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Assessing the Impact of Thermodynamic and other Modelling Choices in MEA-based CO_2 Capture Simulations

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ABSTRACT

Process modelling is essential to improve carbon capture unit design. However, depending on the modelling decisions made, such as the thermodynamic model and calculation method, the results obtained may vary significantly, hindering reliable process design. Nevertheless, studies that decouple the effects of thermodynamic packages and model approximations on simulation results are not well established. This contribution focuses on clarifying these effects and providing guidelines for the simulation of a CO_2 capture process with monoethanolamine (MEA) at different liquid-to-gas (L/G) ratios and CO_2 partial pressures in Aspen Plus. The calculations are validated with eight pilot campaign runs. The analysis reveals that the use of rate-based with kinetic reactions significantly improves the accuracy of the simulations. This approach, combined with the ENRTL-RK thermodynamic model, using Peng-Robinson for the vapor phase, provides the best performance, with average deviations below 3% in terms of CO_2 capture efficiency and energy requirements. On the other hand, strategies to improve convergence success in closed-loop simulations include replacing a single heat exchanger with two heater blocks, and a calculator block to automate mass-balance calculations and account for losses.

Keywords: Climate Change, Carbon Capture Utilization Storage (CCUS), Post Combustion Carbon Capture (PCC), Monoethanolamine (MEA), Aspen Plus Simulation

INTRODUCTION

The recent thirtieth conference of the parties (COP30) in Belém, Brazil, acknowledged the likelihood of overshooting the 1.5°C set during the Paris Agreement [1]. To limit global warming to 1.5°C requires rapid and deep emissions reductions of greenhouse gas (GHG) emissions such as carbon dioxide (CO_2) [2]. One of the key technologies that can curb these emissions, also reported in the Industrial Carbon Management (ICM) by the EU, is Carbon Capture, Utilization and Storage (CCUS) [3]. As the deployment of CCUS accelerates globally, rigorous process modelling becomes central to designing efficient and reliable CO_2 capture systems. Among different CO_2 capture technologies, the most mature and adaptable system at both pilot and industrial scale is post-combustion capture with monoethanolamine (MEA) [4].

Despite extensive literature on MEA capture systems, the bibliography on this topic remains fragmented and many results differ from one another. The main reason for these discrepancies is related to the choice of thermodynamic models, calculation methods (model complexity) and closed-loop convergence challenges. Most published works omit these details that matter in practice.

To address this gap, we investigate the independent effects and interactions between two different thermodynamic packages and calculation methods and document convergence tactics that enable stable solutions. The novelty of this study lies in the decoupling of thermodynamic models from calculation methods, along with the development of modelling strategies that facilitate convergence.

Specifically, the study compares the new unsymmetric electrolyte NRTL model (ENRTL-RK) for liquid with the Peng–Robinson Equation of State (EOS) for vapor phase, with ENRTL-RK combined with the Perturbed-Chain Statistical Association Fluid Theory (PC-SAFT). Furthermore, different degrees of model complexity,

such as equilibrium-stage, rate-based modelling, and chemical reactions are also revised to check their impact on Key Performance Indicators (KPIs). These KPIs include CO_2 capture efficiency (%) and thermal energy requirement (MJ/kg CO_2). Flowsheet convergence tips are also described to help in achieving closed-loop simulation convergence success.

The goal is to provide practical guidelines to follow when modelling post-combustion CO_2 capture processes using chemical absorption, especially at varying liquid-to-gas (L/G) ratios and CO_2 partial pressures.

PILOT PLANT SPECIFICATIONS

In this work, the pilot plant at the University of Kaiserslautern reported in [5] has been used for the validation of the process model developed in this work. The absorber and stripper column internals and the range of operating conditions are reported in Table 1. One of the parameters analyzed in this pilot plant was the variation in the L/G ratio while maintaining a constant gas flow rate. Two series of experiments were used for comparison: one with a low CO_2 partial pressure of 54 mbar (cases A1–A6) and another with a higher CO_2 partial pressure of 102 mbar (cases A7–12). In this work, eight of these experiments, covering both low and high CO_2 partial pressures and L/G ratios, were validated.

