Modelling the Performance of a CO_2 Absorber Containing Structured Packing

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A comprehensive mathematical model was developed to simulate the absorption of carbon dioxide (CO_2) into aqueous solutions of monoethanolamine (MEA) in a packed column containing Sulzer DX structured packing. Experimental work was conducted to generate absorption data that were used to verify the model. Simulation results showed that the model predicted the performance of the packed column with reasonable accuracy. The average absolute deviation (AAD) of the model was 28%. Nonlinear regression techniques were used during the formulation of the model to develop a new correlation for predicting the effective surface area (A_e) of Sulzer DX structured packing. This work has demonstrated the value of such correlations for simulating the absorption performance of different types of packing. Future work will develop similar A_e correlations for various types of random and structured packing.

1. Introduction

The world is searching for a solution to the greenhouse gas emission problem, since there is significant concern over the release of CO_2 into the atmosphere. A variety of projects at the International Test Centre for Carbon Dioxide Capture are working toward improving the CO_2 absorption process and reducing the cost of CO_2 capture. As part of these efforts, a series of computer models have been developed to predict the performance of absorption columns. Accurate computer models are extremely advantageous for engineering research, because the need for costly experiments can be minimized. Furthermore, successful computer models can be used to aid in the design and scaleup of chemical engineering processes.

Much work has been reported in the literature on the development of accurate computer models that simulate the performance of absorption columns. For example, Nardini et al.[1] developed liquid holdup and effective surface area (A_e) correlations for a model they used to simulate the absorption of acid gases into sodium hydroxide solutions. Their system modeled an absorber containing Sulzer BX structured packing. The model worked well, and their work showed that only the dynamic liquid holdup needed to be considered when determining effective packing surface areas. Launaro and Paglianti[2] also developed a model for the absorption of acid gases into sodium hydroxide solutions. Their column contained HelieR structure packing and the model focused on the packing wetted area, as well as the pressure drop across the column. Aroonwilas et al.[3] developed a model for three different types of structured packing that simulated the mass transfer and hydrodynamics inside CO_2 absorption systems using sodium hydroxide (NaOH) and MEA solutions. The model can be used to design, simulate, and optimize CO_2 absorption columns. More recently, Aboudheir et al.[4] developed a comprehensive model that predicts CO_2 absorption into MEA solutions when using a randomly packed column. The model was very accurate and could predict packed bed heights to within an error of 1%.

In the current work, the original Aboudheir model was modified to simulate the absorption of CO_2 in a small absorption

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Table 1. Packed-Column Characteristics

description	Sulzer DX
packing data	
surface area	900 m²/m³
crimp height	2.9 mm
corrugation base	6.4 mm
crimp angle	60°
void fraction	0.775
packed column data	
diameter	0.028 m
number of packing elements	40
element length	0.054 m
total packed height	2.16 m
total available surface area	1.20 m²

column containing Sulzer DX structured packing. Previously, the model was only capable of simulating CO_2 absorption in columns that contain random packing. Absorption data from bench-scale laboratory experiments were used to verify the model. The computer model was able to predict the CO_2 concentration profile along the column with an AAD of 16.8%. To successfully adapt the Aboudheir model, an A_e correlation developed by Henriques de Brito et al.[5] was modified using nonlinear regression techniques. This resulted in an improved A_e correlation that contained coefficients that were more suitable for the structured packing used in this study. Sulzer DX structure packing is typically used for laboratory-scale projects. Future work will evaluate other varieties of random and structured packings that are suitable for larger industrial applications.

