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Improving on the CCSI model for MEA-based CO_2 capture

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Abstract

The U.S. Department of Energy's Carbon Capture Simulation Initiative (CCSI) developed and published a "gold-standard" CO_2 capture process model in 2018 for monoethanolamine (MEA) solvent. This model was created in Aspen Plus by regressing parameters for mass transfer and column hydraulic correlations to minimize the differences between the process model predictions and laboratory-scale CO_2 capture[1] and was subsequently validated against pilot plant data[2]. The source file for the CCSI process model was made publicly available and it has since been widely used for other CO_2 capture studies (e.g., refs.[3,4]). However, there are some underreported issues with the model which constrain its range of validity. In this work, we show how these limitations can affect the accuracy of process model predictions compared to large-scale pilot data and present results from an alternative CO_2 capture model for MEA which is substantially more versatile than the CCSI model. We also present process modelling results for new data from the Haifeng CO_2 capture pilot plant in China.

Detailed and accurate process models are crucially important to facilitate deployment of CO_2 capture technology and establish related government policies because they are the foundation for meaningful performance and techno-economic assessments. Rate-based process models are considered more deterministic and accurate than empirical equilibrium stage models for regenerative amine solvent absorption processes[5]. Prior studies that developed and validated amine solvent-based absorption process models (e.g., refs.[6,7]) relied on data from laboratory-scale equipment that is several orders of magnitude smaller than equipment relevant for industrial-scale applications. Further, the laboratory tests used columns that were substantially shorter than typical industrial designs and focused on a relatively narrow range of column liquid fluxes that is not representative of all CO_2 capture applications. The mass transfer and column hydraulic models commonly used in process simulations are based on a variety of empirical relationships that deviate substantially based on fluid thermodynamic properties, packing parameters, and superficial velocities. The CCSI development sought to address this by validating their model against small-scale pilot data from the National Carbon Capture Center (c. 4-9 tCO_2/d), but the data was limited to flue gas from coal fired power generation which constrained the range of operating conditions.

The CCSI model uses a variation of the Tsai correlation to determine interfacial area for inter-phase mass transfer[8]; this correlation is normally a function of the Weber number and Froude number. However, due to a Fortran programming error, the dependence of interfacial area on the Froude number was omitted in their parameter regression and model validation[9]. This results in the interfacial area calculated by the CCSI model having a substantially higher dependence on liquid flux than the original Tsai correlation. Furthermore, the CCSI model uses a simplified chemistry model based on two reactions which do not consider all ionic species (excludes H_3O^+, OH^-, and CO_3^{2-}). Although the simplified reactions combined with the thermodynamic parameters used in the CCSI model provide reasonable predictions of equilibrium CO_2 partial pressure for the CO_2-MEA-water ternary system for many practical combinations of CO_2 loading and temperature, there are some conditions relevant for CO_2 capture systems where this is not the case. For example, the CO_2 partial pressure predicted by CCSI at 120ºC (typical

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regenerator temperature for MEA) and CO_2 loading between c. 0.30-0.42 mol_{CO2}/mol_{MEA} aligns well with reported data, but at higher loading the predicted partial pressure deviates considerably above the range of reported data (e.g., +44% compared to Aronu et al.[10] at 0.499 mol_{CO2}/mol_{MEA}). The CCSI model is also limited to a specific type of structured packing (Mellapak 252Y), which may be suboptimal for some applications, and a narrow range of operating conditions because of its reliance on parameters for mass transfer and hydraulic calculations that were regressed based on a limited set of experimental data. Finally, the CCSI model does not consider kinetic limitations in the reaction scheme used in the regenerator model (assumes equilibrium).

An alternative rate-based model for CO_2 capture with MEA has been created to address these issues using modern mass transfer correlations developed at the University of Texas[11]. These mass transfer correlations are based on an extensive dataset generated with 39 different random and structured packings, including the data utilized in the original Tsai effective area correlation, and account for the effect of viscosity on the liquid mass transfer coefficient. The new process model incorporates a rigorous chemistry model which considers all relevant ionic species, was validated against published vapour-liquid equilibrium data for CO_2-MEA-water, and includes forward/reverse kinetic limitations in both the absorber and regenerator. We validated the model over a wider range of scale/conditions than the CCSI model using five datasets from four different facilities: laboratory-scale data (0.1 tCO_2/d, 5.5%mol CO_2 flue gas)[12], the US National Carbon Capture Center pilot plant (8 tCO_2/d, 11%mol CO_2 flue gas)[2], Technology Centre Mongstad (78 tCO_2/d, 4%mol CO_2 flue gas)[13,14], and the China Resources Power (Haifeng) Plant Carbon Capture Test Platform (38 tCO_2/d, 13%mol CO_2 flue gas).