Key performance indicators

To validate the model using the experimental data from the pilot plant, two KPIs were defined, namely the CO_2 capture efficiency (η_{cap}) and thermal energy requirement (e_{req}). The following equations (1 – 3), based on the work of [6] were used to calculate these KPIs.

$$\dot{m}_{CO2,abs} = \dot{m}_{CO2,in} - \dot{m}_{CO2,out} \quad (1)$$

$$\eta_{cap} = \frac{\dot{m}_{CO2,abs}}{\dot{m}_{CO2,in}} \bullet 100 \quad (2)$$

$$e_{req} = \frac{\dot{Q}_{reb}}{\dot{m}_{CO2,abs}} \quad (3)$$

Here, $\dot{m}_{CO2,abs}$ is the absorbed CO_2 mass flow, $\dot{m}_{CO2,in}$ and $\dot{m}_{CO2,out}$ are the mass flow rates of CO_2 in the flue gas entering and exiting the absorber in kg/h, respectively, and $\dot{Q}_{reb}$ is the reboiler duty in MJ/h.

Model validation

The deviations between the experimental data and simulations results are given by the relative error (ε) and the percentage average absolute relative deviation ($\%AARD$). Equations (4 – 5) are used to calculate these deviations.

$$\varepsilon = \frac{x_{sim} - x_{exp}}{x_{exp}} \bullet 100 \quad (4)$$

$$\%AARD = \frac{\sum_1^n |\varepsilon|}{n} \quad (5)$$

where, x_{sim} is the simulation result, x_{exp} is the experimental value, and n is the number of data points.

METHODOLOGY

Process flowsheet

Aspen Plus v14 was used to build the flowsheet and simulate the MEA-based CO_2 capture process as depicted in Figure 1. The flue gas enters the bottom of the absorber while the lean solvent is introduced at the top. After absorption, the solvent is loaded with CO_2 and becomes the rich solvent. The rich solvent stream exits from the bottom of the absorber and is pumped through the heater block (half-heat exchanger), to finally enter the stripper, where the process is reversed. Following the stripper, the lean amine stream exits at the bottom and enters the second heater block (which acts as a cooler). This lean amine stream is mixed with the MEA and water makeups which are necessary to account for losses.

In the simulation, it is possible to use a single rigorous heat exchanger (HeatX) model to pre-heat the rich solvent and cool the lean solvent stream. However, for a closed-loop system, this approach creates two nested convergence loops: one for the HeatX block and the second one for the solvent recycle loop. This increases model complexity, making it prone to convergence issues, mostly related to temperature crossovers. To avoid this, two heater blocks connected using a heat stream are used instead of the single HeatX model [7]. In addition, for maintaining overall mass (material) balance, a calculator block is created in order to close the recycle solvent loop. This facilitates the convergence of the recycle stream by ensuring mass balances are accurate through the calculation of the required MEA and H_2O makeup streams.

Thermodynamic method and reactions

One of the most fundamental aspects to consider during process modelling is the choice of the thermodynamic method. This is because an incorrect decision of the thermodynamic package can lead to erroneous results in the simulation.

In this study, two slightly different thermodynamic methods are compared. The first uses the Electrolyte Non-Random Two-Liquid (ENRTL-RK) property method with the Peng–Robinson (PR) EOS to compute liquid and vapor properties, respectively [8]. This model was recently used by [9] and found to provide good predictions of the experimental data. The second thermodynamic package also uses the ENRTL-RK to calculate liquid phase properties but applies the PC-SAFT EOS for the calculation of the vapor phase fugacity coefficients [10].

