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Validation of the CESAR1 model in CO2SIM based on extensive pilot experiments

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Abstract

The CESAR1 model in the CO2SIM simulator has been updated based on new laboratory experiments covering a broader loading and temperature range compared to previous reported data in the literature. The updated model has been validated and successfully improved by extensive testing at the Tiller pilot plant, which operated under a wide range of conditions including CO_2 concentration, liquid flow rate, gas velocity, and absorber and stripper temperature. The simulator contains a range of models with different degrees of complexity. For the VLE model, we have chosen to follow a simplified "soft model"- implementation. Such a model does not calculate species and a full equilibrium of all components, such as for example the NRTL model. It is thus much faster and much less prone to over-fitting. The simulated performance of the process aligns very well with the pilot plant performance across 36 various steady state runs. It is concluded that with this updated version, the simulator is well-suited for simulating CO_2 capture plants to be integrated with various types of industrial process- and power plants. The main objective is focusing on operational aspects such as total energy requirements, actual performance data such as loading levels, circulation requirements and unit operation sizes. Here, the validation procedures includes a combined plant simulation including absorber, desorber and connected unit operations. Emphasis has been focusing on standardized software for mass validation of test campaign runs.

Keywords: Post combustion carbon capture; amine based CO_2 absorption; CESAR1 Solvent; solvent and process modelling; steady state model validation

1. Introduction

Design of full-scale CO_2 capture plants to meet certain operating and product specification is challenging especially if there are large variations in the flue gas. While these operating and product specifications mainly concern the CO_2 capture rate, amine emission limits, CO_2 quality, and minimizing utility consumption (energy, process and cooling water) and solvent loss, it is essential to have knowledge about all the aspects contributing to optimal plant design. Valuable insights into these aspects are achieved from pilot testing combined with simulations. However, despite the extensive testing over the last 20-30 years in a number of pilots of different sizes and at different locations, there are still knowledge gaps related to these aspects. In the ongoing EU-funded project AURORA (https://aurora-heu.eu/)

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both extensive pilot testing in three different pilots combined with modelling and simulation are important parts of the project for closing such gaps.

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 newly published 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 are now being implemented in Aspen Plus as well as in the SINTEF inhouse simulator CO2SIM.

The 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. The CESAR1 model was originally implemented in CO2SIM in the CESAR project[3] and has occasionally been updated since then. However, now in the AURORA project, a more thorough re-evaluation and update of the CESAR1 thermodynamic and physical property model framework has been conducted.

As indicated previously, pilot testing is also an important part of the AURORA project. As one of four planned test campaigns (in three different pilots), the pilot at SINTEF's CO_2 laboratory (Tiller pilot) was in operation with the CESAR1 solvent from September 2024 to April 2025. The tests involved a broad range of operating conditions related to varying CO_2 concentration, liquid flow-rate, gas velocity, and absorber and stripper temperature. The tests served the purpose of generating a broad set of data, *e.g.,* for investigation of capture rate variations up to 98% with different flue gases, and variation in absorber packing height and specific liquid load, enabling an improved basis for simulating full scale plants. The steady state conditions for some of the variations have been used to validate the updated CO2SIM model for the CESAR1 solvent.

2. Results

Sub-models. As indicated the underlying models describing the CESAR1 solvent have been re-evaluated. The most important model in such systems is the one describing the VLE relations, which is the sole contributor to yield the driving forces for the reactions and thus the applicability of the overall capture process. In Figure 1, the results of the VLE model and experimental data for 9 isotherms are shown. It covers the relevant temperature ranges for an absorber/stripper process. Especially data for low loadings and higher temperature are provided in the AURORA project and in total 13 different datasets (including datasets from literature) are used as indicated in the figure. It should be noted that the VLE for low loadings and elevated temperature is difficult to measure, while at the same time these data are important as this condition is found in the reboiler and lower part of the stripper. Another noteworthy point is that typical lean ranges for the total loading level for CESAR1 is very low, in the ranges of around 0.03 mol/mol, which shows that the CESAR1 solvent is easily stripped provided sufficient vapor dilution.

