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Validation of the CESAR1 solvent model based on data from TCM demonstration campaign

F. Andrew Tobiesen[a], Hanne M. Kvamsdal[a]*, Thor Mejdell[a], Karl Anders Hoff[a], Koteswara Rao Putta[b]

[a] *SINTEF Industry, 7034 Trondheim, Norway*
[b] *Technology Center Mongstad (TCM), N-5954 Mongstad, Norway*

Abstract
The aim of the AURORA project has been to qualify the open and non-proprietary CESAR1 solvent technology for commercial deployment. As part of this qualification there have been two major test campaigns in pilots (the Tiller pilot and the Technology Centre Mongstad -TCM) and validated process models based on these test campaigns are further used for determining the solvent performance for a broad range of flue gas conditions (CO_2 concentration, water content, flue-gas flowrate, temperature) relevant for four distinct process plants (two refineries, one cement producer and one materials recycling plant). Two different steady state simulators are used for the process simulations, Aspen Plus and CO2SIM. The latter being an inhouse rate-based CO_2 capture simulator was established for efficient development of various solvent systems. Within the AURORA project, the simulator has been extensively upgraded with respect to the procedure for validation of the process model including pre-assessment of the data quality prior to comparison of the experimental and simulated data. Furthermore, an extensive work has been done to update the underlying CESAR1 solvent models (thermodynamics, kinetics, and property data) as well as improvements of the enthalpy balance of the process models. While the validation procedure and validation against the Tiller pilot have been previously presented [1], the focus here is the validation against the data from the TCM demonstration campaign using CO2SIM software.

Several tests were conducted during the 5 months test campaign at TCM in 2025. These tests enabled large variations in the flue gas conditions and based on the results; 8 different steady state data sets were selected for validation of the process models implemented in CO2SIM. For each data sets, measured operating data are converted into fully specified thermodynamic state variables (temperature, pressure, flow and composition) for the measured selected key streams. These inputs are stored in excel files and imported into CO2SIM using an automated sequence to ensure repeatability and consistent treatment across the campaign datasets. To limit error propagation through the full flowsheet, the validation is performed in stages by simulating the absorber first, followed by a final integrated full-plant validation. Figure 1 shows the flowsheet of the overall TCM plant represented in the CO2SIM simulator.

In the standalone absorber validation, the setup is driven by measured boundary conditions in and out of the absorber

* Corresponding author. Tel.: (+47) 93059222, *E-mail address:* Hanne.Kvamsdal@sintef.no

unit. In Figure 2 a) and b) parity plots for comparing simulated and experimental CO_2 mass transfer rates based on liquid and gas phases, respectively, are given. As shown, the gas-side mass transfer shows good agreement, while the liquid-side parity plot shows some scatter, particularly for dataset number 4, which exceeds the 10% error margin. This deviation is likely attributed to uncertainties in the specific liquid flow or composition measurements for that data-set, rather than hydraulic- and other model deficiencies. It should be noted that the experimental mass balance (Gas vs. Liquid) was inspected for the 8 datasets and an Average Absolute Deviation (AAD) of 5.3% was determined. This value serves as the baseline for model accuracy meaning that simulation errors near or below this threshold indicate the model is statistically indistinguishable from measurement uncertainty. We can see that this is indeed the results from the simulations as the AAD for the simulation versus experimental is 3.5% for the liquid and 4.7% for the gas side mass-balance.

Following the absorber-only validation, a full plant validation was performed by combining the absorber and stripper into an integrated simulation case (Figure 1). For each data-sets, the flow sheet model is constrained using measured campaign conditions, including solvent concentration, reboiler duty based on calculated steam conditions, key heat exchanger temperatures, and operating conditions and sizes of each unit. Validation is performed by comparing simulated and measured mass transfer data and other key parameters, as well as overall CO_2 mass balance closure across absorber and stripper. Figure 3 shows parity plot for mass transfer when the full plant simulation is performed. Figure 4 a and b show parity plots of the SRD based on CO_2 captured in the liquid and the CO_2 product stream (stream V11), respectively. As can be seen the deviations are within or slightly higher than the 5% error band except for data-set number 4.

Based on a full analysis it can be concluded that the model, using the newly implemented CESAR1 thermodynamic- and rate-based framework, successfully captures the mass and energy performance of the TCM plant. More results and discussions will be presented in the conference paper and in the presentation at the conference.

