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# ASPEN HYSYS AND ASPEN PLUS SIMULATIONS FOR AMINE BASED ABSORPTION PROCESS COMPARED TO RESULTS FROM EXPERIMENTS IN CO<sub>2</sub>-RIG

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## Abstract

In this study, equilibrium-based and rate-based simulations in Aspen HYSYS and Aspen Plus were performed to compare the removal efficiency and physical properties of density and viscosity in a CO<sub>2</sub> absorption column. The experimental results from our previous study were used for comparison. In the equilibrium-based simulations, removal efficiency at 40 kg/hr of solvent flow rate was fitted with simulation by adjusting the Murphree efficiency of 12% in all stages. Accordingly, the equilibrium-based performed for other considered flow rates by keeping adjusted constant Murphree efficiency for all the stages in the absorber column. The variations of physical properties like density and viscosity were simulated and compared with measured properties under three different liquid to gas (L/G) ratios. Performed rate-based simulations with default molar volume/density and viscosity models of Clarke model and Jones-Dole model respectively were able to predict the properties with acceptable accuracy, but a deviation of 25% between measured and simulated viscosities for the lean MEA mixture was observed.

**Keywords:** *Equilibrium-based, Rate-based, CO<sub>2</sub> capture, MEA*

## 1. Introduction

Process simulation provides the ability to understand the process behavior under various process conditions and help to identify optimum conditions. The process of post-combustion carbon dioxide (CO<sub>2</sub>) capture through amine based absorption process has been evaluated in various ways through mathematical modelling and simulations to identify the key factors in order to optimize the configuration and efficiency of the process [1-4].

Aspen HYSYS and Aspen Plus are two process simulation packages that are widely used in the industry for steady state process simulations and calculations of equilibrium data for various gas liquid mixtures. Two approaches of equilibrium-based and rate-based modelling are facilitated for simulation of the amine-based post-combustion CO<sub>2</sub> capture process. For equilibrium-based modelling, an amine package with Kent-Eisenberg [5] and Li-Mather [6] equilibrium models is available in Aspen HYSYS. The equilibrium-based column model can be refined using a Murphree efficiency on each stage. For rate-based modelling, the Electrolyte-NRTL equilibrium that is based on Austgen *et al.* [7] model is adopted to model the vapour-liquid equilibrium of the reacting system in Aspen Plus. The column can be modelled based on both equilibrium stages with Murphree efficiencies and rate-based approaches.

In literature, studies related to process simulations using Aspen HYSYS and Aspen Plus are widely available for amine based post-combustion CO<sub>2</sub> capture. An Aspen Plus model was developed by Lim *et al.* [8] and performed a validation against a pilot plant operated at Boryeong, South Korea. There was a good agreement for the estimation of CO<sub>2</sub> loading, heat duty and temperature in the stripper between developed model and pilot plant

results. Plaza *et al.* [9] worked with absorber and stripper models in Aspen Plus in which a thermodynamic model proposed by Hilliard [10] was used for modeling CO<sub>2</sub> removal from aqueous MEA (monoethanol amine). Zhang and Chen [11] also performed validation of a rate-based MEA model in Aspen Plus with a pilot plant. The study extended from simulation model for CO<sub>2</sub> absorption with MEA to both absorption and desorption process and was validated against recently published pilot plant data. For Aspen HYSYS simulation, different absorption and desorption configurations were investigated using an equilibrium-stage model in Aspen HYSYS for natural gas based pilot plants [12]. A comparison between equilibrium-based model in Aspen HYSYS and rate-based model in Aspen Plus was performed by Øi [1] for the CO<sub>2</sub> absorption into MEA from atmospheric gas. Results show that it is difficult to conclude which model gives more accurate predictions. According to Zhang and Chen [11], a rate-based model is capable of predicting the overall performance of the CO<sub>2</sub> capture system excellently.