For both property methods, the pure and binary parameters have been regressed or validated against available experimental data [8, 10]. Moreover, the following

chemical equilibrium reactions (equations (6 – 10)) were considered.

$$2H_2O \leftrightarrow OH^- + H_3O^+ \quad (6)$$

$$H_2O + HCO_3^- \leftrightarrow CO_3^{2-} + H_3O^+ \quad (7)$$

$$2H_2O + CO_2 \leftrightarrow HCO_3^- + H_3O^+ \quad (8)$$

$$H_2O + MEACOO^- \leftrightarrow MEA + HCO_3^- \quad (9)$$

$$H_2O + MEAH^+ \leftrightarrow MEA + H_3O^+ \quad (10)$$

Equilibrium constants of reactions (6)–(10) for both thermodynamic packages were calculated using the Gibbs free energy change described by equation (11).

$$\ln(K_j) = -\frac{\Delta G^o_{i,j}}{RT} \quad (11)$$

Here, K_j denotes the chemical equilibrium constant, $\Delta G^o_{i,j}$ is the standard free energy of formation of component i, R is the universal gas constant, and T is the temperature in Kelvin.

On the other hand, carbamate and hydrolysis reactions are typically expressed as kinetically controlled reactions, given by equations (12 – 13). Kinetic constants for these reactions can be found in [10].

$$MEA + CO_2 + H_2O \rightarrow MEACOO^- + H_3O^+ \quad (12)$$

$$MEACOO^- + H_3O^+ \rightarrow MEA + CO_2 + H_2O \quad (13)$$

Equilibrium-stage modelling

The Aspen Plus RadFrac block allows two calculation methods: equilibrium and rate-based modelling. Furthermore, in both methods it is possible to consider equilibrium or kinetic reactions in the liquid phase.

In this work, equilibrium-stage modelling was the first approach used, setting the number of stages to 20 for both columns. This approach assumes perfect mixing and does not take into account mass-transfer. Nonetheless, it is recommended as a first step because it facilitates the convergence of the closed-loop simulation, producing initial column estimates (such as temperature and composition) that are useful when moving to the more advanced rate-based modelling. Additionally, for the same equilibrium model, different model complexities regarding reaction information can still be applied, as reported in [11].

The first model used in this paper was the equilibrium-stage with chemical equilibrium reactions (EQ). Then, after successful convergence of the closed-loop simulation, the complexity can be increased to equilibrium-stage using kinetic reactions (EK). Nonetheless, when switching to EK model, data for liquid holdup or liquid residence time is required. In this contribution, the liquid holdup values reported by [12] were used. After successful convergence of the EK model, the columns can then be switched to rate-based modelling to account for mass transfer phenomena.

Rate-based modelling

In reality, the previous equilibrium-stage assumptions are never satisfied because of the highly non-ideal behavior of CO_2 capture systems. To address these limitations, the rate-based model is also tested. The rate-based model accounts for both mass and heat transfer. The mass transfer is explained by the two-film theory (Figure 2), which uses the Maxwell-Stefan approach [13].

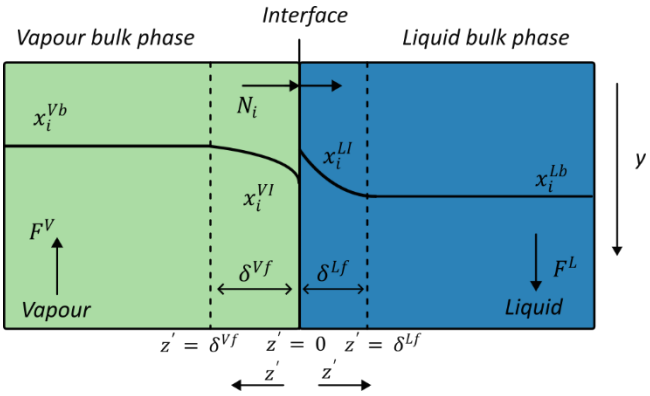


Figure 2. Two-film theory (model) for a packing segment adapted from [13].