2. Experimental Work

CO_2 was absorbed from a simulated flue gas stream (air + CO_2) using aqueous MEA solutions. Sulzer DX structured packing was used inside the column to promote contact between the gas and liquid phases. Structured packing was chosen because Aroonwilas et al.[6] and deMontigny et al.[7] have shown that it offers superior performance when compared to random packings. Recently, the use of structured packing has been increasing in industry. Its high-efficiency performance allows for the construction of smaller process units. Table 1 lists the geometric characteristics of Sulzer DX structured packing, as well as the characteristics of the absorber used in this study.
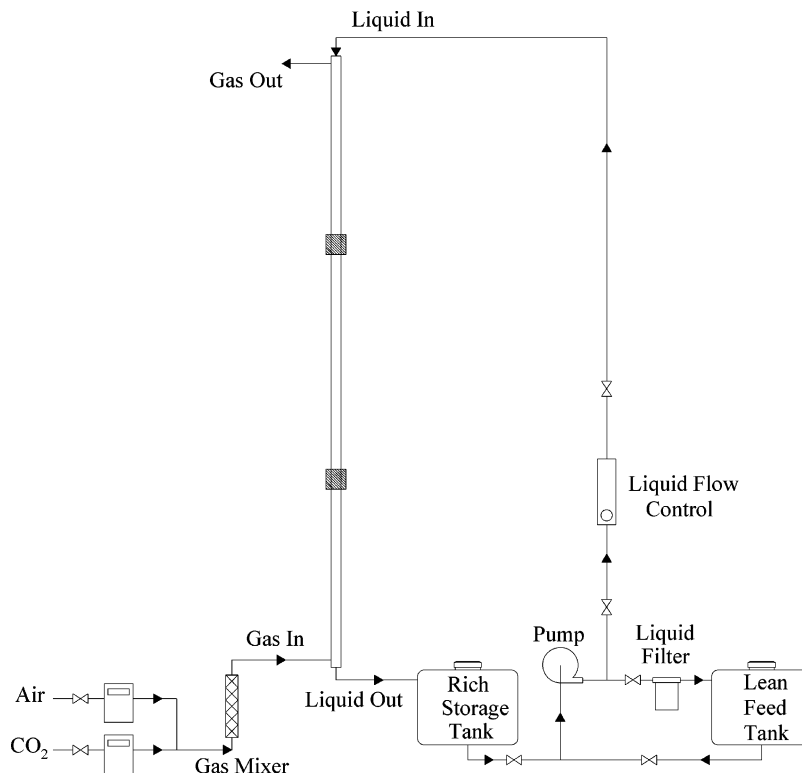
Figure 1. Schematic of experimental CO_2 absorption apparatus.

Table 2. Experimental Operating Conditions

operating conditions	range
inert gas flow rate	30.7−30.9 kmol m^{-2} h^{-1}
liquid flow rate	5.4−12.6 m^3 m^{-2} h^{-1}
MEA concentration	1.0−3.0 kmol/m^3
CO_2 feed concentration	13.9%−14.5%
feed solution CO_2 loading	0.03−0.20 kmol/kmol

A detailed description of the packed column design and experimental procedure has been provided elsewhere.[8] In short, the column was 2.40 m tall with an inside diameter of 28 mm. The column was insulated and the system was operated under counter-current flow configurations. A simulated flue gas stream (air + CO_2) entered at the bottom of the column and flowed upward, while lean MEA solution was pumped to the top of the column and flowed downward. Experiments were conducted in a batch mode without solution regeneration. During steady-state operation, the concentration of CO_2 in the gas phase was measured along the length of the column, using an infrared gas analyzer. A mass balance calculation at the end of each experiment was performed to confirm the validity of the run. Figure 1 shows a schematic of the experimental apparatus, and Table 2 lists the experimental operating conditions used in this study.

3. Model Development

A rigorous computer program developed by Aboudheir et al.[4] was modified to model a packed column that contained Sulzer DX structure packing. This model was based on three main components: (1) a material and energy balance model developed by Pandya,[9] (2) a vapor−liquid equilibrium (VLE) model and termolecular-kinetics model developed by Aboudheir et al.,[4] and (3) physical properties published in the literature. Pandya's material and energy balance model was the first work on design techniques for gas absorption with chemical reaction in adiabatic packed towers. The model considers heat effects from absorption, solvent evaporation, and condensation, and it accounts for the chemical reaction in the liquid phase as well as the heat- and mass-transfer resistances in both phases. Both Tontiwach-wuthikul et al.[10] and Pintola et al.[11] successfully used Pandya's model to predict the CO_2 concentration and temperature profile along the length of the packed columns. Their working models were accurate at low solvent concentrations and solution loadings, but not at high solution loadings. Errors between experimental and predicted results were attributed to the simplified methods used to calculate the enhancement factor, VLE data, and the kinetics of reaction. Therefore, Aboudheir et al.[4] developed more-accurate VLE and termolecular-kinetics models to calculate the reaction rate constants along the length of the packed column. The original Aboudheir model was written in FORTRAN 90 and works very well, predicting the packed height in absorber columns to within 0.8% of the actual value. Recently, the model was adapted to predict the absorption of CO_2 into aqueous solutions of 2-amino-2-methyl-1-propanol in columns that contained random packing.[12] In the current work, the original Aboudheir model was modified to simulate the absorption of CO_2 into MEA in absorption columns that contained Sulzer DX structured packing.