In this work, CO<sub>2</sub> absorption into MEA was studied using the two simulation packages Aspen HYSYS (equilibrium-based model) and Aspen Plus (equilibrium and rate-based models). Series of laboratory experiments have been performed in an experimental CO<sub>2</sub>-rig located at the University of South-Eastern Norway [13]. The experiments were done to investigate the CO<sub>2</sub> removal efficiency under different inlet CO<sub>2</sub> concentrations and solvent flow rates. The measured physical properties of density and viscosity at the absorber top for lean MEA and the bottom for rich MEA were compared with rate-based simulations from Aspen Plus.

## 2. Murphree efficiency based and rate – based simulation

### 2.1 Murphree efficiency

In distillation and absorption, the tray efficiency is described in several ways [14]. The point efficiency is defined as the ratio of change of composition at a point to the change of composition that would occur on a theoretical stage. Instead of a single point, Murphree efficiency is defined for the entire tray as given in Eq (1).

$$E_M = \frac{(y_n - y_{n-1})}{(y_n^* - y_{n-1})} \quad (1)$$

Where,  $y_n^*$  is the composition of vapour in equilibrium with the liquid leaving the tray,  $y_n$  is the actual composition of vapour leaving the tray.

The overall column efficiency  $E_o$  is given as

$$E_o = \frac{\text{number of ideal stages}}{\text{number of real stages}} \quad (2)$$

And these two efficiencies can be related as

$$E_o = \frac{\ln\left[1 + E_M\left(\frac{mV}{L} - 1\right)\right]}{\ln\left(\frac{mV}{L}\right)} \quad (3)$$

Where,  $m$  is the slope of the equilibrium line,  $V$  and  $L$  are molar flow rates of the vapour and liquid respectively.

For a packed column, Murphree efficiency of a tray is applicable for a packing section with a certain height.

### 2.2 Rate-based model

The rate-based approach considers the mass and heat transfer and chemical kinetics as the governing phenomena in the separation process. The driving force for the mass transfer is directly proportional to the deviation from the equilibrium between gas and liquid and is proportional to the contact area between the two phases [15]. The reaction model for MEA + CO<sub>2</sub> + H<sub>2</sub>O is given in reactions R1 to R5 as described by the Austgen *et al.* [7] for primary and secondary amines.

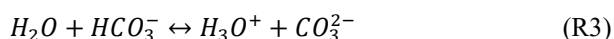
Ionization of water



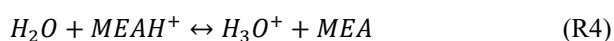
Dissociation of carbon dioxide



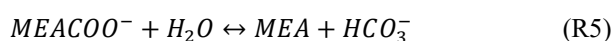
Dissociation of bicarbonate



Dissociation of protonated MEA



Carbamate reversion to bicarbonate



## 3. Methodology

### 3.1 Pilot plant and process description

An amine-based laboratory CO<sub>2</sub>-rig located at the University of South-Eastern Norway is shown in Figure 1. The process is consisting of absorption and desorption columns for chemical absorption and stripping of CO<sub>2</sub>. Feed with air and CO<sub>2</sub> pass through the absorber countercurrently with aqueous MEA and the structured packing enhances the mass transfer between CO<sub>2</sub> and absorbent. The absorber column is filled with Sulzer 250Y packing to build a packing section with 1500 mm height. Detailed information about the laboratory CO<sub>2</sub>-rig can be found in a previous publication with a piping and instrumentation diagram (P&ID) [13].



Figure 1: Amine based CO<sub>2</sub> capture pilot plant at USN

### 3.2 Experiments

#### 3.2.1 CO<sub>2</sub> rig experiments

A controlled flow of CO<sub>2</sub> with purity 99.5% from AGA Norge AS was mixed with constant air supply to achieve 5% and 10% CO<sub>2</sub> concentration (mol%) in the gas feed. The solvent flow rate was adjusted from 10 kg/hr to 100 kg/hr with 10 kg/hr increments. Finally, the CO<sub>2</sub> concentration of the treated gas was measured to determine the CO<sub>2</sub> removal efficiency. All the gas analysis were performed by an NDIR (Non-Dispersive InfraRed) instrument from ADC.

For the study of physical property variations of the absorber column, experiments that were performed in our previous work [16] were used for the simulations. There, three different liquid flows were considered. Samples were taken from liquid streams at the top and the bottom of the absorber and the temperatures were recorded in each case. Density and viscosity of collected samples were measured in the laboratory.