Unlike CCSI, we did not regress mass-transfer correlation parameters to avoid overfitting the data and retain the applicable range of the original correlations. For each datapoint, the overall system mass-energy balance was modelled by adjusting the lean solvent CO_2 loading to match the predicted mass transfer in the absorber and regenerator columns with the regenerator heat input, absorber vapour inlet conditions, and other process parameters fixed based on the measured data. Predicted CO_2 capture rate, lean solvent CO_2 loading, and absorber/regenerator temperature profiles from each model were compared with the measured data.

The gross-CO_2 capture rate and lean solvent loading predicted by the process model developed in this study more closely align with laboratory-scale measurements reported in Notz et al.[12] than the performance predicted by the CCSI model (**Figure 1**), with root-mean-squared deviations (RMSDs) of 4.0 pp and 0.009 mol/mol versus 6.6 pp and 0.014 mol/mol respectively. The two process models predict similar column temperature profiles which closely align with the measured data in Notz et al.[12]. Comparisons of model predictions and measurements for data from Technology Centre Mongstad (**Figure 2**) yield similar results with the model developed in this study more closely predicting gross-CO_2 capture rate and lean solvent loading (RMSDs of 1.4 pp and 0.010 mol/mol) than the CCSI model (RMSDs of 3.3 pp and 0.024 mol/mol). The gap between the absorber temperature profile predicted by the CCSI model and measured data from Technology Centre Mongstad increased substantially as the absorber solvent flux decreased below the range used to regress the CCSI mass transfer parameters (10-31 m^3/m^2-h) (e.g., RMSD of 0.9ºC at 8 m^3/m^2-h vs. 3.9ºC at 4 m^3/m^2-h in **Figure 3**), while the temperature profile predicted by the model in this study closely aligned with the reported data (RMSD 0.6-1.2ºC) over the full range of absorber liquid fluxes. The two models provide similar results for the National Carbon Capture Center and Haifeng datasets – e.g., 97.5% gross-CO_2 capture (this study) and 98.5% (CCSI) versus 97.8% measured for the Haifeng pilot plant – as the absorber liquid flux for the coal power exhaust composition is aligned with the range of liquid fluxes used for the CCSI parameter regression and the generally higher capture rates in the coal power datasets lead to absorber mass transfer limitations based on equilibrium.

The new CO_2 capture process model will enable more accurate predictions of performance and process conditions for engineering design and techno-economic analyses across a wider range of process conditions and packing than the incumbent CCSI model.

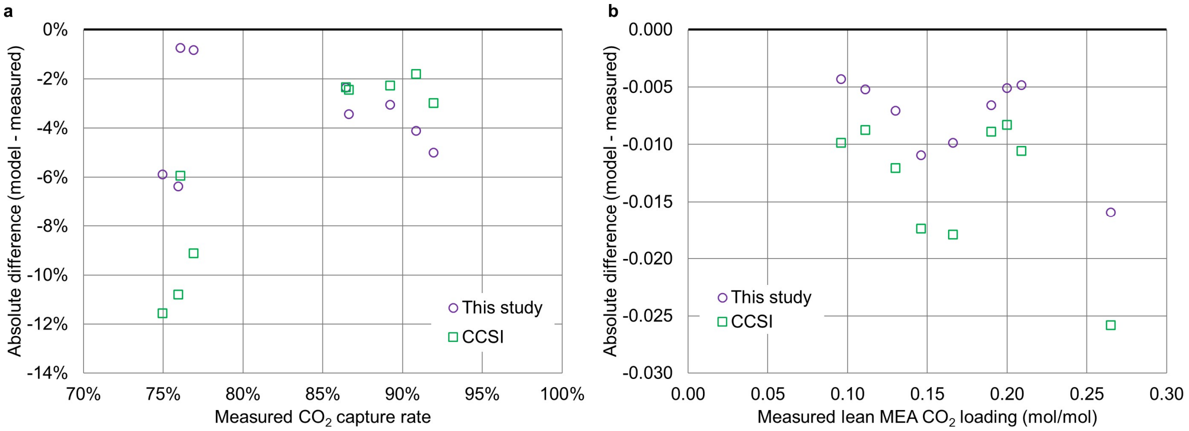

Figure 1. *Comparison of predictions from the process model developed in this study (purple circles) and the CCSI model (green squares) with laboratory-scale measurements.* ***a*** *Difference between model predicted gross CO_2 capture rate and measured data versus measured gross CO_2 capture rate.* ***b*** *Difference between model predicted lean solvent loading and measured lean solvent loading versus measured lean solvent loading (mol_{CO2}/mol_{MEA}).Laboratory-scale data from Notz et al.[12].*