Validation. The Tiller pilot was simulated using automated routines that directly captures the relevant time series from the plant over an OPC-UA server. A full reproduction of the plant is thus modelled with identical measured operating conditions for each specific steady state run (36 steady state runs very chosen for the validation purpose), with varied operating conditions and inlet CO_2.concentrations. The software thus inserts specific unit data from the pilot plant into the flow sheet model and autogenerates the 36 runs for simulation. This thus enables efficient simulations with no need for manual case creation, it is all simulated in batch. Figure 2 shows a parity plot of the simulated versus experimental CO_2 production out of the stripper condenser. For the 36 simulated cases, which including the relevant unit operations in a closed system, the average deviation (AD) and average absolute deviation

(AAD) for the set is around 5%, indicating both high accuracy and precision, and in the same range as the deviation in the pilot dataset. This can also be seen in the plot. There is a slight systematic deviation at increasing capture rate. At low inlet concentrations, at around 2-3% CO_2 the simulations, shown in red dots, underpredict capture, and is slightly outside the 5% band, whereas at large capture rates it is systematically slightly overpredicted. It is argued that heat loss can be a reason for this discrepancy. Heat loss from such small pilot plants are significant, especially at low circulation rates where the solvent retention time through the plant gets higher. Although the pilot is equipped with thorough heat tracing systems and insulation, heat losses will still be a function of the circulation rate, where the relative loss is larger the lower this is. In this work, a non-linear heat loss correlation is used as function of liquid flow-rate, as we believe the loss will be slightly exponential at low flows.

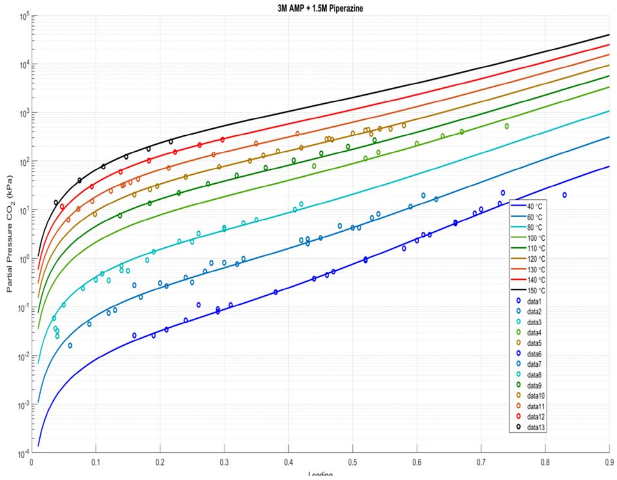

Figure 1: Results of a fitted Soft VLE model for various isotherms compared to experimental data from the AURORA project and from literature (13 data sets).

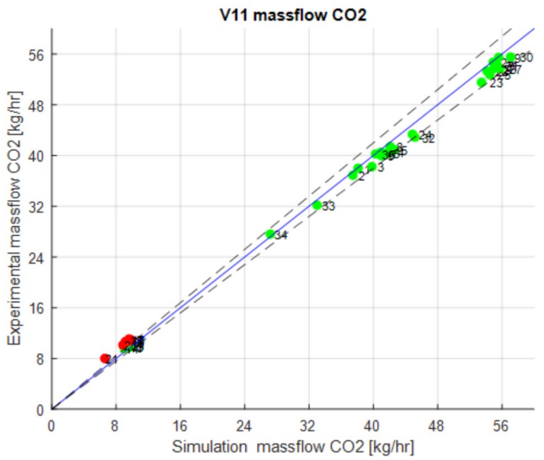

Figure 2: Parity plot showing total CO_2 flow [kg/h]out of stripper condenser for all pilot runs. Tiller pilot versus simulated for various operating conditions.