Similar to equilibrium modelling, rate-based models also accept two approaches to define chemical reactions. The first one is rate-based model with chemical equilibrium reactions (RE), while the second one uses also the rate-based model but with kinetic (RK) and film reactions. This last model is considered the most complex.

In rate-based modelling, the column geometry must be specified for both absorber and stripper. To this end, data presented in Table 1 is utilized to replicate the pilot plant that will be used for validation. On the other hand, Table 2 reports the model parameters used for the rate-based model, which are common for the two thermodynamic models used in this work. For the liquid, vapor mass transfer, and interfacial area factor, the correlation by [14] is used. The heat transfer has been modeled using [15] and the liquid holdup was calculated by [16]. Additionally, the liquid film was discretized into 5 points and the reaction condition factor was set to 0.9 as suggested by [17].

Combining equilibrium-stage and rate-based modelling, along with equilibrium and rate-limiting kinetic reactions, and two thermodynamic packages, a total of eight different calculation models were tested.

Table 1: The main pilot plant specifications [5].

Parameter	Data	Unit
Flue gas source	Natural gas burner	(-)
CO_2 concentration in the flue gas	3–14	(vol%)
Liquid flow rate	20–350	(kg/h)
Flue gas flow rate	30–100	(kg/h)
Liquid load in the absorber	2–28.5	($m^3/(m^2h)$)
Electrical heat duty of evaporator	0–30	(kW)
Absorber pressure	Atmospheric pressure	(bar)
Stripper pressure	1.0–2.5	(bar)
	Absorber Geometry	
Total height of packing in absorber	4.25	(m)
Column internal diameter	0.125	(m)
Type of packing	BX 500	(-)
	Stripper Geometry	
Total height of packing in stripper	2.55	(m)
Column internal diameter	0.125	(m)
Type of packing	BX 500	(-)

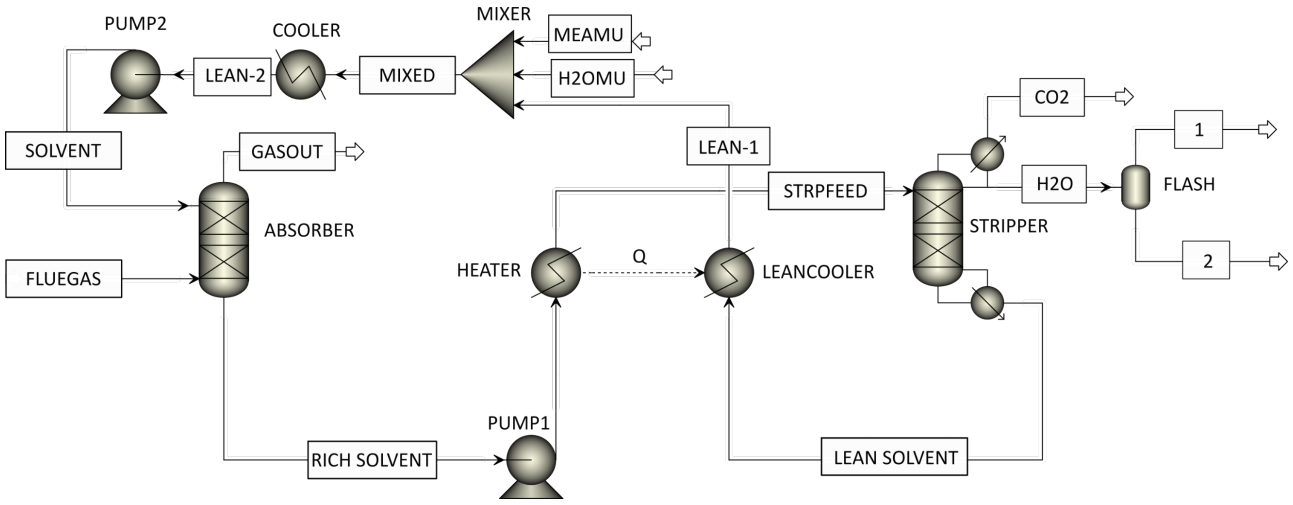


Figure 1. Process flowsheet of MEA CO_2 capture process.