#### 3.2.2 Density measurements

Density measurements of the liquid MEA + H<sub>2</sub>O + CO<sub>2</sub> mixtures were performed using a DMA 4500 density meter from Anton Paar. A liquid volume of 5 ml approximately was injected into the U-tube of the density meter using a syringe. The temperature was set as it was recorded at the sampling point. The measurements were

repeated three times to verify the repeatability of the measurements and the average was taken as the final reading. A density check was performed with degassed water frequently to verify the validity of the previous calibration at 293.15 K.

### 3.2.3 Viscosity measurements

Viscosity measurements of the MEA + H<sub>2</sub>O + CO<sub>2</sub> mixtures were carried out using a Physica MCR 101 rheometer from Anton Paar. A double-gap measuring system was adopted, as it was suitable for low viscous fluids. The calibration of the rheometer was performed using a standard calibration fluid S3S from Paragon Scientific Ltd. The viscosities of the calibration fluid measured were compared with the standard given by the supplier. The deviations of the measurements were noted at different temperatures and viscosities of the MEA + H<sub>2</sub>O + CO<sub>2</sub> mixtures and corrected accordingly.

### 3.3 Simulations

The equilibrium-based simulations were carried out in Aspen HYSYS V10 environment. The amine package with Kent-Eisenberg [5] model was used to perform relevant calculations in the vapour and liquid phases. An absorber with four stages with defined Murphree efficiencies in each stage simulated the CO<sub>2</sub> removal efficiencies under different flow conditions.

In Aspen Plus rate-based simulations, an absorber column developed from RadFrac absorber model was used for the simulations. The property method of Electrolyte-non-random two-liquid (ELECNRTL) was selected as the mixture behaves as an electrolyte. All the simulations were performed under open-loop conditions.

For the physical properties, it is possible to regress experimental density and viscosity results of MEA + H<sub>2</sub>O + CO<sub>2</sub> from Weiland *et al.* [17] or Hartono *et al.* [18] to estimate relevant model parameters in Aspen Plus. The Clarke model, called VAQCLK in Aspen Plus for liquid molar volume is available with regressed model parameters. The model calculates liquid molar volume of aqueous electrolytes solutions using Amagat's law as given in Eq (4) and the relationship between partial molar volume of an electrolyte and its mole fraction in the solvent as given in Eq (5) [19].

$$V_m^l = \sum_i x_i V_i \quad (4)$$

Where,  $V_m^l$ ,  $x_i$  and  $V_i$  are molar volume of the mixture, mole fraction and the molar volume of component respectively.

$$V_{ca} = V_{ca}^\infty + A_{ca} \frac{\sqrt{x_{ca}}}{1 + \sqrt{x_{ca}}} \quad (5)$$

Where,  $V_{ca}$  is the partial molar volume of electrolytes,  $x_{ca}$  is the apparent electrolyte mole fraction and  $V_{ca}^\infty$ ,  $A_{ca}$  are regression parameters.

The option code 1 represents the quadratic mixing rule for solvent in which the interaction parameter VLQKIJ for MEA and H<sub>2</sub>O can be regressed against MEA + H<sub>2</sub>O density data from Kapadi *et al.* [20] and Han *et al.* [21]. The Clarke model parameters  $V_{ca}^\infty$  named as VLCLK/1 can also be regressed for the main electrolyte (MEA<sup>+</sup>,

HCO<sub>3</sub><sup>-</sup>), (MEA<sup>+</sup>, MEACOO<sup>-</sup>) and (MEA<sup>+</sup>, CO<sub>3</sub><sup>2-</sup>) against experimental MEA + H<sub>2</sub>O + CO<sub>2</sub> density data. The Jones-Dole electrolyte correction model, referred as MUL2JONS in Aspen Plus can be adopted to model the liquid viscosities in a MEA + H<sub>2</sub>O + CO<sub>2</sub> mixture. Due to the presence electrolytes, model calculates the correction to the liquid mixture viscosity of a solvent mixture. The Jones-Dole electrolyte correction model is given as follows [19],

$$\eta = \eta_{solv} (1 + \sum_{ca} \Delta\eta_{ca}) \quad (6)$$

Where,  $\eta$ ,  $\eta_{solv}$  and  $\Delta\eta_{ca}$  are viscosity of the liquid mixture, viscosity of the liquid mixture calculated by the Andrade/DIPPR model and contribution to the viscosity correction due to apparent electrolyte  $ca$  from cation  $c$  and anion  $a$  respectively.

