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Validation of process simulator with new plant data for MEA and CESAR1

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Abstract

Process simulators are frequently used to design and optimize CO_2 capture plants. Aqueous monoethanolamine (MEA) is the most studied solvent with CESAR1 (aqueous blend of 2-Amino-2-methylpropan-1-ol and piperazine) being considered the next benchmark solvent for post-combustion carbon capture. Although the physicochemical properties of several open solvents such as aqueous solutions of MEA and CESAR1 are reasonably well described in the literature, comparison with plant data under PCCC conditions are less commonly found. In this work, the commercial process simulator ProTreat® is used to simulate data points obtained in 3 different plants, namely: (i) TNO's mini plant I and (ii) II both using 30wt% MEA and (iii) RWE pilot plant using CESAR1. The simulations are compared to the experiment data in terms of rich loadings, temperature profiles, duties, etc. The ProTreat® process simulator was used to model the experimental campaigns with good accuracy. Therefore, process design using it can be regarded with good level of confidence. Besides, ProTreat® showed exceptional speed and convergency rates for the cases studied and an easy user interface to set up simulations.

Keywords: CO_2 capture; pilot campaign; MEA; CESAR1;

1. Introduction

Carbon capture and storage (CCS) is acknowledged as a necessary tool to support the energy transition and achieve carbon neutrality [1], [2]. Chemical absorption using amine-based solvents is the state-of-the-art process for post-combustion CO_2 capture with several plants under operation. Process simulators are often used to design, simulate and optimize such plants. Although the physicochemical properties of several open solvents such as aqueous solutions of monoethanolamine (MEA) and CESAR1 (aqueous blend of 2-Amino-2-methylpropan-1-ol and piperazine) are reasonably well described in the literature, comparison with plant data under PCCC conditions are less commonly found. In this work, the commercial process simulator ProTreat® is used to simulate data points obtained in 3 different plants, namely: (i) TNO's mini plant I and (ii) II both using 30wt% MEA and (iii) RWE pilot plant using CESAR1.

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The simulations are compared to the experiment data in terms of rich loadings, temperature profiles, duties, etc. This work intends to validate the simulator and identify the most important properties to be accurately represented that will have a significant impact on the design of novel capture plants.

2. Studied plants

A typical absorption process consists of an absorption and desorption (closed) loop as shown in the simplified diagram presented in Figure 1. The main equipment is the absorber and desorber towers, heat exchangers, fan and pumps. Most of the times, the absorber column also hosts the water wash section. To adjust the flue gas temperature (and sometimes, contaminant levels) to absorber conditions, a direct contact cooler (not shown) is often employed prior to the absorber.

Due to the exothermic reaction between CO_2 and the solvent, the temperature of both gas and liquid will rise inside the absorber. The increase in temperature has an adverse effect in the solvent capacity, and to better control it and maintain a higher absorption capacity, an absorber intercooler stage is sometimes placed.

Although, the plants studied in this work have different characteristics as shown in Table 1, they share the same basic absorption-desorption loop shown in Figure 1.

TNO has two mobile mini plants to test the capture performance of solvents operating with real flue gas at industrial locations, or with artificial flue gas at a controlled lab environment. They are both part of the ECCSEL research facilities infrastructure [3], while mini plant II is also ATEX-compliant, thus it can be used in potentially hazardous or explosive atmospheres, such as refineries. The mini plants have been used in various projects (ALIGN-CCUS, LAUNCH-CCUS, REALISE, NEWEST) to study the removal capacity as well as stress-test the stability of different solvents with flue gas from different industries, investigate emission mitigation technologies and research solvent degradation. Both plants have an absorber diameter of 44.96 mm and packing heights of approximately 4.3 m. TNO's mini plants have capacity to process up to 5 Nm^3/h of gas, producing up to 1 $kgCO_2/h$.

RWE operates a CO_2 capture pilot plant at their lignite power plant in Niederaussem. The plant treats 1150 Nm^3/h of flue gas. Two long-term testing campaigns with MEA (30 wt.%) have been conducted (after the commissioning in 2009 (5,000 hours [4]) and within the ALIGN-CCUS project (18,000 hours [5]) campaign with MEA, and an even longer campaign (more than 28,000 hours [6]) with CESAR1 is on-going as part of the LAUNCH project. The absorber diameter and packing heights are 0.61 m and 18 m, respectively.

