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Advanced and efficient modelling of the CESAR1 solvent

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Abstract

The overarching aim of the AURORA project is to qualify the CESAR1 solvent for commercial deployment. This is done through a dedicated qualification procedure [1], which ensures that important knowledge gaps are identified based on results from previous projects (e.g., CESAR, ALIGN-CCUS, and SCOPE) and closed through extensive pilot testing and solvent and process modelling and simulation. In a review article [2] based on open literature, the knowledge gaps related to modelling, degradation, solvent management, and pilot testing of the CESAR1 solvent were identified. Based on this, experiments in the lab related to solubility, kinetics, density and viscosity have been performed and improved models established. These models have implemented in the SINTEF inhouse simulator CO2SIM.

The CO2SIM simulator provides a flexible and extensive simulation framework for solving a wide range of chemical processes related to CO_2 capture technologies. It is a powerful tool for solvent development and preliminary design of solvent-based carbon capture plants. The former is enabled through the development of "soft models" for solvents for which limited data are available in the first stage of development or for complex system like the CESAR1 solvent which consists of two amines (AMP and piperazine) with a large variety in the individual properties. In brief, these soft models do not calculate species and a full equilibrium of all components, such as for example the NRTL model, although such models are available in CO2SIM also. It is an explicit equilibrium model primarily as function of temperature and bound CO_2 in the solvent.

Within the AURORA project the model implementation has been revised and a new thermodynamically consistent mechanistic model approach based on full speciation is developed. Additionally, the enthalpy formulations have been updated enabling improved validity for a broader operating pressure in the stripper. These updates are briefly described in the following. More details will be given in the conference paper and in the presentation.

Improved overall VLE and kinetics framework

The novel contribution is the formulation a thermodynamically sound, yet computationally efficient and simpler

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equilibrium solver for the blended amine system, that still yields predictive species concentrations by calculating the complete speciation chemistry. The model needs high quality experimental equilibrium partial pressure data and reaction kinetics. We do not calculate individual component activities, thus avoiding a full eNRTL-type activity model, which is computationally expensive and prone to other issues such as overfitting. But we use this fugacity model, which we call the “Soft-model fit”, to directly do a full solvent speciation equilibrium calculation.

This primary measurement point, the fugacity or assumed partial pressure, is fixed, and the dissolved free CO_2 in solution is calculated using Henry’s law. We then solve the solvent electroneutrality and compute the implied loading in the solution after obtaining the solvent speciation (Figure 1). This implied loading needs to iteratively match the measured experimental loading at the given temperature requiring a robust numerical solver. We thus enforce elemental balance and charge neutrality in a similar fashion as a full equilibrium species calculation. The system is solved robustly and fast using a bracketed hybrid Newton-bisection method, ensuring a single valued convergence even in very nonlinear regimes. The activities are not calculated per species, but effective equilibrium constants are regressed against the equilibrium pressure model (Figure 2a), yielding lumped activities that are offsets of the measured equilibrium constants found from literature.