The following assumptions were used in the model to write the main equations for the mass and energy balances:

(1) The reaction is fast and occurs in the liquid film such that the bulk liquid is in equilibrium,

(2) Liquid-phase heat-transfer resistance is small, when compared to the gas phase,

(3) Mass-transfer resistance for water in the liquid phase is negligible,

(4) The interfacial area for heat and mass transfer is the same, and

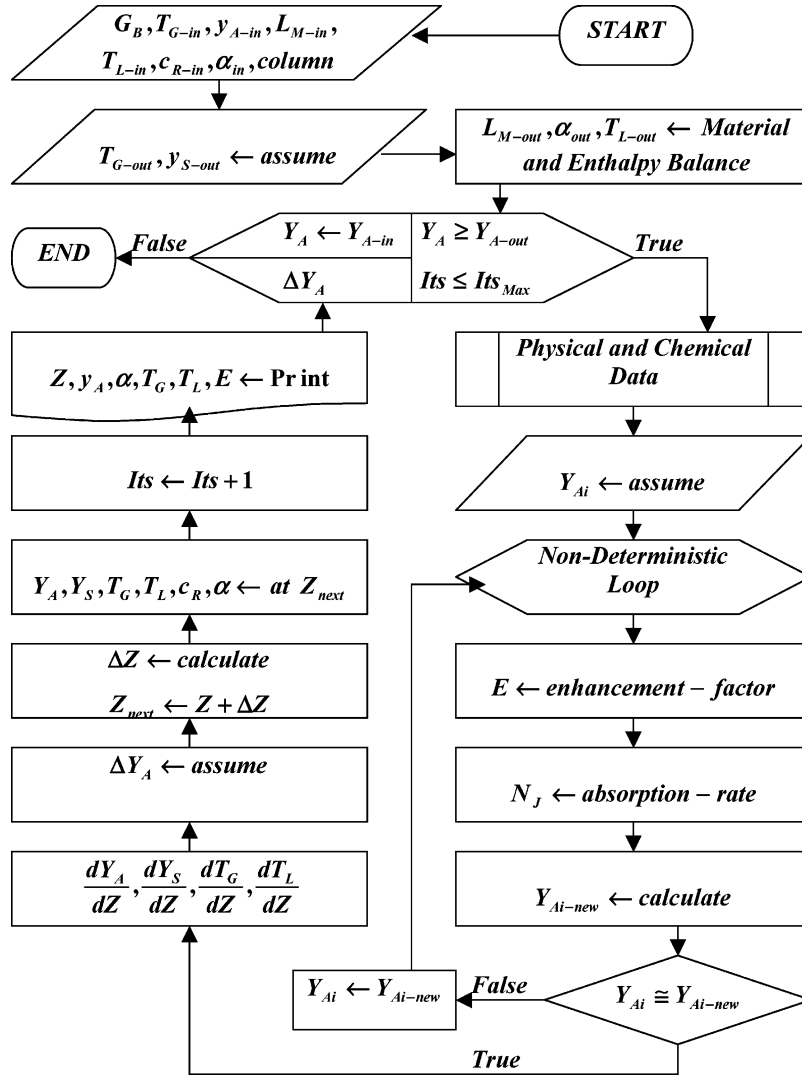(5) Only CO_2 and water vapor can cross the gas/liquid interface.

START

$G_B, T_{G-in}, y_{A-in}, L_{M-in},$
$T_{L-in}, c_{R-in}, \alpha_{in}, column$

$T_{G-out}, y_{S-out} \leftarrow assume$

$L_{M-out}, \alpha_{out}, T_{L-out} \leftarrow Material$
$and\ Enthalpy\ Balance$

$Y_A \leftarrow Y_{A-in}$ | $Y_A \geq Y_{A-out}$
ΔY_A | $Its \leq Its_{Max}$

False — END

True

$Z, y_A, \alpha, T_G, T_L, E \leftarrow Print$

Physical and Chemical Data

$Its \leftarrow Its + 1$

$Y_{Ai} \leftarrow assume$

$Y_A, Y_S, T_G, T_L, c_R, \alpha \leftarrow at\ Z_{next}$

Non-Deterministic Loop

$\Delta Z \leftarrow calculate$
$Z_{next} \leftarrow Z + \Delta Z$

$E \leftarrow enhancement - factor$

$\Delta Y_A \leftarrow assume$

$N_J \leftarrow absorption - rate$

$\dfrac{dY_A}{dZ}, \dfrac{dY_S}{dZ}, \dfrac{dT_G}{dZ}, \dfrac{dT_L}{dZ}$

$Y_{Ai-new} \leftarrow calculate$

$Y_{Ai} \leftarrow Y_{Ai-new}$ False $Y_{Ai} \cong Y_{Ai-new}$

True

Figure 2. Flowchart for the CO_2-MEA simulation model in FORTRAN 90.