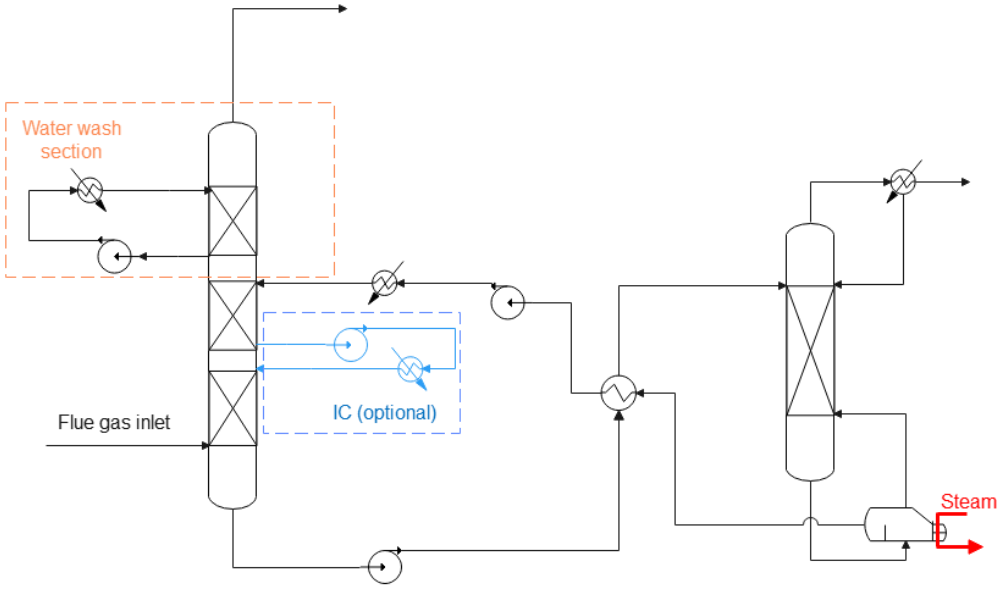

Figure 1: Simplified flow diagram from a typical CO_2 capture plant.

Table 1: Studied plant's data.

		TNO mini plant I	TNO mini plant II	RWE pilot
Absorber				
Packing type	-	Sulzer BX SS	Sulzer BX SS	Confidential
Packing height	m	4.30	4.25	(4x) 4.5
Diameter	m	0.045	0.045	0.60
Inter cooler		No	No	Yes
Stripper				
Packing type	-	Sulzer BX SS	Sulzer BX SS	IR40
Packing height	m	2.04	1.53	(2x) 5
Diameter	m	0.045	0.045	0.45
Absorber water wash				
Packing type	-	N/A	Sulzer BX SS	Confidential
Packing height	m	N/A	1.53	3
Diameter	m	N/A	0.045	0.60

3. Methodology

In total 16 experimental runs were validated: 7 from TNO mini plant I, 4 from TNO mini plant II and 5 from RWE pilot plant. The simulations were performed considering every plant characteristic. The direct contact cooler was not modelled in this work, and the absorber gas inlet input was taken at the corresponding gas conditions. For the cross-heat exchanger, the rich outlet temperature was set.

For the RWE plant, the absorber packing was not disclosed. So, Mellapak 250X was assumed and the interfacial area factor was adjusted to fit the rich loading data. A single optimal interfacial area factor was found and used to simulate all runs. The reboiler duty was used as input, and the reboiler temperature and other variables were calculated.

For the runs evaluated from TNO's mini plants, the reboiler temperature was set in the simulations instead of the reboiler duty since the mini plants' heat losses and limited absorber height do not allow for generating representative energy numbers. The packing used in the mini plants was not available in ProTreat®, so we selected Mellapak 500X and set the interface area factor to 0.88.

4. Results and discussion

In this section, the results from the simulations are shown and discussed. To validate the experiments, a mass balance check was performed. This was aimed to validate and give confidence to the measurement techniques used in the campaigns. The mass balance was performed on the CO_2 produced calculated via the gas (flow rate of CO_2 in the stripper) and liquid phases (liquid flow rate and amine/CO_2 concentration).