The interaction parameters between MEA and H<sub>2</sub>O in the Aspen liquid mixture model, MUKIJ and MULIJ, can be regressed against experimental MEA + H<sub>2</sub>O viscosity data. Further, the Jones-Dole model parameters in  $\Delta\eta_{ca}$ , IONMUB, for MEA<sup>+</sup> and MEACOO<sup>-</sup> are possible to regress against MEA + H<sub>2</sub>O + CO<sub>2</sub> viscosity data [22]. The data regression to estimate parameters is beyond the scope of this study, and density and viscosity predictions were obtained using default parameter values in Aspen Plus.

The experimental input data for the physical property simulations are given in Table 1 and Table 2. The Aspen Plus simulations were performed in the Aspen Plus V10 environment.

Table 1: Scenarios considered in CO<sub>2</sub>-rig experiments

Case no	Air flow rate (Nm <sup>3</sup> /hr)	Liquid flow rate (kg/hr)	CO <sub>2</sub> in feed (%)	T <sub>Absorber,in</sub> (°C)
Case 1	15	47.92	10.2	19.5
Case 2	15	106.56	9.9	25.7
Case 3	15	151.17	9.9	30.1

Table 2: Lean amine loading with corresponding (L/G) in mass basis

Case no	Liquid flow rate (kg/hr)	(L/G)	Lean MEA loading (mol CO <sub>2</sub> / mol MEA)
Case 1	47.92	2.3	0.213
Case 2	106.56	5.4	0.280
Case 3	151.17	7.8	0.279

## 4 Results

### 4.1 CO<sub>2</sub> removal efficiency

For the investigation of CO<sub>2</sub> removal efficiency, two case studies were performed by keeping inlet gas CO<sub>2</sub> concentration at 5% and 10% (mole basis) of total gas flow. Figure 2 illustrates the variation of CO<sub>2</sub> removal efficiency under different liquid flow rates from 10 kg/hr to 100 kg/hr, which is equivalent to a range of liquid to gas (L/G) ratio from 0.3 to 3 on a mass basis approximately.



As shown in Figure 2 the CO<sub>2</sub> removal efficiency increases with the increase of liquid flow rate. Under low flow rates, the driving force for the mass transfer is reduced as the aqueous amine solution reaches high CO<sub>2</sub> loadings rapidly. This is reversed under high flow rates as more liquid with high driving force increase the CO<sub>2</sub> removal efficiency. Further, the increase of amine flow enhances the gas/liquid interfacial area while passing through the structured packing. This effect also increases the mass transfer through the gas/liquid interface.

In the equilibrium-based model, the Murphree efficiency on each of four plates were fitted to 12% for 40 kg/hr to get equal CO<sub>2</sub> removal efficiency in simulation and experiment. At other liquid flows the Murphree efficiency were kept constant at 12%. The rate-based simulations in Aspen Plus were performed by adjusting the interfacial area factor (IAF) to 1.98 to achieve a similar removal efficiency at 40 kg/hr compared to experiment. The results for other flow rates were taken at the adjusted IAF of 1.98.

This high interface area factor indicates that the rate-based model does not describe the absorption mechanisms accurately. Because the IAF is expected to increase with increasing liquid flow, the liquid flow influence on removal efficiency with a constant IAF in Figure 2 is opposite of what was expected. In Table 3 the IAF shows a more reasonable dependence of increasing liquid flow. A possible factor that may also influence on the CO<sub>2</sub> removal efficiency is the temperature, which may vary in the measured data in Figure 2.

