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ADVANCING THE LARGE-SCALE DEVELOPMENT OF PCC PROCESSES BY PROVIDING ESSENTIAL VLE DATA FOR AQUEOUS SOLUTIONS OF AMINES

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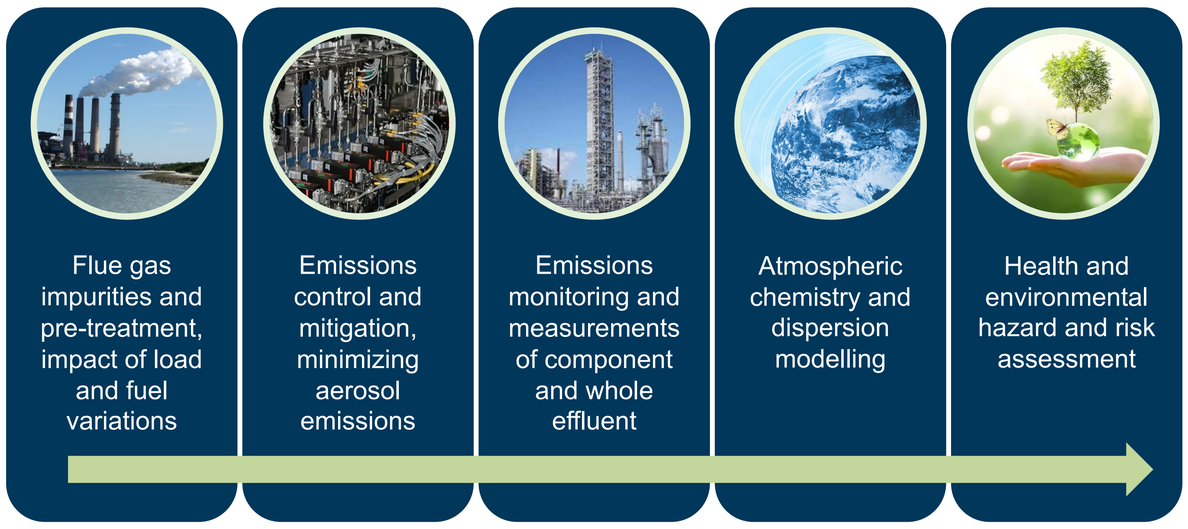
OBJECTIVES

Accelerate development and deployment of CO_2 capture technologies by providing essential **VLE data for the improvement of rigorous thermodynamic models** required in the design and optimization of amine-based carbon capture processes. This will help to:

- Improve the **prediction of amine emissions** from solvent-based carbon capture technologies
- Enable the **implementation of advance emission control strategies** in a range of industrial carbon capture applications
- Strengthen the **risk assessment** related to flue gas emissions at CO_2 capture facilities

SCOPE's project governing approach



VLE EBULLIOMETRIC DATA AND THERMODYNAMIC MODEL FOR AMP/PZ/H_2O SYSTEM

New VLE ebulliometric data for unloaded (i.e., without CO_2) aqueous AMP and PZ solutions are presented at 30 °C, 40 °C and 50 °C, and AMP:PZ ratios of 3:1.5/4:1/6:1 (Fig. 1). These solutions are representative of those measured in water wash systems placed at the top of absorber columns [1].

New VLE data complement existing VLE data in literature (Fig. 2) [2] and are correlated to further improve an **eNRTL thermodynamic model** (Table 1) implemented in Aspen Plus to be used in rate-based absorption process models **for rigorous design of absorber columns and water wash systems**.

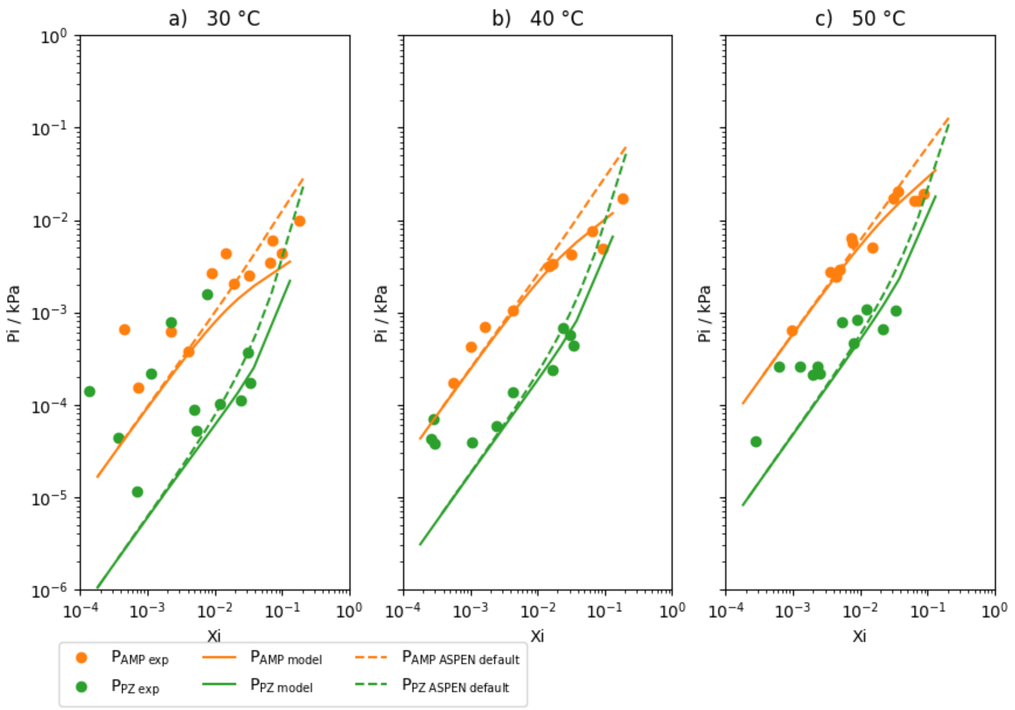


Fig. 1| Volatility of AMP & PZ and representation of the eNRTL model for the unloaded ternary system at temperatures: (a) 30 °C, (b) 40 °C, and (c) 50 °C and AMP:PZ ratios of 3:1.5/4:1/6:1. *Lines: eNRTL model in Aspen; ● New experimental VLE data*