4.1. Mass balance

The mass balance check was performed for all experimental runs. The CO_2 produced was calculated via both the gas and liquid phases. The mass balance calculated from RWE agrees within 1% deviation. For TNO's mini plants the deviations are somewhat higher. However, as shown in

Figure 2, most of the results agree within 20% deviation (dashed lines) which is acceptable for small pilot plants. Given the small size of the pipes, heat losses are practically unavoidable which could lead to, for instance, condensation drastically affecting measurements (e.g., gas flow rate). This could explain why, in general, the results from the mini plants seem to predict a higher CO_2 production from the liquid phase.

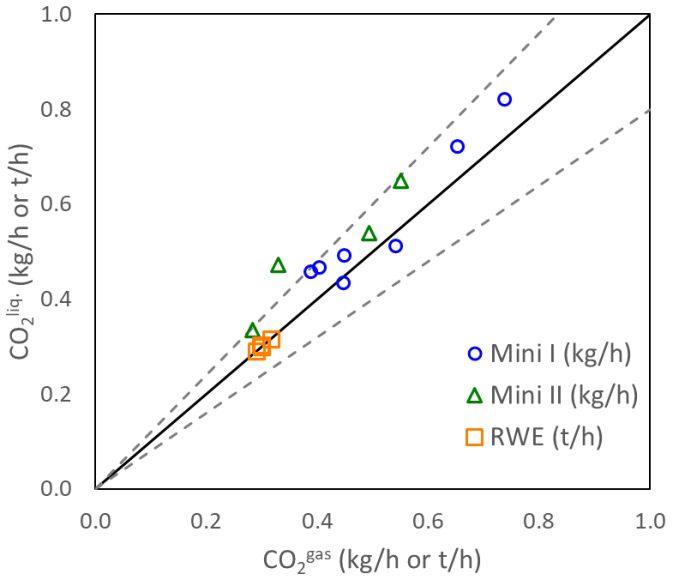

Figure 2: Mass balance check for the experimental runs. Solid line (y=x), Dashed lines: ±20%.

4.2. Simulation results

As mentioned above, for RWE simulations the reboiler duty was set and variables such as lean loading, reboiler temperature, and absorber outlet temperature were calculated by the simulation. The ratio between calculated and experimental measurements are shown in Figure 3. The reboiler temperature shows good agreement and is calculated within 1% deviation. The interfacial area factor was varied to match the experimental rich loading since the packing was not disclosed. The results show a good agreement within 5% with slightly higher deviation (<10%) seen for run #5. The lean loadings, on the other hand, present higher deviations, except at run# 3. The experimental lean loadings were very lean ranging from 0.02 to 0.06 (except at run# 3 where lean loading was 0.17) which small absolute deviation would give large relative deviations. For instance, run# 2 presents the lowest experimental lean loading, i.e. 0.023, and calculated lean loading was 0.062 (about 167% deviation). When comparing to run# 3 (higher lean loading, 0.168), the deviation reduces drastically about 13%. For the other runs (with lean loadings ranging from 0.05 to 0.06), the deviations are calculated between 36 to 50%.

Although ProTreat® is a fully rate-based simulator, for the post-combustion plant, the stripper calculations rely mostly on the equilibrium calculations. In a P_{CO2}-α diagram, the pressure presents a very steep behavior in the low loading region, and a small deviation in the partial pressure will lead to a significant deviation in the loading. When fitting a thermodynamic model, the low loading range usually presents higher deviations. This is also related to the uncertainty of the experiments. Since RWE mass balance is calculated within 1% deviation, it is believed that the lean loading deviation is caused by the expected uncertainty of the model in this region. As shown in Ferron et al.[7], the equilibrium data at stripper conditions (above 100˚C) do not cover very lean loadings region. Under the transnational project SCOPE (Sustainable OPEration of post-combustion Capture plants, ACT 3 Project No 327341), new data will be generated and ProTreat® model will be refitted for both MEA and CESAR1. This could improve the accuracy of the model and lean loadings calculations.

The lean loadings deviation will direct impact the CO_2 produced calculations. In the RWE case, the calculated lean loadings were consistently higher than experimental (and rich loadings with little deviation) which will result in the underprediction of the CO_2 produced and overprediction of energy requirements. As seen in Figure 3, the specific reboiler duty (SRD) was consistently higher than experimental and calculated within 10% deviation for most runs.