Table 3. IAF and CO<sub>2</sub> out (%) in treated gas

Case no	IAF	CO <sub>2</sub> out (%) in treated gas
Case 1	1.04	5.8
Case 2	1.37	4.8
Case 3	1.43	4.1

As shown in Figure 2, the equilibrium-based model with constant Murphree efficiency predicted removal efficiency closer to the experiments at low flow rates below 50 kg/hr. The deviation between measured and simulation increases at higher flow rates. For the rate-based model, predictions are closer to the experiment at higher flow rates and the deviations are greater at low flow rates.

Neither the equilibrium based nor the rate-based model give a good qualitative description of the CO<sub>2</sub> removal as a function of liquid flow. This was also the conclusion in comparisons of equilibrium-based and rate-based models with performance data at TCM Mongstad [4]. The accuracy in simulated CO<sub>2</sub> removal efficiencies shown in Figure 2 are however reasonable for both models.

In Aspen HYSYS simulations, the removal efficiency increased with liquid flow rate, until it reached 30 kg/hr. Subsequently, the removal efficiency became a steady value after 30 kg/hr of liquid flow rate. Similar behavior was observed for 10% inlet CO<sub>2</sub> concentration in which a steady removal efficiency of 33% after 60 kg/hr of liquid flow in the HYSYS simulation.

In case of using a rate-based model in Aspen Plus, the absorption efficiency will vary slightly with the liquid

flow and the removal efficiency as a function of liquid flow will be expected to be simulated more accurately.

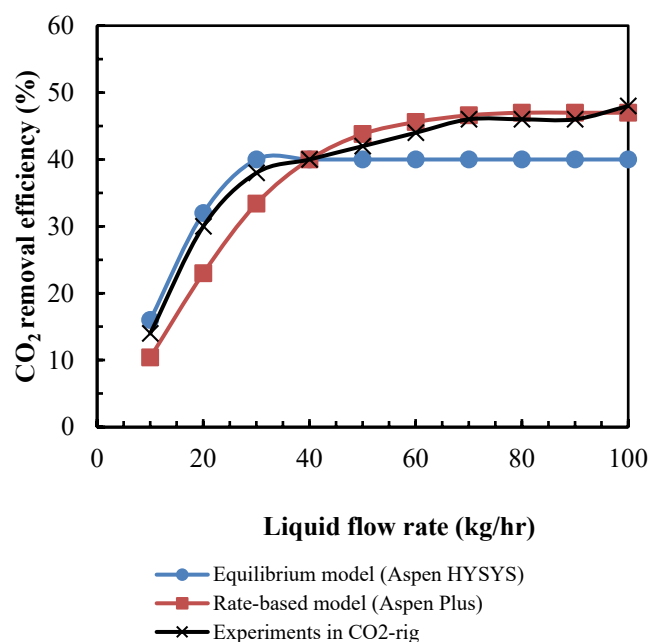


Figure 2: Comparison of CO<sub>2</sub> removal efficiency from experiments, equilibrium-based model and rate-based model

#### 4.2 Physical property analysis

Density and viscosity of the lean and rich MEA solvent have been measured at three different liquid flow rates as shown in Table 1 [16] were used for the rate-based simulations in Aspen Plus. For each case, the interfacial area factor was adjusted to achieve the removal efficiency observed during the experiments. IAF was adjusted by trial and error until the relative deviation between measured and simulated CO<sub>2</sub> concentrations at the treated gas becomes < 1%. The simulated CO<sub>2</sub> concentration of the treated gas at absorber out and corresponding IAFs are given in Table 3.

Accordingly, the corresponding density and viscosity of the lean and rich amine stream were evaluated. Figure 3 compares the experimental results with the simulation of the density variations in the liquid stream at the top and bottom of the absorber. Absorption of CO<sub>2</sub> increases the CO<sub>2</sub> loading in the solvent. The experiments revealed that the density of the MEA + H<sub>2</sub>O + CO<sub>2</sub> increased at the absorber bottom compared to the absorber top even though the temperature increases due to the exothermal reaction between MEA and CO<sub>2</sub>. The simulations were able to predict this trend as shown in Figure 3. The maximum relative deviation of measured density from the simulation is 6%. The model called VAQCLK with option code 1 in the property set was adopted to simulate the measured densities.