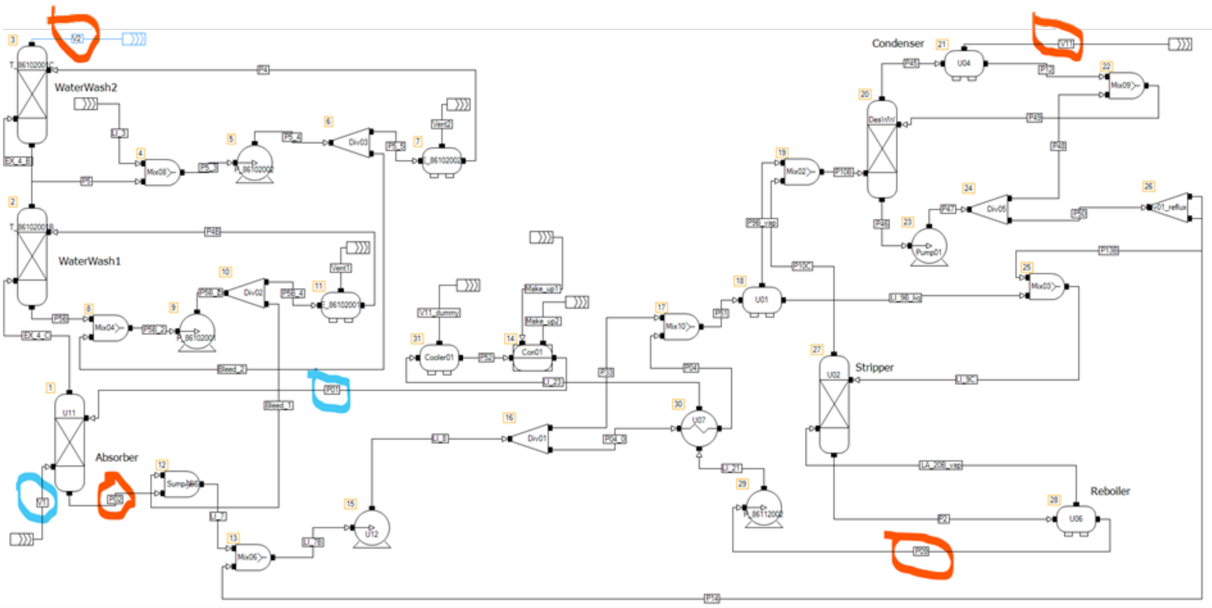
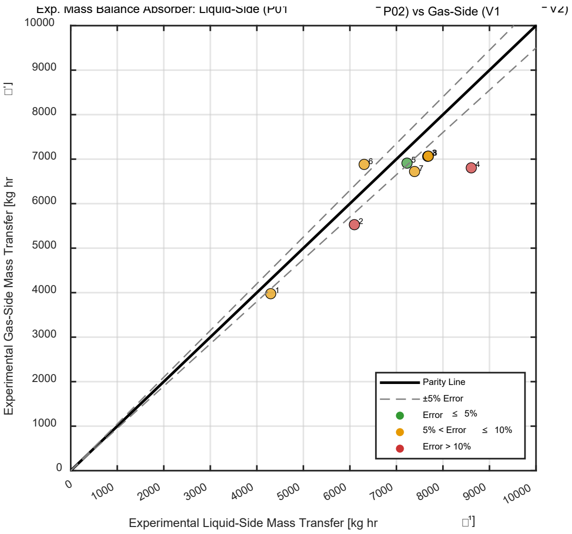
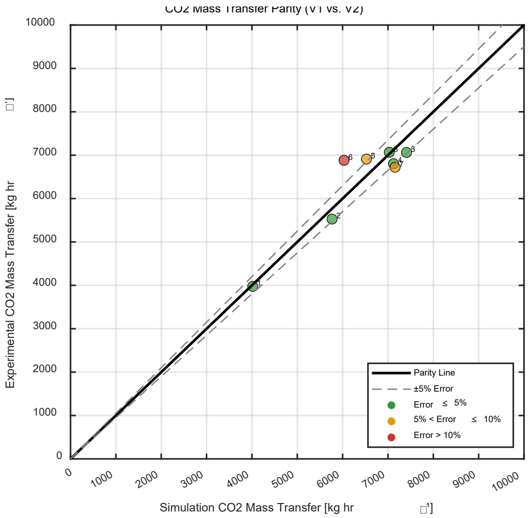


Figure 1: CO2SIM flowsheet for the TCM plant. The blue and red circles show input and output streams, respectively, that are used to validate the solvent models. Two independent experimental data sets for each stream exist from the pilot plant, which enables a thorough experimental mass balance analysis prior to simulation. After this, a simulation study can be conducted.