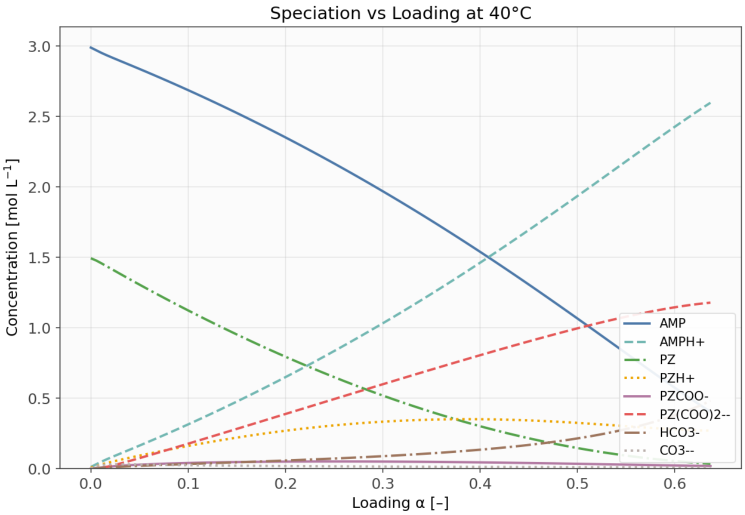
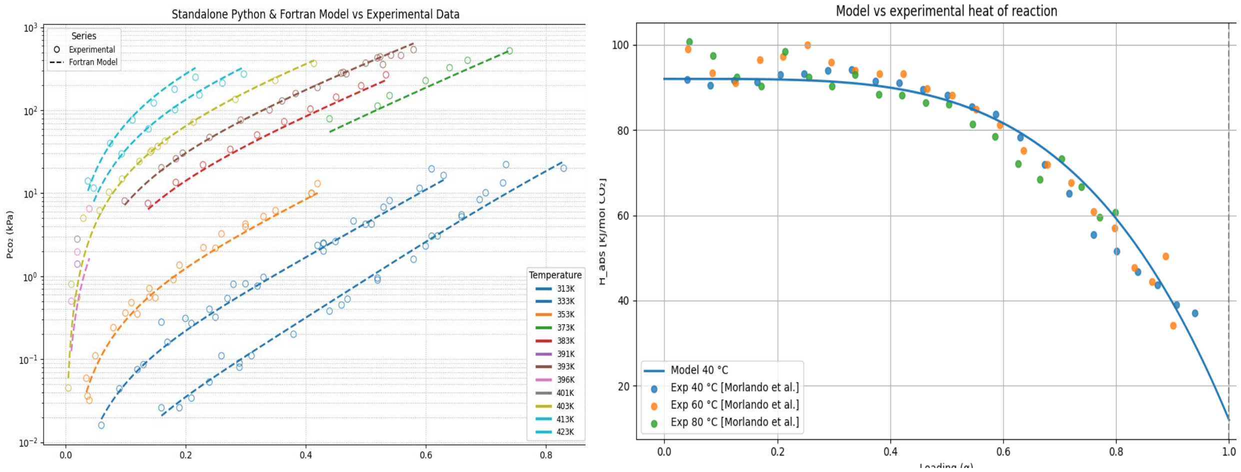


Figure 1: Speciation plots as function of loading for CESAR1 using the speciation model at 40°C



(a) (b)

Figure 2: (a) The VLE-model fit, (b) The fitted heat of reaction model that is subsequently used in the enthalpy model

Two forms of kinetic models are thus used optionally. Either speciation can be used directly in the kinetic model, or a simplified kinetic model can be used based on the assumption that piperazine is fully consumed first forming carbamates, followed by accumulation of the “carrying amine” AMP to form bicarbonate. This can be described by a stoichiometric relationship, and we call this the “depletion rule”-model. Figure 3 presents Different plots showing the flux and enhancement at different temperatures for CESAR1, based on the two different kinetic models used. It can be seen that the rapid pseudo-kinetic model is mostly very close to the rigorous model using the full speciation set from the VLE model.

