IEAGHG 8th Post Combustion Capture Conference

16th to 18th September 2025 Marseille, France

Development of a new CESAR1 carbon capture model across various scales and inlet CO_2 contents

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Abstract

Post-combustion Carbon Capture (CC) appears essential to capture CO_2 from various industrial point sources. Amine(s)-based carbon capture is currently the most mature carbon capture technology and it can be relatively easy to apply it as an end-of-pipe unit with limited adaptations to the upstream industrial process. However, this CC process is characterized by a significant heat consumption for regenerating the solvent, requiring the use of more advanced solvents and/or process configurations for reducing its energy consumption. In this context, the CESAR1 solvent, an aqueous blend composed of 27 wt.% of 2-amino-2-methyl-1-propanol (AMP) and 13 wt.% of pipezarine (PZ), offers a promising alternative. This solvent was developed under the European-funded project CESAR [1] and pilot-scales tests have reported 20% less energy consumption compared to the conventional monoethanolamine (MEA) 30 wt.% solvent [2]. Moreover, the International Energy Agency Greenhouse Gas R&D program (IEAGHG) introduced CESAR1 as the new benchmark solvent [3]. To date, most studies on AMP/PZ have focused on pilot-scale experiments, with still limited data available for industrial applications. Predicting CC performance in industrial applications can be performed through numerical simulations. However, detailed modelling of the CC process with CESAR1 remains limited and no AMP/PZ model, to our knowledge, is currently available in open access libraries (e.g. in Aspen Plus® software). Therefore, developing a new detailed AMP/PZ model in Aspen Plus® is relevant. In this context, this work aims to develop a high-reliability AMP/PZ model in Aspen Plus® to assess the CESAR1 performances in industrial applications. The AMP/PZ solvent model is implemented in a comprehensive manner, ensuring consistency across thermodynamics, physico-chemical properties, and kinetics submodels. The model is first validated using the micro pilot-scale CC unit at University of Mons (UMONS). Once validated at micro-pilot-scale, the model is used to evaluate the performance of a small-scale industrial CC unit under varying CO_2 concentrations in flue gases, representative of applications from gas turbines (4 vol.%) to lime plants (24 vol.%).

The development of the AMP/PZ model is based on the accurate modelling of thermodynamics, physico-chemical properties and kinetics. Yi et al. [4] developed an open-access electrolyte NRTL (Non-Random Two Liquid) thermodynamic model for aqueous AMP, PZ and AMP/PZ solutions in Aspen Plus®. The model has shown good prediction of the CO_2 solubility and the heat of absorption for the CESAR1 composition [4]. Physico-chemical properties were modelled using built-in Aspen Plus models® and related database parameters. However, the viscosity