Run #3, where the lean loading was higher (i.e., 0.168), the SRD is calculated with less than 1% deviation. The same is observed for the CO_2 produced.

The absorber liquid outlet and lean outlet of cross heat exchanger temperatures were mostly calculated within 10% deviation. As seen, the absorber liquid outlet temperature is overpredicted indicating that either a possible heat loss in that section of the plant or the heat model is predicting higher heat of absorption. For the cross-heat exchanger we used a simple model which does not account to any operational issues (e.g., heat transfer resistance). Nevertheless, 10% deviation on those temperatures is acceptable for these simulations.

For TNO simulations, given the uncertainty in the reboiler duty measurements, we opted to set the reboiler temperature and calculate the other variables. However, the calculated lean loading ranged from 20 to 40% lower than the experimental. Small changes in the reboiler temperature, nevertheless, could lead to significant changes in the lean loadings. It was, therefore, decided to adjust the reboiler temperature to match the experimental lean loading. In ProTreat® this can be easily done using the solver block.

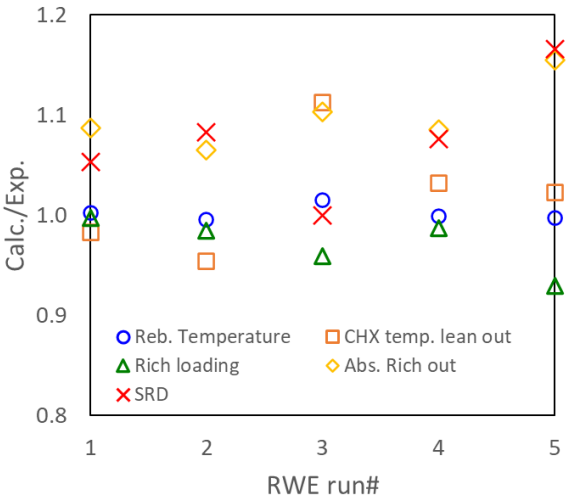

Figure 3: RWE pilot plant simulation results for CESAR1.

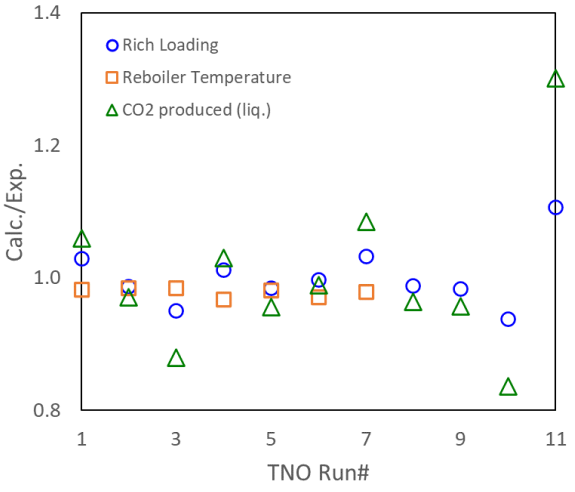

Figure 4: TNO mini plants simulation results for 30 wt.% MEA.

Figure 4 shows the results from TNO's mini plants simulation (runs# 1 to 7 for mini plant I and 8 to 11 for mini plant II). Given the size of the pipes and equipment in the mini plants, heat losses are expected to occur. This is seen when comparing the calculated temperature (e.g., absorber liquid outlet). For example, the temperature of the lean solvent entering the cross-heat exchanger should be close (or equal) to the reboiler temperature. For mini plant II, given its configuration, there is a difference in these temperatures of more than 10 degrees Celsius. Since heat losses are known for these pilots, and not considered in the simulations, we are not presenting the temperature comparison around the cross-heat exchanger for TNO results.

Figure 5 shows the absorber temperature profile of selected runs from TNO's mini plant. As seen, the calculated temperature profile follows the same trend as the experimental measurements. Run#1 presented an excellent agreement between the calculated and measured values, with only the temperature on the top of the column being underestimated. For the other runs, especially at the upper part of the column, the deviations were more significant with the measured values consistently higher than the calculated.

This behavior could be explained by the small diameter of the absorber. When small diameters are used, there is a potential for wall effect to take place. If the liquid at the top of the absorber is not properly contacted with the gas flowing upwards, less effective heat transfer will occur resulting in a higher outlet temperature. The simulation does not consider these potential effects and will consider a perfect distributed liquid (and wet packing) able to exchange heat and mass between liquid and gas.