Table 2: Rate-based model parameters used.

Parameter	Specification
Number of segments	20
Flow model	Mixed
Mass transfer coefficient method	Brf-85
Heat transfer coefficient method	Chilton and Colburn
Interfacial area method	Brf-85
Interfacial area factor	1
Liquid holdup correlation	Brf-92
Reaction condition factor	0.9
Film discretization ratio	5

RESULTS AND DISCUSSION

Effect of thermodynamic and model complexity

The process modelling results of the eight runs carried out at the University of Kaiserslautern are evaluated. The CO_2 capture efficiency (%) and the thermal energy requirement (MJ/kg CO_2) are the two KPIs evaluated and compared for the four different model complexities.

A summary of the %AARD in all KPIs for these models is given in Table 3. Both thermodynamic models predict the KPIs with an AARD of less than 10%. Among the KPIs, the thermal energy requirement is the one that can

be most accurately predicted. Nonetheless, some differences arise regarding the use of different model complexities. Including kinetically-controlled reactions significantly impact the results when using rate-based models. As an example, for the ENRTL-RK with Peng–Robinson, the model predicts the CO_2 capture efficiency and thermal energy with an AARD of 9.23% and 7.96%, respectively, when using rate-based model with equilibrium reactions (RE), but improves to 2.46% and 2.84%, respectively, when including kinetic reactions (RK). When using ENRTL-RK with PC-SAFT, the same pattern is noticed, but with minor improvements, especially for thermal energy requirement.

Lastly, the incorporation of mass-transfer kinetics also has a significant influence on the results, particularly when using ENRTL-RK with Peng–Robinson. Switching from equilibrium to rate-based model, when already considering kinetically controlled reactions (i.e., from EK to RK), improves predictions of CO_2 capture efficiency from 8.31% to 2.46%. Likewise, using PC-SAFT for the same KPI, the deviations decrease from 7.97% to 5.46%. For the thermal energy requirement, predictions improve by 61% (i.e., from 7.23% in EK to 2.84% in RK) when using Peng–Robinson and by 8% (from 7.05% to 6.47%) if using PC-SAFT.

These results highlight the fact that when thermodynamic binary parameters from both models have been properly validated against experimental data (heat capacity, density), they play a minor role compared with model complexity. In this case, where the same property method was used to calculate liquid properties (ENRTL-RK), the choice of different EOS for the vapor phase did not alter the results significantly, achieving minor differences in %AARD between Peng–Robinson and PC-SAFT for the same model complexity. However, for the same thermodynamic model, %AARD changed significantly when moving from classic equilibrium-stage model to the more advanced rate-based model with kinetic reactions.

Effect of L/G ratio and CO_2 partial pressure

After checking the average patterns from the two KPIs, this subsection examines these KPIs for each run analyzing the impact of the L/G ratio and CO_2 partial pressure. Figure 3 depicts the relative errors of the calculated CO_2 capture efficiency at low (A1, A4, A5, and A6) and high (A9, A10, A11, and A12) CO_2 partial pressure across various L/G ratios using the two thermodynamic methods.

It is apparent from Figure 3 that both thermodynamic methods perform well and are comparable to each other, although slight differences arise. At both, low and high CO_2 partial pressures and L/G ratios, the two thermodynamic models overestimate experimental results by 5–11% when using chemical equilibrium reactions (EQ and RE). However, when using kinetically-controlled reactions (RK, crimson-red) PC-SAFT underestimates experimental results by 1–11%, whereas, with Peng–Robinson, simulation results either underestimate or overestimate experimental values in the range of (-5%)–2%, showing excellent agreement with the data at high CO_2 partial pressures. Switching the mass-transfer model to EK (light blue), results in overestimation of the calculations by 0–11% for both thermodynamic packages.