Furthermore, the system is assumed to operate under steady-state conditions. Based on these assumptions, the main equations required for the mass and energy balances were written. For the concentration gradients of the gas species, Pandya[9] wrote

$$\frac{dY_A}{dZ} = \frac{-k_{A,G}aP(y_{A,G} - y_{A,i})}{G_B} \quad (1)$$

$$\frac{dY_S}{dZ} = \frac{-k_{S,G}aP(y_{S,G} - y_{S,i})}{G_B} \quad (2)$$

Temperature gradients were written for both the gas and liquid phases:

$$\frac{dT_G}{dZ} = \frac{-h_G a(T_G - T_L)}{G_B(C_{PB} + Y_A C_{PA} + Y_S C_{PS})} \quad (3)$$

$$\frac{dT_L}{dZ} = \frac{1}{L_M C_{PL}} \left(\begin{array}{l} G_B(C_{PB} + Y_A C_{PA} + Y_S C_{PS})\dfrac{dT_G}{dZ} + \\[2mm] G_B(C_{PS}(T_G - T_o) + \lambda_S)\dfrac{dY_S}{dZ} \\[2mm] + G_B(C_{PA}(T_G - T_o) - \Delta H_R((T_o, P))\dfrac{dY_A}{dZ} \end{array} \right) \quad (4)$$

Within each differential section of the column, the gas-phase mole fraction of CO_2 at the interface can be expressed by eq 5, which results from the mass flux balance equations in the gas and liquid phases. The liquid-phase mole fraction of CO_2 is expressed using Henry's Law ($c_{Ai} = He \times p_{Ai}$). The system of differential equations defined by the model is integrated simultaneously to calculate composition and temperature profiles along the column.

$$p_{Ai} = \frac{p_A + \dfrac{k_{LA}^0 E}{k_{GA}}C_{Ae}}{1 + \dfrac{k_{LA}^0 E}{k_{GA}}He} \quad (5)$$

For modeling purposes, the inlet gas and liquid conditions are usually known, with the outlet conditions being uncertain. The original Aboudheir model solves this two-point boundary value problem using the shooting method. By initially assuming that the temperature and moisture content of the outlet gas are in equilibrium with the inlet liquid, the outlet liquid conditions can be determined by applying mass and energy balances across the packed column. The shooting method solution progresses upward along the column, computing profiles for the temperature and concentration until the specified CO_2 outlet concentra-

tion is achieved. If the calculated conditions at the top of the column do not converge with the initially assumed values, new outlet gas conditions are assumed and procedure is repeated. This procedure is outlined in Figure 2, which shows a simplified flowchart for the FORTRAN 90 program that solves the system of eqs 1−5. The parameters demanded by the model for each absorption case are obtained from available experimental measurements or correlations. These parameters are programmed into subroutines that are called by the main program under each operating condition. Further details about the model are provided in Aboudheir et al.[12]

One of the challenges faced when simulating chemical absorption system is the proper calculation of the enhancement factor. In this work, we opted to use one of the proposed solutions in the literature. Wellek et al.[13] reviewed and compared several approximate solutions with a precise numerical solution and found that Yeramian et al.[14] presented one of the best explicit approximations:

$$E = \frac{E_1{}^2}{2(E_i - 1)} \left(\sqrt{1 + \frac{4(E_i - 1)E_i}{E_1{}^2}} - 1 \right) \qquad (6)$$

The above expression for the enhancement factor was used in the current work, and further details can be found in Aboudheir et al.[4]

3.1. Correlations Used in the Packed-Column Model. Three important parameters in the model are A_e, the gas-phase mass-transfer coefficient (k_G), and the liquid-phase mass-transfer coefficient (k_L). These values were calculated using correlations published in the literature. Since the original Aboudheir model was developed for absorption in randomly packed columns, correlations published by Onda et al.[15] were used to calculate the A_e and k_G values. Although Onda also proposed a correlation to calculate k_L, a separate correlation developed by Cho[16] was used instead because it has been shown to produce better results.[4,10] A detailed study is required to determine why the Cho k_L correlation produced more accurate results than Onda's, but this level of analysis is outside the scope of the current study. Unfortunately, the lumped parameters in the coefficient of Cho's correlation do not offer any clues. Table 3 lists the correlations that were used in the original model, as well as the correlations that were used to modify Aboudheir's model for structured packing.

To adapt the original Aboudheir model for Sulzer DX structured packing, the A_e, k_G, and k_L correlations had to be changed. A review of the literature did not reveal any publications that presented specific correlations for Sulzer DX packing; therefore, several published correlations were evaluated. Research collaboration between Bravo et al.[17] and Fair et al.[18] has produced a large number of papers over the years on mass transfer in structured packings. Their mechanistically based correlations require much packing property data and were not used in the current modeling work. Rather, the correlations presented by Henriques de Brito et al.[5] were chosen, in part for their simplicity, but also because they are the best-suited for the current experimental conditions. This decision is supported by the remaining discussion.

