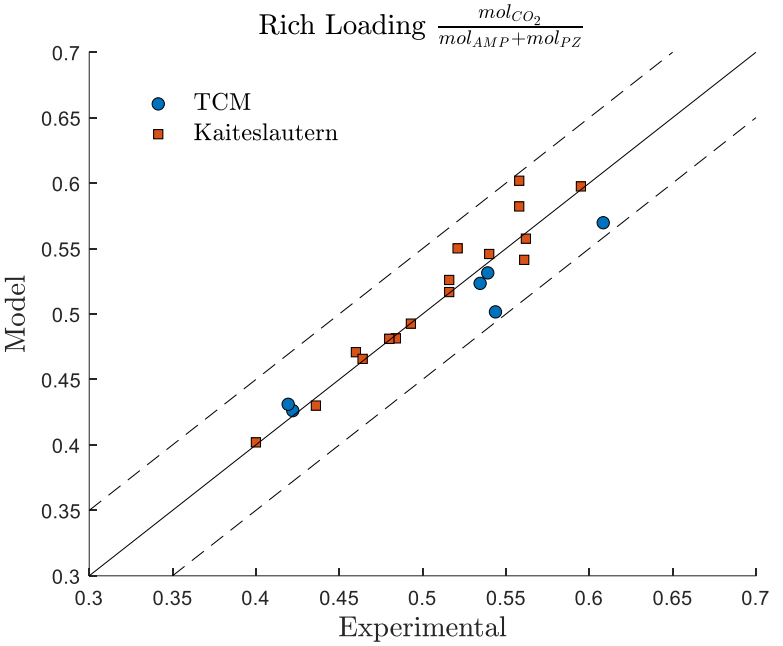

Figure 2: Comparison of the simulated and experimental CO_2 rich loading, (● [9], ■ [8]), the dashed line indicates a ± 5 % deviation.

To conclude, at PCCC-8 we plan to present a new model for CO_2 absorption using aqueous AMP/PZ solutions. The

model performance will be assessed by comparing the model predictions with experimental lab scale data and pilot plant data.

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Keywords: Post-combustion Carbon Capture,amine-based absorption; thermodynamic Modeling, CESAR1 Solvent; Process modelling; Aspen Plus.

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