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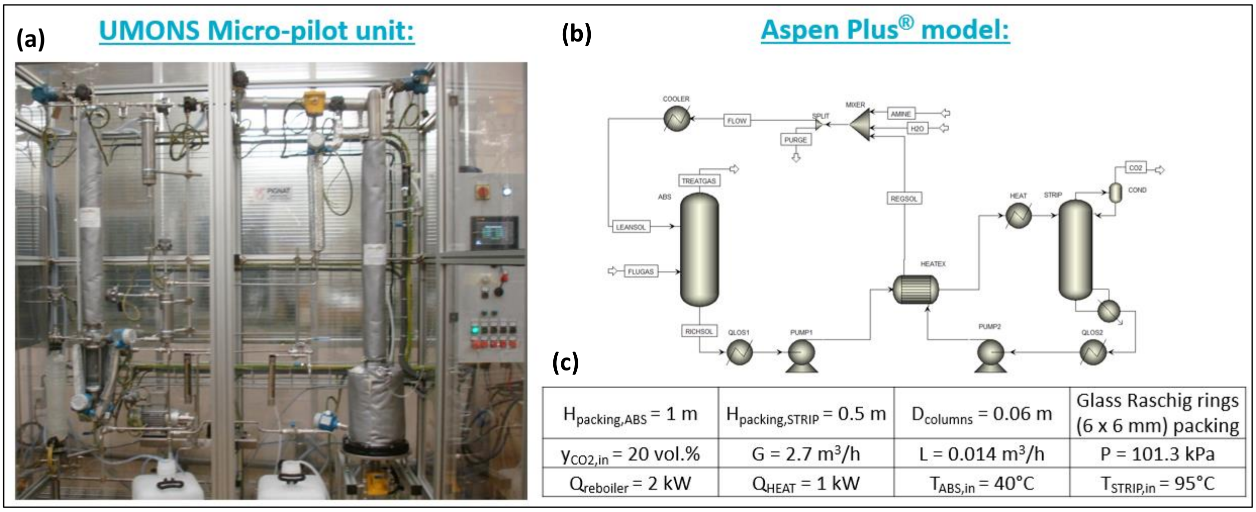
modelling, using the Jones Dole model, requires additional parameters regression, which was performed using viscosity measurements from literature for AMP-H_2O, AMP-PZ-H_2O and AMP-PZ-H_2O-CO_2 systems [5]. The various properties were validated against experimental data from the literature. Regarding kinetics and equilibria, the implemented reactions mechanism as well as the kinetic/equilibrium laws for the rate-controlled reactions are given in Table 1.

Table 1. AMP-PZ-CO_2 reaction mechanism and kinetic/equilibrium laws

	Reactions	Kinetic/Equilibrium law
1)	$2\ H_2O \leftrightarrow H_3O^+ + OH^-$	Gibbs free energy minimization
2)	$H_2O + HCO_3^- \leftrightarrow H_3O^+ + CO_3^{-2}$	Gibbs free energy minimization
3)	$PZH^+ + H_2O \leftrightarrow PZ + H_3O^+$	Gibbs free energy minimization
4)	$H^+\ PZCOO^- + H_2O \leftrightarrow PZCOO^- + H_3O^+$	Gibbs free energy minimization
5)	$CO_2 + OH^- \rightarrow HCO_3^-$	Pinsent et al. [6]
6)	$HCO_3 \rightarrow CO_2 + OH^-$	Pinsent et al. [6]
7)	$PZ + CO_2 + H_2O \rightarrow PZCOO^- + H_3O^+$	Bishnoi and Rochelle [7]
8)	$PZCOO^- + H_3O^+ \rightarrow PZ + CO_2 + H_2O$	Bishnoi and Rochelle [7]
9)	$PZCOO^- + H_2O + CO_2 \rightarrow PZ(COO)^{-2} + H_3O^+$	Bishnoi and Rochelle [7]
10)	$PZ(COO)^{-2} + H_3O^+ \rightarrow PZCOO^- + H_2O + CO_2$	Bishnoi and Rochelle [7]
11)	$H_2O + AMPH^+ \leftrightarrow AMP + H_3O^+$	Gibbs free energy minimization
12)	$AMP + CO_2 + H_2O \rightarrow HCO_3^- + AMPH^+$	Saha et al. [8]

The validation of the AMP/PZ model has been performed using the UMONS micro-pilot CC unit (see Figure 1). The micro-pilot unit, completely described in [9], has been simulated using the rate-based approach. For all the operating points, the inlet gas flow rate is 2.7 m^3/h with a CO_2 content of 20 vol.%. The solvent is regenerated at atmospheric pressure. The comparison of experimental and simulated absorption rate and Specific Reboiler Duty (SRD) is shown in Figure 2. The comparison shows good agreement across different solvent compositions, demonstrating the model validity at the micro-pilot scale under these specific conditions. Further validation at larger scales and different operating conditions is required to extent the applicability of the model.