The wetting of the packing surface area by the liquid solvent is an important aspect of the absorption process. Obviously, it is desirable to have as much of the packing surface area wetted as possible, thus maximizing the surface area of liquid exposed to the gas phase. Typically, packing is said to have a total available surface area and an effective surface area. The effective surface area represents the amount of packing that is wetted by

Table 3. Correlations from Different Sources for Predicting A_e, k_G, and k_L in Packed Columns

correlation

Onda et al.[15]

$$\frac{A_e}{A_T} = 1 - \exp\left[-1.45 \left(\frac{\sigma_C}{\sigma_L} \right)^{0.75} \left(\frac{L}{A_T \mu_L} \right)^{0.1} \left(\frac{L^2 A_T}{\rho_L{}^2 g} \right)^{-0.05} \left(\frac{L^2}{\rho_L \sigma_L A_T} \right)^{0.2} \right]$$

$$k_G = 5.23 \left(\frac{D_G A_T}{RT} \right) \left(\frac{G}{A_T \mu_G} \right)^{0.7} \left(\frac{\mu_G}{\rho_G D_G} \right)^{0.33} (A_T d_P)^{-2.0}$$

$$k_L = 0.0051 \left(\frac{L}{A_e \mu_L} \right)^{0.67} \left(\frac{\mu_L}{\rho_L D_L} \right)^{-0.5} (A_T d_P)^{0.4} \left(\frac{\rho_L}{\mu_L g} \right)^{-0.33}$$

Cho[16]

$$k_L = (2.4 D_A)^{0.5}$$

Henriques de Brito et al.[5]

$$\frac{A_e}{A_T} = 0.465 \left(\frac{\rho_L u_L}{A_T \mu_L} \right)^{0.3}$$

$$k_G = 0.0338 \left(\frac{D_G}{d_h} \right) \left(\frac{\rho_G u_G d_h}{\mu_G \cos 45°} \right)^{0.8} \left(\frac{\mu_G}{\rho_G D_G} \right)^{0.33}$$

$$k_L = \frac{(D_L k_2 C_{A,L})^{0.5}}{Ha}$$

the liquid at any given time during steady-state operations. Work by Weiland et al.[19] stated that effective surface areas can be a substantial fraction of the total surface area but will certainly not be equal to the total surface area. This report is in direct contrast to the work completed by Henriques de Brito et al.,[5] which found that the effective area could exceed the total geometric area of the packing. They attributed this phenomena to either instabilities such as ripples or waves in the liquid surface, or to a splitting of the liquid film into multiple smaller liquid showers that lead to an increased effective area. Whatever the case, one way to increase the wetted area, as suggested by Nawrocki et al.[20] is to increase the liquid load and the number of distribution points in the liquid distributor at the top of the column. Another suggestion is to select an appropriate type of packing, because the surface characteristics of packing material affect wettability. For instance, packing that is composed of gauze mesh promotes wetting better than solid-surfaced packing. This is the case with Sulzer DX structured packing, because it is made from a stainless steel gauze mesh. Bravo et al.[17] reported that gauze surfaces promote capillary action, causing the liquid to spread into a liquid film that covers most of the available surface, even at low flow rates. According to Helling and DesJardin,[21] this capillary action is dependent on the liquid density, surface tension, and contact angle for wetting of liquids on solids.

3.2. Adapting the Correlations. The new model used correlations proposed by Henriques de Brito et al.[5] The k_G correlation was used as presented. The correlation for k_L did not produce good results; therefore, the correlation by Cho[16] that appeared in the original Aboudheir model was retained. Finally, the Henriques de Brito correlation for A_e required modification to account for differences in the Sulzer DX packing. First of all, the cos 45° term in the k_G correlation was changed to cos 60°, which is the inclination angle of Sulzer DX structured packing. Further differences in the system were taken into account by conducting a nonlinear regression analysis on the Henriques de Brito A_e correlation to identify new coefficients X_1 and X_2:

Table 4. Experimental CO$_2$ Absorption Data Using Monoethanolamine (MEA) Solution in a Sulzer DX Packed Column

description	DX-1	DX-2	DX-3	DX-4	DX-5	DX-6	DX-7	DX-8
inert gas flow (kmol m^{-2} h^{-1})	30.9	30.9	30.9	30.9	30.9	30.7	30.7	30.7
liquid flow rate (m^3 m^{-2} h^{-1})	5.4	6.7	8.4	10.6	12.6	8.4	8.4	8.4
MEA concentration (kmol/m^3)	2.0	2.0	2.0	2.0	2.0	1.0	2.0	3.0
CO$_2$ loading (kmol/kmol)								
inlet	0.06	0.10	0.15	0.17	0.19	0.03	0.20	0.19
outlet	0.52	0.47	0.45	0.41	0.39	0.58	0.49	0.39
column temperature (°C)								
top	18.7	19.9	17.9	19.8	17.6	21.3	21.7	19.7
bottom	20.8	21.8	18.7	20.5	18.1	21.3	22.7	20.6
mass balance error (%)	−3.9	−3.6	−3.9	−2.8	−3.1	−5.2	−2.6	−5.3
gas-phase CO$_2$ concentration (%)								
sampling point 11 (2.35)[a]						0.00		
sampling point 10 (2.12)[a]						0.09		
sampling point 9 (1.88)[a]						0.20		
sampling point 8 (1.65)[a]						0.31		
sampling point 7 (1.41)[a]	0.00				0.00	0.64	0.00	
sampling point 6 (1.18)[a]	0.14	0.00	0.00		0.03	1.51	0.39	0.00
sampling point 5 (0.94)[a]	0.38	0.14	0.14	0.00	0.14	4.12	0.65	0.39
sampling point 4 (0.71)[a]	1.24	0.49	0.61	0.38	0.49	5.53	1.77	1.03
sampling point 3 (0.47)[a]	4.31	2.18	2.48	1.89	2.00	8.50	4.70	3.20
sampling point 2 (0.24)[a]	10.33	8.09	8.08	6.56	6.79	11.85	9.70	8.00
sampling point 1 (0.00)[a]	14.23	14.35	14.38	14.50	14.35	13.92	14.43	14.54