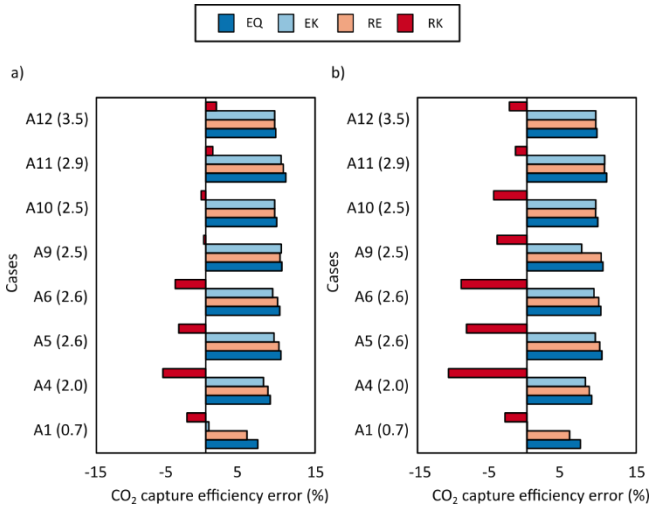


Figure 3. Relative error (%) for CO_2 capture efficiency using: (a) ENRTL-RK with Peng–Robinson and (b) ENRTL-RK with PC-SAFT. L/G ratio value in brackets.

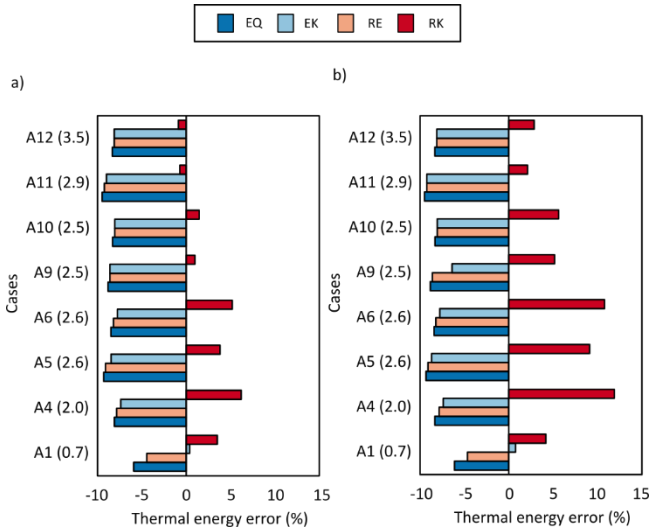


Figure 4. Relative error (%) for thermal energy requirement using: (a) ENRTL-RK with Peng–Robinson and (b) ENRTL-RK with PC-SAFT. L/G ratio value in brackets.

Figure 4 illustrates the relative errors of the calculated thermal energy requirement for both low and high CO_2 partial pressures and L/G ratios. As shown in the figure, the differences between the results using the two thermodynamic models are comparatively small, with the

Table 3: % AARD between the pilot plant data based on 8 runs and the process modelling results using different model complexities and two thermodynamic methods.

Thermodynamic method	Model complexity	CO_2 capture efficiency (%)	Thermal energy requirement ($MJ/kgCO_2$)
ENRTL-RK Peng–Robinson	EQ	9.66	8.35
	EK	8.31	7.23
	RE	9.23	7.96
	RK	2.46	2.84
ENRTL-RK PC-SAFT	EQ	9.68	8.39
	EK	7.97	7.05
	RE	9.25	7.98
	RK	5.46	6.47

exception of the RK model.

Interestingly, when using chemical equilibrium reactions (EQ and RE) the calculated values consistently underestimate the thermal energy requirement in the range of (-9%)–(-4%), irrespective of the mass-transfer method. Conversely, using kinetically-controlled reactions (RK, crimson-red) with PC-SAFT clearly over-predicts the experimental results in the range of 2–12%.