$H_{packing,ABS}$ = 1 m	$H_{packing,STRIP}$ = 0.5 m	$D_{columns}$ = 0.06 m	Glass Raschig rings (6 x 6 mm) packing
$y_{CO2,in}$ = 20 vol.%	G = 2.7 m^3/h	L = 0.014 m^3/h	P = 101.3 kPa
$Q_{reboiler}$ = 2 kW	Q_{HEAT} = 1 kW	$T_{ABS,in}$ = 40°C	$T_{STRIP,in}$ = 95°C

Figure 1. UMONS micro-pilot unit (a), associated Aspen Plus® model (b) and micro-pilot data (c).

After validating the model at micro pilot-scale, simulations of a small-scale industrial CC unit, representative of larger pilot-scale CC unit, have been performed. These simulations are based on a previous work where a rate-based MEA CC model for micro gas turbine application was developed, characterized by a CO_2 content of 4.3 vol.% in the flue gas [10]. The gas flow rate for this unit is about 1000 m^3/h. A comparison between CESAR1 and the conventional

MEA 30 wt.% solvent is conducted. For each case, the solvent liquid-to-gas ratio (L/G) has been varied to find the minimum SRD (Figure 3), the capture efficiency being kept at 90%.

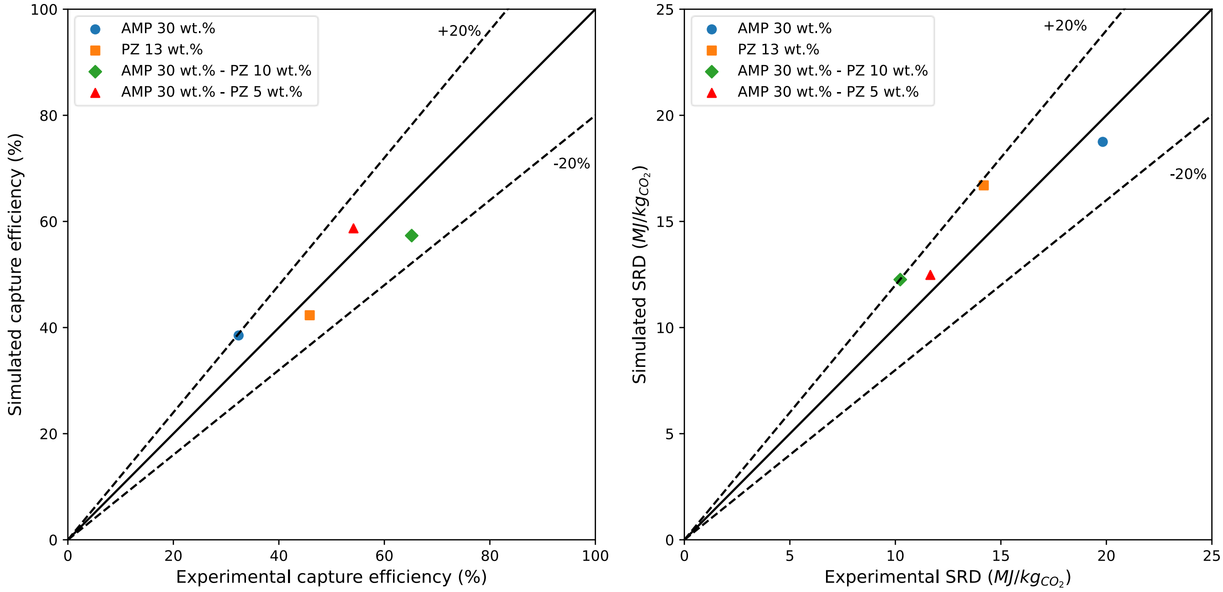


Figure 2. Comparison between experimental and simulated capture efficiency (left) and SRD (right).