[a] The value given in parentheses is the height of the sample from the bottom of the column (in meters).

surface area correlation:
$$\frac{A_e}{A_T} = X_1\left(\frac{\rho_L u_L}{A_T \mu_L}\right)^{X_2} \quad (7)$$

The BCLSF subroutine from the IMSL MATH Library[22] was used to obtain optimum fitting parameters. A few steps were required to complete this process. The original Henriques de Brito A_e correlation did not produce results that fit the data; the model was run using a *reverse-engineering* approach. Instead of running the model with the A_e correlation, it was bypassed and an A_e value was entered manually. This was done on a trial-and-error basis for each experiment until a suitable A_e value had been identified. Once an acceptable A_e value had been found, it was recorded in a data file, along with the relevant Reynolds number (Re) for that particular run. These data file was then used as an input database for the nonlinear regression subroutine. The BCLSF subroutine could then be run to evaluate the fitted data parameters and determine the optimum fitting coefficients that would minimize the error in the Henriques de Brito A_e correlation. The nonlinear regression program minimized the following error function:

$$F(I) = A_e(I)|_{\text{Fitted}} - (A_T \times X(1) \times Re(I)^{X(2)}) \quad (8)$$

where $X(1)$ and $X(2)$ are the coefficients in the Henriques de Brito A_e correlation.

4. Results and Discussion

Eight experiments were conducted in the packed column: five that varied the liquid flow rate, and three that varied the solution concentration. The experimental results are listed in Table 4 for all eight runs. These experiments were modeled using the original Onda and Henriques de Brito correlations. The Onda-based simulation was not expected to provide an accurate prediction, because it was developed for columns that contain random packings. The Henriques de Brito system was developed for Sulzer Mellapak (125.Y, 250.Y, 500.Y) structured packing and provided better results; however, the accuracy remained poor. The mediocre results of the original Henriques de Brito system can be explained by considering the A_e correlation. First of all, the current system contains Sulzer DX structured packing,
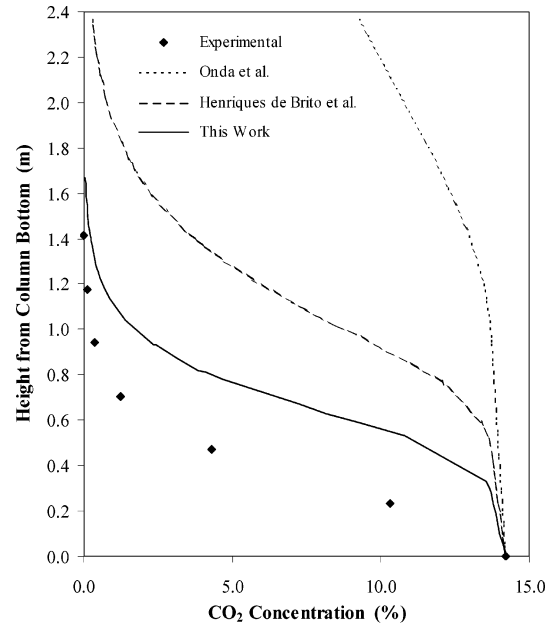

Figure 3. Simulation results for experimental run DX-1.

whereas the Henriques de Brito A_e correlation was developed using Sulzer Mellapak. Second, the original correlation was developed using a constant liquid density and viscosity, whereas these values vary as a function of temperature in the Aboudheir packed-column model.