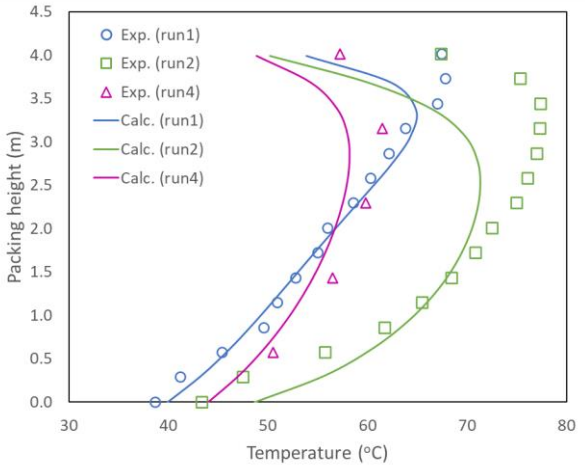

Figure 5: Absorber temperature profile for runs 1, 2 and 4 for TNO's mini plant I using 30 wt.% MEA.

For RWE plant, the exact position (in meters) for thermocouples were not available. They were placed at the top of the packing sections. For illustration purposes, we assume that these were 4.5, 9.0, 13.5 and 18.0 m. As seen in Figure 6, The temperature profile in the absorber follows the experimental trend. It is possible to see the effect of the inter cooler (at the bottom packing section) which modify the bulge temperature profile. In general, the model predicts a higher temperature than the experimental. This can be caused by some heat loss in the redistribution section in-between packing sections. The difference is more pronounced in runs #1 and 2 as these present leaner loadings and will react with more CO_2 producing more heat (compared to run #3). At the top of the packing, the deviation is higher as seen from TNO's plant.

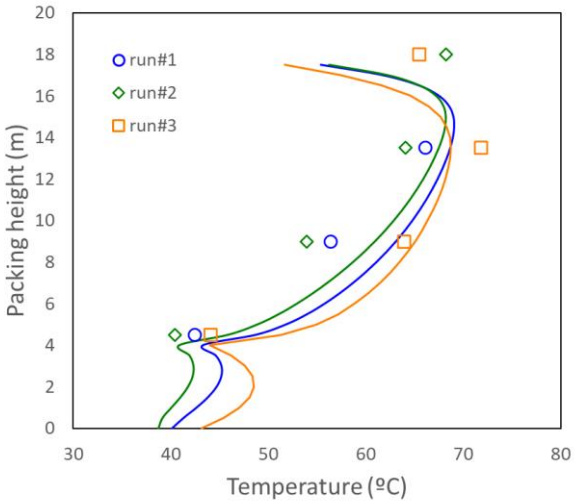

Figure 6: Absorber temperature profile for runs 1, 2 and 3 for RWE plant using CESAR1.

5. Conclusions

Three pilot campaigns were modelled using the commercial process simulator ProTreat®. In general, the calculated results presented good agreement with experimental data for all plants. Some adjustments were necessary to make in the simulations to account for unknown parameters. For instance, the packing of RWE absorber pilot plant was not disclosed, and an adjustment on the interfacial area factor was performed to match the rich loading.

Smaller pilots are flexible and offer the possibility of on-site measurements with real flue gas. However, due to its smaller size, heat losses and channeling effect are pronounced with potential impact on the measurements. As seen in the campaigns analyzed in this work the smaller pilots presented higher deviations, mostly due to the abovementioned issues. Nevertheless, the deviations encountered were within reasonable range. For TNO's mini plants, energy requirements could not be properly measured. The plant, however, is well equipped and other relevant data (such as temperatures, flows, etc.) can be easily assessed. The plant is suited to measure the solvent behavior of solvents at different flue gas conditions.

Larger pilots are usually not mobile, but channeling and heat losses are less pronounced. As a result, these plants can show more accurate the process' energy requirements. As seen in the RWE campaign, the mass balance (CO_2 produced calculated via gas and liquid phases) agrees within 1%.

The ProTreat® process simulator was used to model the experimental campaigns with good accuracy. Therefore, process design using it can be regarded with good level of confidence. Besides, ProTreat® showed exceptional speed and convergency rates for the cases studied and an easy user interface to set up simulations.

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