Rate-based simulations for the density of liquid streams were able to predict the trend of density variation with the increase of liquid flow in the absorber. Further simulations follow the trend of increase of density in the rich amine solution compared to that of lean amine. The temperature obtained through the simulations for rich amine mixture deviates around 5% from the measured.

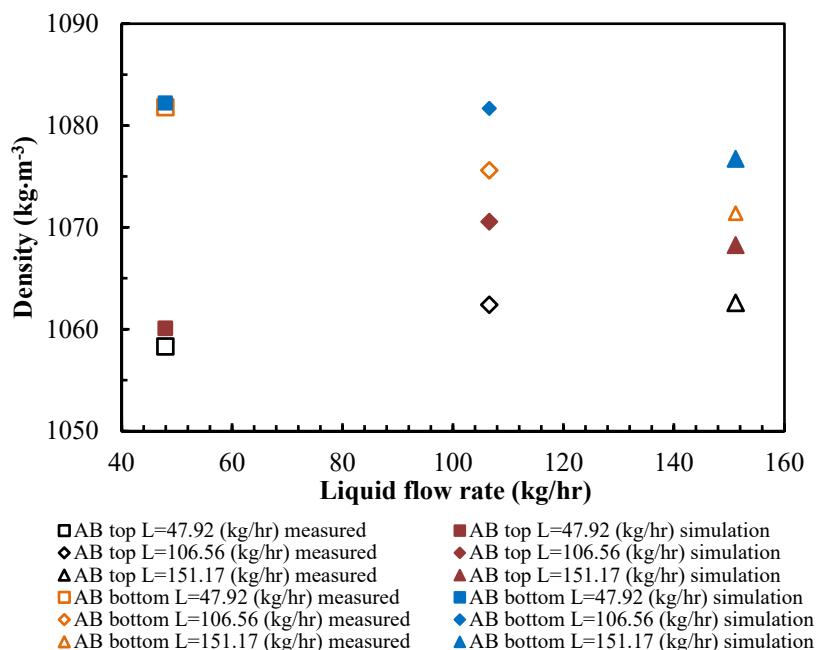


Figure 3: Comparison of the measured densities with the simulation

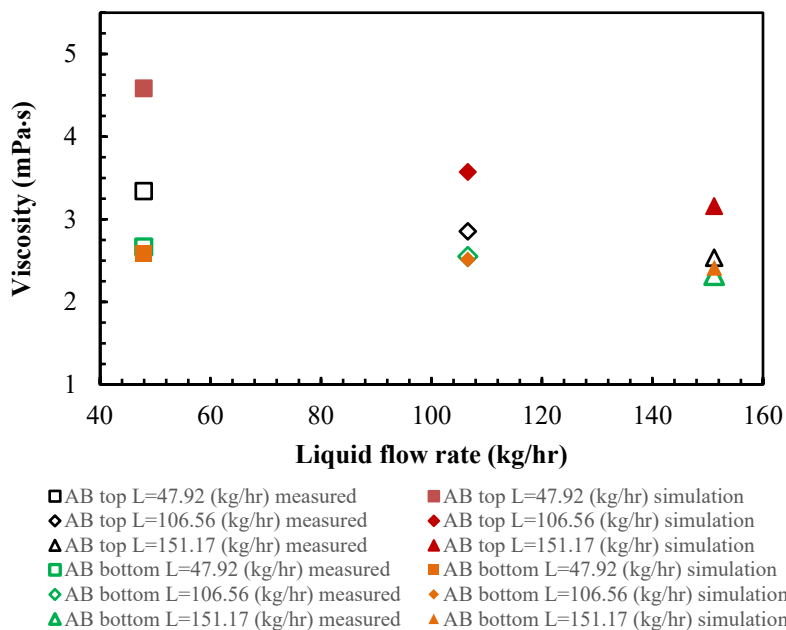


Figure 4: Comparison of the measured viscosities with the simulation

For the viscosity predictions based on rate-based simulations in Aspen Plus, Figure 4 illustrate the comparison between simulated viscosities and measured data at both lean and rich amine solutions. As shown by the experiments, viscosity at the lean MEA solution is higher than that of rich MEA. Generally, the increase of CO<sub>2</sub> in MEA + H<sub>2</sub>O + CO<sub>2</sub> mixture increase the viscosity [17, 23], but the increase of temperature dominate to reduce the viscosity at rich MEA mixture.