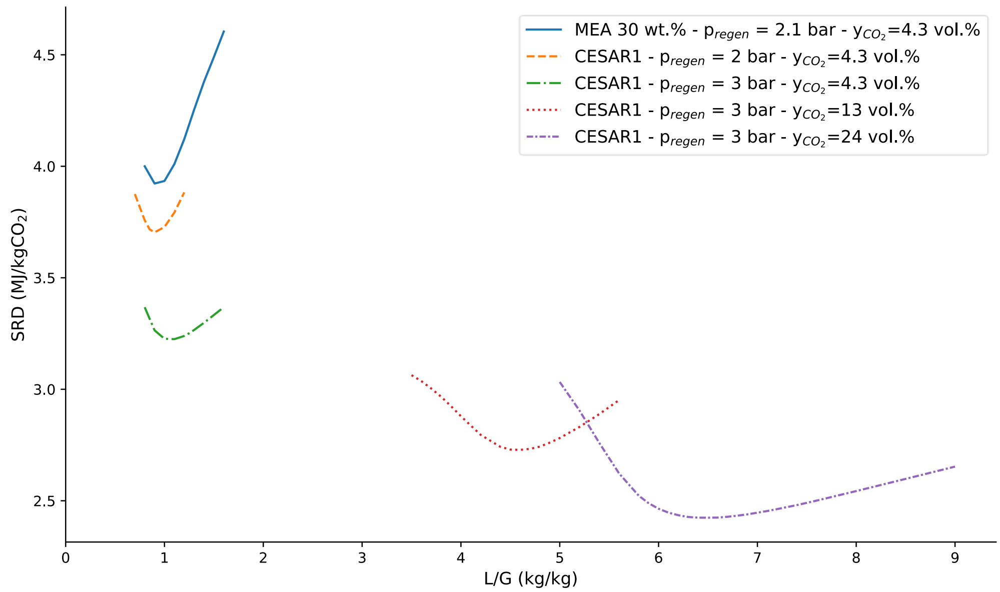


Figure 3. SRD as a function of the L/G for MEA 30 wt.% and CESAR1 for different flue gas CO_2 contents

At equivalent stripper pressures (2 bar for CESAR1 and 2.1 bar for MEA), the minimum SRD for CESAR1 (3.70 MJ/kg_{CO2}) is slightly lower compared to MEA (3.92 MJ/kg_{CO2}). Since CESAR1 is more resistant against thermal degradation, the stripper pressure can be increased up to 3 bar [11], leading to an optimized SRD of 3.22 MJ/kg_{CO2}, representing a 17.7% reduction compared to the MEA case. The obtained reboiler duties are consistent with those reported in the IEAGHG report for natural gas fired power plants [3].

To assess performance of CESAR1 for different industrial applications, additional simulations were conducted with increased CO_2 concentrations in the inlet flue gases (Figure 3). It can be seen that the SRD is strongly reduced at higher CO_2 contents with CESAR1. More specifically, for higher CO_2 contents, the optimal solvent flow rate increases significantly to achieve 90% capture. For a CO_2 content of 13 vol.%, representative of coal-fired power plants or waste incinerator, the optimal SRD is 2.73 MJ/kg_{CO2}. For a CO_2 content of 24 vol.%, typical of lime plant applications, the optimized SRD further decreased to 2.44 MJ/kg_{CO2}. These values are consistent with results reported in literature for similar applications [3,12], highlighting the model precision and robustness.

As a conclusion, a new comprehensive AMP/PZ model in Aspen Plus® has been developed in this study, which has been validated at micro-pilot scale under specific operating conditions. The model has been extended to a small-scale industrial CC unit applied to a micro gas turbine, demonstrating that CESAR1 outperforms conventional MEA solvent. Moreover, simulations with higher CO_2 concentrations in the inlet gas, representative of realistic applications, resulted in low specific reboiler duties, comparable to literature values, demonstrating the broad applicability of the model. Based on this model, future work will involve full-scale simulations of the CC unit for different applications, including techno-economic assessment, as well as the development of dynamic simulations with the CESAR1 solvent, which will be particularly innovative.

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Keywords: Amine-based CO_2 capture process ; CESAR1 solvent ; Aspen Plus® simulation ; Experimental validation ; Variable CO_2 contents.

Acknowledgments: Wallonia is warmly acknowledged for the funding of the NKL project in the framework of the Recovery and Resilience Plan (PNRR), initiated and financed by the European Union.