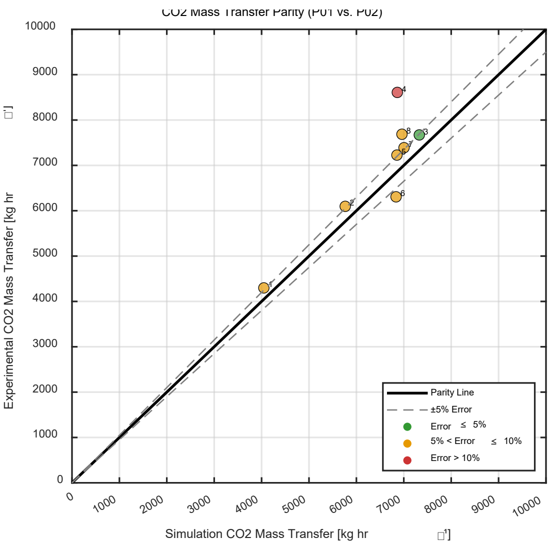


(a: exp liquid phase)

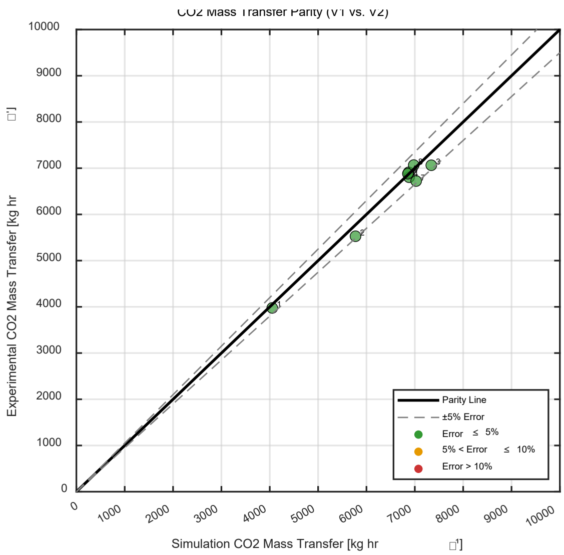


(b: exp gas side)

Figure 2: Absorber validation: (*a) shows a parity plot comparing experimental CO_2 mass transfer rates along gas and liquid phases, (b) shows the simulation results compared to the gas phase measurements.*

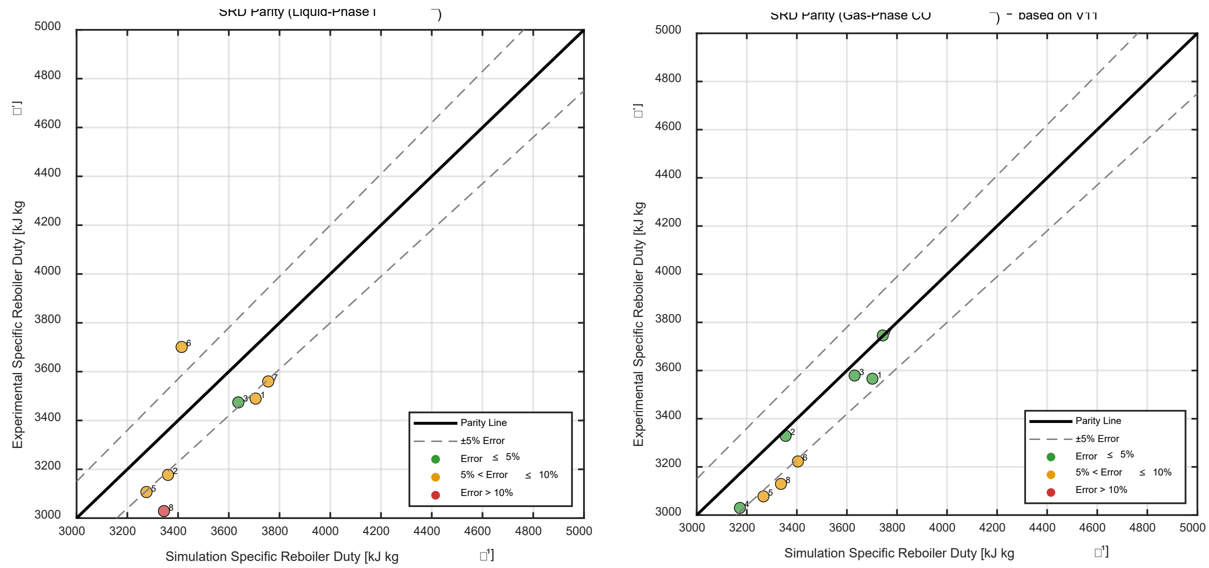


(a)



(b)

Figure 3: Full plant validation (*a) shows a parity plot comparing simulated vs. experimental CO_2 mass transfer rates the absorber liquid phase, (b) shows the simulation results compared to the gas phase measurements.*



(a) (b)

Figure 4: *SRD for the runs, based on the liquid phase, (b) calculated from the product gas flow (V11)*

Acknowledgments

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References

[1] F.A. Tobiesen, H.M. Kvamsdal, T. Mejdell, and K.A. Hoff, Validation of the CESAR1 model in CO2SIM based on extensive pilot experiments, presentation at the IEAGHG 8th Post Combustion Capture Conference, Marseille, France (16th to 18th September 2025)

Keywords: post-combustion carbon capture; Amine based CO_2 absorption, CESAR1 solvent; pilot testing; model validation