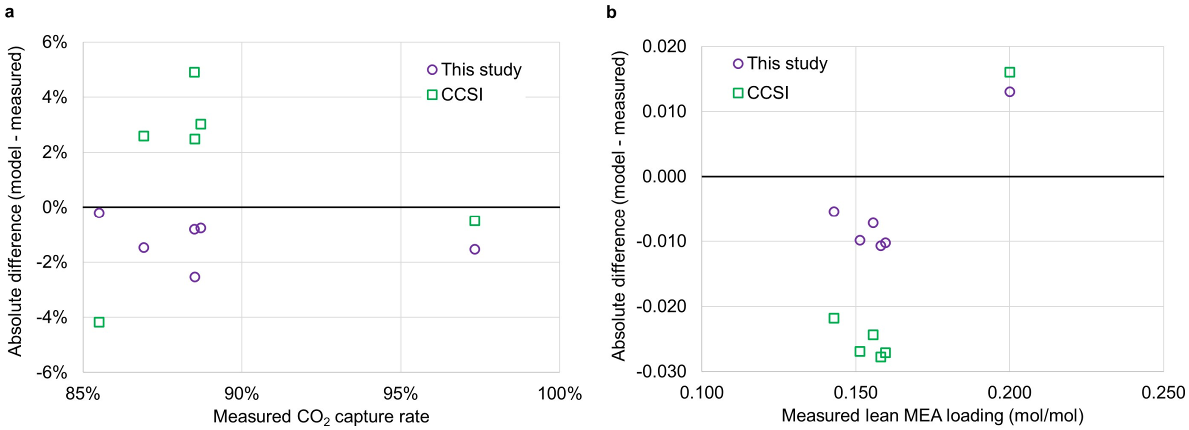

Figure 2. *Comparison of predictions from the process model developed in this study (purple circles) and the CCSI model (green squares) with pilot plant data from Technology Centre Mongstad.* ***a*** *Difference between model predicted gross CO_2 capture rate and measured data versus measured gross CO_2 capture rate.* ***b*** *Difference between model predicted lean solvent loading and measured lean solvent loading versus measured lean solvent loading (mol_{CO2}/mol_{MEA}). Pilot plant data from Faramarzi et al.[13] and Bui et al.[14].*

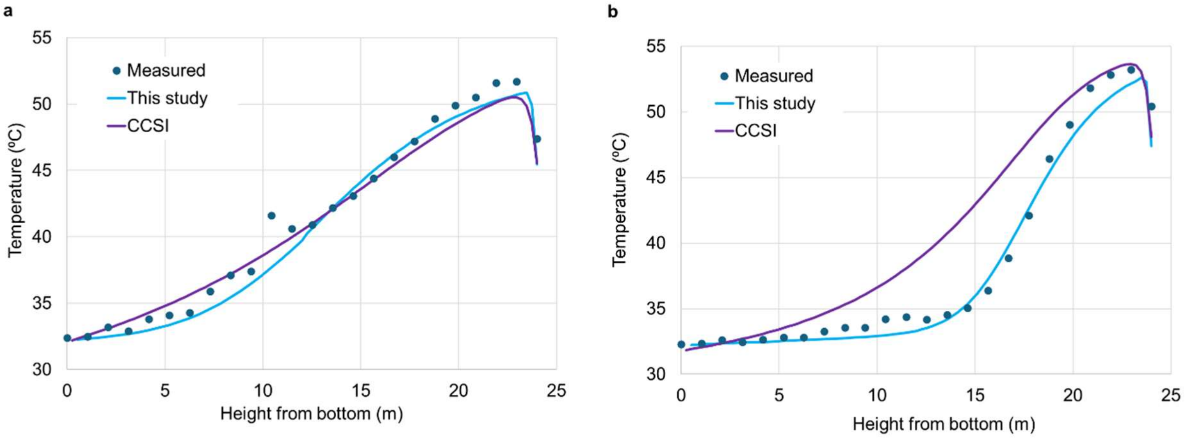

Figure 3. *Comparison of predicted absorber temperature profile from the process model developed in this study (purple circles) and the CCSI model (green squares) with pilot plant data from Technology Centre Mongstad.* ***a*** *Absorber temperature profile for data from Faramarzi et al.[13] with absorber liquid flux of 8 m^3/m^2-h.* ***b*** *Absorber temperature profile for data from case ICL11 in Bui et al.[14] with absorber liquid flux of 4 m^3/m^2-h.*

Keywords: Carbon capture; absorption; regeneration; process modelling; monoethanolamine

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