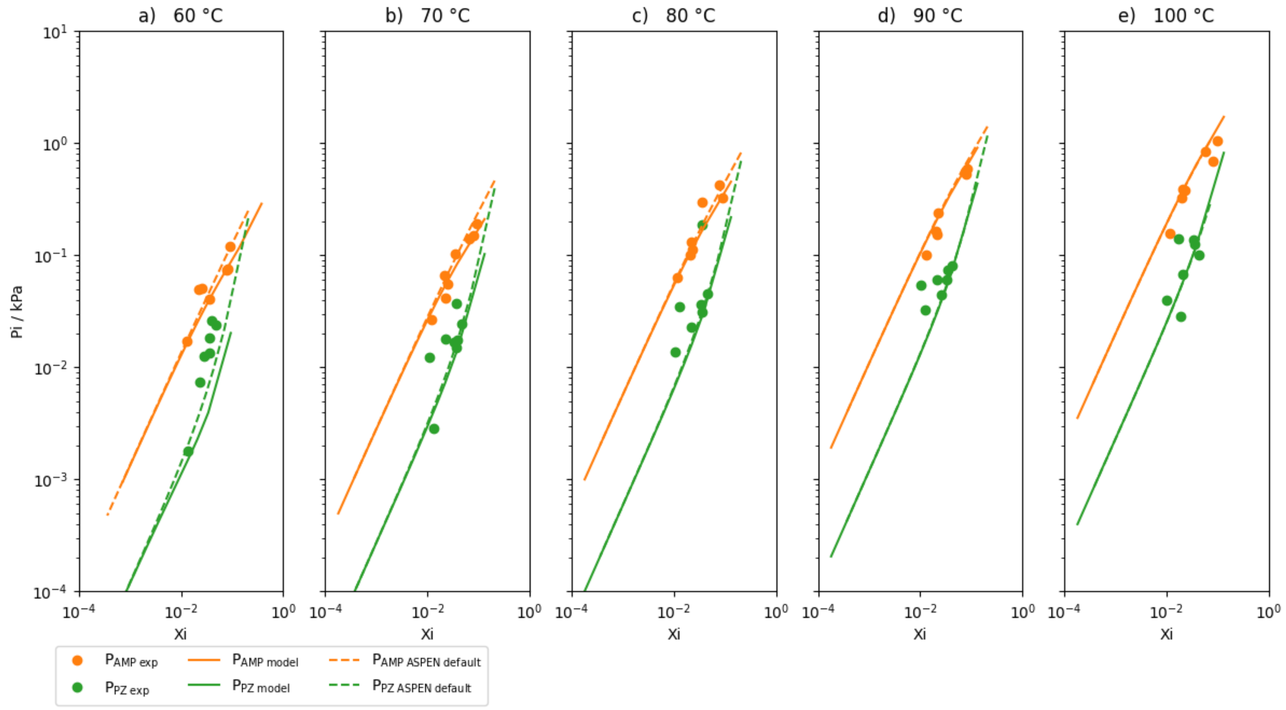


Fig. 2| Volatility of AMP & PZ and representation of the eNRTL model for the unloaded ternary system at temperatures: (a) 60 °C, (b) 70 °C, (c) 80 °C, (d) 90 °C, and (e) 100 °C. *Lines: eNRTL model in Aspen; ● Experimental data in [2]*

CONCLUSIONS

- **VLE data at low temperatures and concentrations of amines** (measured in water washer systems [1]) have proven to be extremely challenging to collect.
- In this work, **we push the equipment limits** by collecting VLE data of AMP and PZ at low concentrations and low temperatures.
- **With the new VLE data we aim to improve the existing model predictions** by providing essential data, currently lacking from literature, for improving the binary interaction parameters between the AMP and PZ of the eNRTL thermodynamic model.
- Additional measured VLE data will be added to further improve the predictions of the presented eNRTL thermodynamic model.

Table 1| Binary interaction parameters of AMP(1) + PZ(2) + H2O(3) for the eNRTL model.

System	Parameter	Quantity	Parameter	Quantity
AMP(1) + H_2O(3) [a]	a_{13}	-0.34	a_{31}	4.49
	b_{13}	-546.90	b_{31}	-372.00
PZ(2) + H_2O(3) [a]	a_{23}	-0.60	a_{32}	5.32
	b_{23}	-698.51	b_{32}	-1280
AMP(1) + PZ(2) [b]	a_{12}	0	a_{21}	19.10
	b_{12}	0	b_{21}	-7049.14

(a) Regressed in Hartono et al. 2013 [2]
(b) Regresses in this work

REFERENCES

[1] Moser, P. et al. *Int. J. Greenh. Gas Control* 109, 103381 (2021)
[2] Hartono, A. et al. *Chemical Engineering Science*, vol. 91, pp. 151–161 (2013)

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