Initially, all eight runs were analyzed in the nonlinear regression. Two of the runs (DX-1 and DX-6) did not have ideal simulation results and, therefore, were left out of the final nonlinear regression. Figure 3 shows the poor results of the model when simulating the DX-1 run. There are a few possible reasons for the poor simulation results of the DX-1 and DX-6 experiments. When we examine the experimental conditions for these two runs, we find that the DX-1 run had the lowest liquid flow rate (5.4 m^3 m^{-2} h^{-1}) and the DX-6 run had the lowest solution concentration (1.0 kmol/m^3). These experimental conditions may be outside the bounds of the model, although a proper sensitivity analysis was not performed to verify this explanation. A more plausible explanation is to consider the liquid inlet

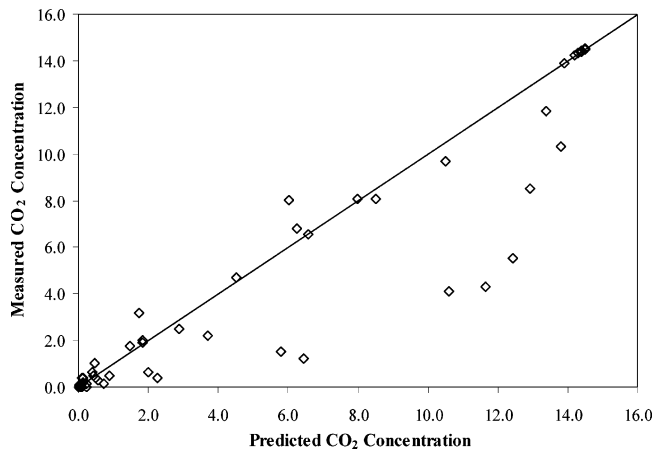**Figure 4.** Parity plot for all eight packed-column runs.

Figure 5. Parity plot for the six packed column runs that produced acceptable results.

solution CO_2 loading, which was low for both of these runs at 0.06 and 0.03 mol CO_2/mol MEA, respectively. All of the other experiments had inlet solution CO_2 loadings of $\alpha > 0.10$ mol CO_2/mol MEA. Because Aboudheir et al.[23] developed the VLE and termolecular-kinetics models in their work for concentrated, loaded MEA solutions, it is quite likely that the accuracy of the simulation reduces when the solution concentration and solution CO_2 loading are low.

The parity plot in Figure 4 shows the results for all eight runs. Some data points clearly have been overpredicted by the model. The average absolute deviation (AAD) of the model, when the correlation was developed using all eight experiments, was 54.3%. Based on these poor results, a decision was made to analyze the nonlinear regression without the results from the DX-1 and DX-6 experiments. Figure 5 shows the parity plot for the remaining six runs. In this case, the AAD for the model was 16.8%, and there was a good comparison between the simulation results and experimental data. Note that the AAD calculations only included data points that had a CO_2 gas-phase concentration that was >1%, as measured by the infrared gas analyzer. This was done to eliminate the misleading error values obtained when comparing low concentrations with model predictions. For example, if the CO_2 concentration was 0.50%, and the model predicted 0.25%, the error would be 50% when, in fact, the results are quite acceptable.

Based on the nonlinear regression analysis, a new A_e correlation was developed for the Sulzer DX packing. The original Henriques de Brito correlation and modified Henriques de Brito correlation (current work) are compared below:

original Henriques de Brito:
$$\frac{A_e}{A_T} = 0.465 \left(\frac{\rho_L u_L}{A_T \mu_L} \right)^{0.3} \quad (9)$$
(Sulzer Mellapak)

modified Henriques de Brito:
$$\frac{A_e}{A_T} = 0.759 \left(\frac{\rho_L u_L}{A_T \mu_L} \right)^{0.254} \quad (10)$$
(Sulzer DX)

Equation 10 can be used with confidence to account for the A_e value in Sulzer DX structured packing, providing that the liquid flow rate, solution concentration, and inlet CO_2 loading are not too low. Simulation results for runs DX-5 are shown in Figure 6, using the modified Henriques de Brito A_e correlation. The new equation clearly provides a more accurate prediction.