Selected case comparison

An arbitrary case was picked, run nr 34, to show simulated against the pilot results. Table 1 shows key simulated performance values for the given case. The loading range is determined based on thermodynamics and rates purely. The findings show that the predictive capability of CO2SIM within the test range is very high, both in terms of balances, thermodynamics i.e. loading ranges and corresponding temperature and enthalpy models. We believe this model is a significant improvement of the previous models we have worked with. Also shown are temperature profiles in the absorber and desorber (Figure 3 and 4, respectively) for this case

Table 1: KPI's of simulation of Run 34 from the Tiller pilot plant

Parameter	Unit	Run 34	Sim 34
CO_2 Inlet (dry)	vol%	11.1	***11.1***
CO_2 Recovery	%	98.4	***96.3***
Gas Inlet Temp (Absorber)	°C	37.6	***37.5***
L/G Ratio	kg/kg	1.35	***1.37***
Lean Loading	mol/mol	0.03	***0.03***
Rich Loading	mol/mol	0.65	***0.65***
Reboiler Duty	kW	25.0	***25.0***
SRD (based on CO_2 produced)	MJ/kg CO_2	3.25	***3.31***
Reboiler Liquid Temp	°C	121.4	***123.1***
Reboiler Vapor Temp	°C	122.6	***123.1***
Cold Rich Temp (TI05)	°C	37.7	***37.4***
Cold Lean Temp (TI08)	°C	40.0	***44.4***
CO_2 Product Flow	kg/h	27.0	***27.2***

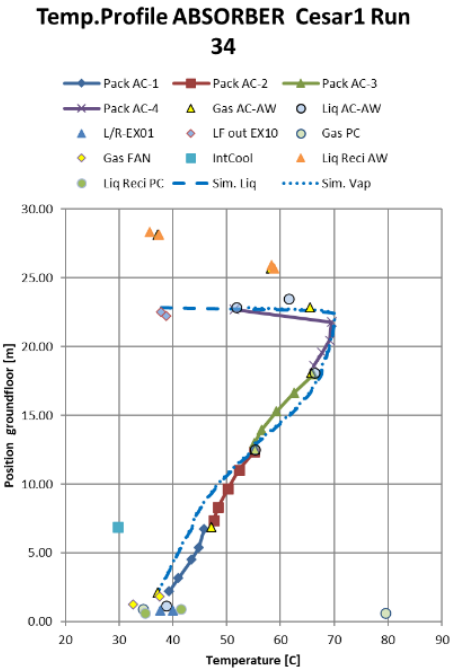

Figure 3: Internal temperature profile for the absorber packing. Simulation versus pilot.

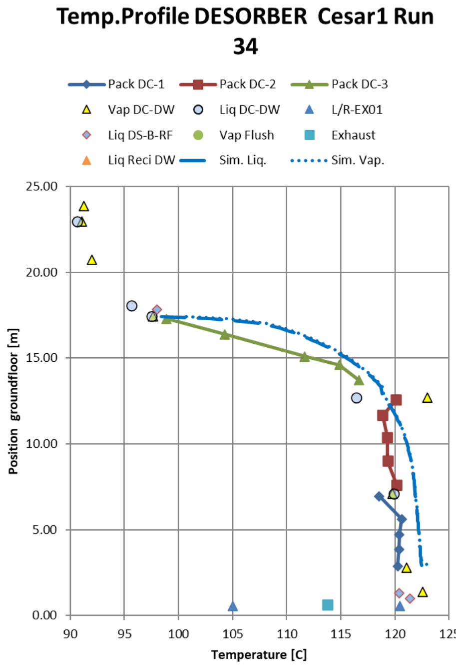

Figure 4: Internal temperature profile for the desorber packing. Simulation versus pilot.

3. Conclusion

The CESAR1 model in the CO2SIM simulator has been updated based on additional experimental data obtained in the AURORA project. The model is validated using extensive plant data from the Tiller pilot, which covers a broader range of CO_2 concentrations, gas and liquid flow-rates and reboiler temperatures than found available in open literature. The predictions of the simulator agree very well with the corresponding values obtained in the pilot plant. Based on this it is concluded that the simulator is well capable of being used for simulation of CO_2 capture plants to be integrated with various types of industrial process- and power plants. More details will be given at the conference.

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