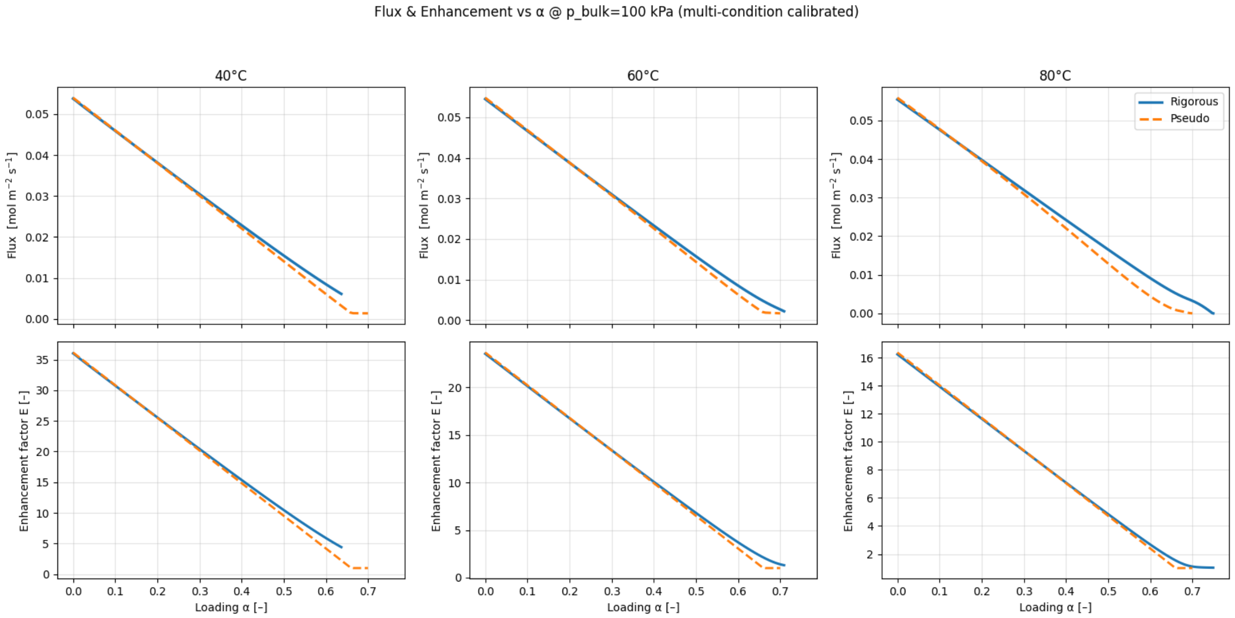


Figure 3: Different plots showing the flux and enhancement at different temperatures for CESAR1, based on the two different kinetic models used

Enthalpy formulations and phase relationships

The basis for the enthalpy description is the generic approach which has been used for most solvent systems used in CO2SIM for many years. This framework has been revised for concentrated CESAR1 solutions by decomposing the stream enthalpy into a physical baseline and a state-dependent chemical contribution. The physical term is constructed from ideal-gas heat capacities and integrated from a common reference state, combined with vaporization enthalpies and partial pressures for the pseudo-amine representing the AMP–PZ blend. The chemical term is introduced through a calorimetric heat-of-absorption correlation $q_{\mathrm{abs}}(T, \alpha)$, expressed as a function of CO_2 loading and temperature (Figure 2b), and integrated with respect to loading to obtain a chemical enthalpy correction consistent with enthalpy as a state function. This formulation preserves energy conservation across the absorption/desorption cycles and correctly embeds loading-dependent reaction effects in the enthalpy surface without double counting physical condensation. The method enables also validating the numerically obtained liquid heat capacity with measurement data (Figure 4).

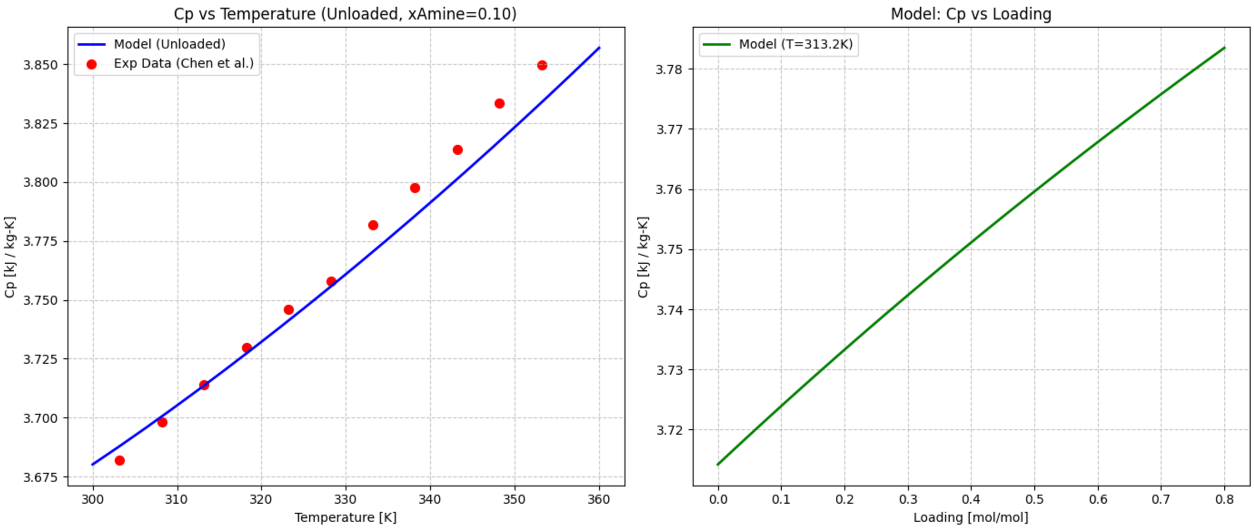


Figure 4: (a) CESAR1 heat capacities of unloaded amine solution compared to experimental data, (b) Heat capacities as function of loading.

The full simulation model is tested against pilot data from both the Tiller pilot plant as well as the TCM demonstration plants in Norway.

Acknowledgments

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