As a final note, earlier in Table 1, the total available surface area for the Sulzer DX structured packing was listed at 900 m^2/m^3. In this work, the model calculated effective packing
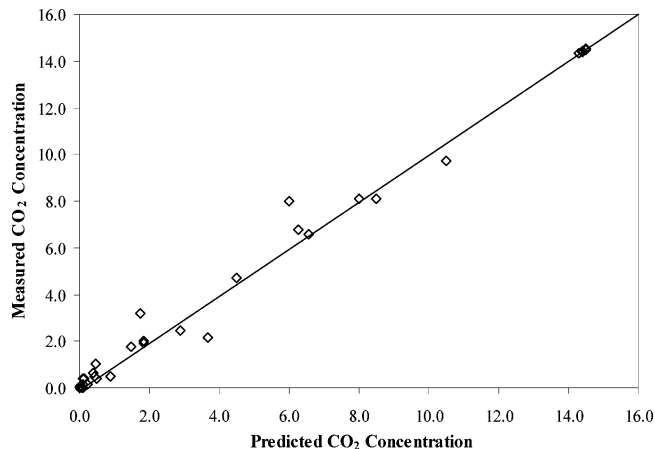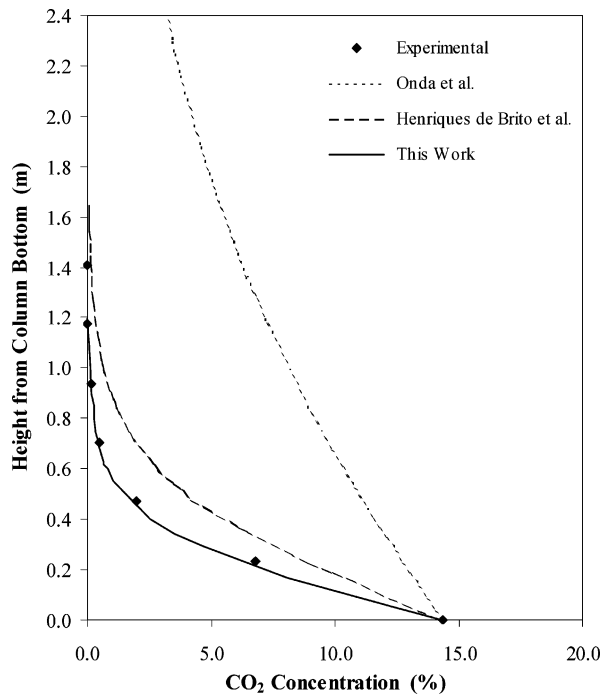

Figure 6. Simulation results for experimental run DX-5.

surface areas in the range of $550-800$ m^2/m^3. This represents a wetted packing efficiency of $61\%-89\%$, when compared to the total available surface area. In analyzing the data, there was no obvious correlation between the liquid flow rate and the A_e value. This is suspicious, because one might expect an increased liquid flow rate to improve the packing wetting. In terms of solution concentration, there was a definite relationship with a decrease in the A_e value as the solution concentration increased. This result can be directly attributed to solution viscosity, which increases as the solution concentrations increase.

5. Conclusions

A bench-scale CO_2 absorption plant was operated using aqueous monoethanolamine (MEA) solutions and Sulzer DX packing. The absorber performed well and presented no operating challenges. An original computer model that was presented by Aboudheir et al.[4] was expanded to simulate absorption systems that contain Sulzer DX structured packing by modifying an effective surface area (A_e) correlation that was developed by Henriques de Brito et al.[5] The new model performed well;

however, the accuracy was reduced when the liquid flow rate, solution concentration, and inlet solution CO_2 loading were low. With this in mind, it is recommended that the new A_e correlation be used for systems containing Sulzer DX packing that operate with liquid flow rates in the range of $6.7-12.4$ m³ m⁻² h⁻¹, solution concentrations of ~2.0 kmol/m³, and solution CO_2 loadings of >0.10 mol CO_2/mol MEA.

This work has shown that it is possible to customize existing absorption models to simulate existing packed columns, using appropriate engineering correlations. The flexibility of Aboudheir's model is valuable to engineers who want to simulate specific varieties of random and structured packing. Although the model developed in this work is limited to Sulzer DX packing, the potential to expand Aboudheir's model to other varieties of packing is huge.

Acknowledgment

Nomenclature

a = interfacial area per unit of packing (m²/m³)

A_e = effective surface area (m²/m³)

C_{Ae} = equilibrium concentration (kmol/m³)

$C_{P,j}$ = heat capacity of component j (kcal kmol⁻¹ K⁻¹)

D_A = diffusivity of component A in the absorption solution (m²/s)

E = enhancement factor

G_B = total molar gas flow rate (kmol m⁻² h⁻¹)

h_G = heat-transfer coefficient (kcal m⁻² h⁻¹ K⁻¹)

He = Henry's law constant (kmol m⁻³ kPa⁻¹)

ΔH_R = heat of chemical reaction between the absorbed gas and amine (kcal/kmol)

$k_{j,G}$ = gas-phase mass transfer coefficient for component j (kmol m⁻² s⁻¹ kPa⁻¹)

k_L = gas-phase mass transfer coefficient for component j (kmol m⁻² s⁻¹ kPa⁻¹)

k_L^0 = physical mass transfer coefficient (m/s)

L_M = liquid mass velocity (kmol m⁻² h⁻¹)

P = total system pressure (kPa)

T = temperature (K)

$y_{j,i}$ = mole fraction of component j at the membrane/liquid interface

y_j = mole fraction of component j

$Y_{j,G}$ = mole ratio of component j in the bulk gas (kmol/kmol)

Z = height of packed column or effective membrane length (m)

α = solution CO_2 loading (kmol CO_2/kmol MEA)

λ = latent heat of vaporization (kJ/kmol)

Subscripts

A = component A, solute gas

B = component B, the nonsoluble carrier gas

G = gas

i = interface

L = liquid

o = base for enthalpy or bulk liquid concentration

P = pressure

S = volatile solvent

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