This also happens when using Peng–Robinson with kinetic reactions (crimson-red), but in these cases the thermal energy has more modest overestimations, with overall deviations between (-1%)–6%.

Additionally, it can be seen that the results using PC-SAFT for RK (crimson-red) overestimate the experimental values compared to Peng–Robinson at both low and high CO_2 partial pressure values (Figure 4). This result was also evident in Figure 3 when predicting CO_2 capture efficiency, yet, in that case, the deviations were causing an underprediction. The analysis shows that the differences between the two thermodynamic models is comparatively small at low CO_2 partial pressure and L/G ratio between 0.7 and 2.6.

However, at high CO_2 partial pressure and L/G >2.5 the choice of the EOS for the vapor phase (Peng–Robinson) affects the results, particularly in rate-based model with kinetic reactions.

CONCLUSIONS

The purpose of the present contribution is to provide a framework for accurately simulating a post-combustion CO_2 capture process using MEA by evaluating the effects of thermodynamic models and mass transfer methods, under different modelling decisions and chemical reactions assumptions.

During process modelling, two strategies were identified to facilitate convergence of closed-loop simulations. The first strategy consisted of replacing a rigorous heat exchanger with two heater blocks connected by a heat stream. The second strategy consisted of using a calculator block to automate the computation of solvent and co-solvent (water) makeup, thereby maintaining material balance in the system automatically.

The two thermodynamic models used were based on the ENRTL-RK method for liquid phase properties, but differing on how vapor phase properties are calculated (Peng–Robinson vs PC-SAFT).

The results indicated that both thermodynamic methods yielded an %AARD below 10% in all cases, showing comparable results in most mass transfer approaches. However, the use of the rigorous RK model revealed that ENRTL-RK with Peng-Robinson was superior to ENRTL-RK using PC-SAFT, reducing average deviation by approximately 50% for both KPIs.

For the computational cost, both equilibrium-stage and rate-based simulations exhibit acceptable performance for isolated runs, in the order of 1.0-2.0s (EQ; the simplest) and 11.0-22s (RK, the most complex) using a 13th Gen Intel(R) Core i7-1355U and 16.0 GB RAM machine. While this difference might seem small in practice, it can become relevant when the process model is embedded within an optimization framework potentially requiring the evaluation of thousands of solutions. Furthermore, the rate-based model provides greater accuracy, yet it requires additional data such as column internals (tray or packing specifications) and reliable mass transfer correlations, which might not always be available in practice. Hence, modellers may select simplified approaches in contexts where deviations on the order of 10% are deemed acceptable.

The current process model was validated using experimental data from a single pilot-plant operating under post-combustion conditions representative of gas-fired and coal-fired power plants. Although the validation considers a reasonably broad range of L/G ratios (0.7-3.5) and inlet CO_2 compositions (CO_2 partial pressures, 54-102 mbar), the applicability to other pilot plants or to op-

erating conditions outside this range cannot be guaranteed. Therefore, this should be regarded as a limitation of the present study.

Nevertheless, the results obtained here provide useful insight into the model performance within the tested domain. In particular, for the cases analysed, the Peng-Robinson equation of state for the gas phase showed better performance at L/G ratios above 2.5, suggesting that it may be a more suitable option for plants operating under similar conditions. The combination of this model within the rate-based with kinetic equations framework assures very good accuracy for the KPIs studied, particularly at higher CO_2 partial pressures. Still, extrapolation to other systems should be carried out with caution. For reliable application to different pilot plants or operating windows, the thermodynamic model should be assessed and, if necessary, fit using experimental data representative of the corresponding conditions. Even in that case, real-world systems may deviate from the assumptions made in the model. This is because the predictive accuracy depends on the quality and availability of data for parameters such as mass transfer coefficients and kinetic constants, which might not always be available in practice.

In conclusion, the results presented in this paper may be used as practical guidelines for the accurate design of post-combustion CO_2 capture systems using rate-based models with kinetic reactions, adaptable to various L/G ratios and CO_2 partial pressures.

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