Rate-based simulations were able to predict the trend of viscosity variation in the absorber column under different liquid flow rates. As described in Figure 4, simulated viscosities showed large deviations around 25% compared to that of measured at the lean MEA mixture. Lower deviations were reported for the viscosity of rich MEA mixture and it was around 4%. The measured

viscosities agree with the viscosity data published for MEA + CO<sub>2</sub> + H<sub>2</sub>O mixtures under different CO<sub>2</sub> loadings and temperatures [18]. A possible cause for such deviations can be that the property model parameters were not regressed against the actual measured data. The causes can be found by performing simulations after estimating the required parameters through a regression.

Several other viscosity models such as Andrade model (MUL2ANDR), TRAPP model (MUL2TRAP) and Eyring-NRTL model (EYRING) for liquid mixture viscosity were also examined and compared with measured viscosities. The predictions deviate highly compared to the Jones-Dole electrolyte viscosity model with a factor around 2. This indicates that the selection of property models needs to be selected carefully to acquire the best results.



### 4.3 Uncertainty of experiments and simulations

The experiments in the CO<sub>2</sub>-rig involve different types of uncertainties. These uncertainties are related to inaccuracies of the measuring instruments and the process samplings. The extracted samples for the density and viscosity measurements should be representative of the system. The CO<sub>2</sub>-rig in USN has performed several modifications in order to achieve theories of process sampling to improve the accuracy of the measurements. In earlier work [13], uncertainties have been evaluated. It has been problems with the consistency in the amount of absorbed CO<sub>2</sub> calculated from the gas and liquid side. The absorbed CO<sub>2</sub> amount calculated from the liquid side has been assumed to have the highest uncertainty due to the uncertainty in measured difference of CO<sub>2</sub> concentration between lean and rich amine. In this work, the CO<sub>2</sub> removal efficiency is calculated based on CO<sub>2</sub> concentrations in the gas in and out which are assumed to have reasonable accuracy.

In the simulations, equilibrium and physical property models have uncertainties due to the assumptions considered during the model developments. Our recent publication on uncertainty analysis of interfacial area and mass transfer coefficient models [24] revealed the propagation of uncertainty of physical properties through such models. Those uncertainties in physical properties can appear from the sampling to measuring device. Uncertainties in viscosity are expected to give more impact on design than uncertainties in density.

### 5 Conclusion

Simulations based on an equilibrium-based model in Aspen HYSYS and a rate-based model in Aspen Plus were performed and compared with CO<sub>2</sub> removal efficiencies obtained via experimental study performed with the CO<sub>2</sub>-rig located at USN, Norway.

In the equilibrium-based model, for the study of 5% CO<sub>2</sub> feed gas concentration, the Murphree efficiency was adjusted to 12% to fit the removal efficiency at 40 kg/hr of liquid flow rate. The assumption of a constant Murphree efficiency is doubtful when variables like gas or liquid flow are varied. But performance data can be fitted by adjusting the Murphree efficiency as a function of gas- or liquid flow.

In case of using a rate-based model, the IAF can be adjusted. So far, neither fitting the Murphree efficiency in an equilibrium model or fitting the IAF in a rate-based model give qualitatively reasonable results. The calculated CO<sub>2</sub> removal as a function of liquid flow are however reasonably accurate for both models.

For the physical properties based on rate-based simulations, the default Jones-Dole model (MUL2JONS) was able to predict the measured viscosities with measurable deviation and may be improved by estimating model parameters through a regression using available measured viscosity data in the literature. Other considered models the Andrade model (MUL2ANDR), TRAPP model (MUL2TRAP) and Eyring-NRTL model (EYRING) for liquid mixture viscosity deviated largely from measured data. Accordingly, they are not adopted in this application. The default molar volume and density

model VAQCLK was able to predict densities in the MEA + H<sub>2</sub>O + CO<sub>2</sub> with acceptable accuracy.

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