DETERMINING THE ABSORPTION EFFICIENCY OF THE SOLVENT ABSORBENTS IN CARBON DIOXIDE CAPTURE PROCESS BY APPLYING THE NUMERICAL METHOD OF LINES

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Abstract- The research focused on the numerical study for the performance of Carbon dioxide capturing by Post-combustion process. The Numerical Method of Lines was applied on the developed Partial Differential Equations to reduce them to Ordinary Differential Equations. The series of equations developed were simulated on Python Computer programme. Three solvent absorbents were investigated in order to determine their absorption efficiency. This was done by calculating the ration of the concentration of Carbon dioxide absorbed to the concentration of the solvent absorbents.

I. INTRODUCTION

Carbon dioxide capture process (CCP) is the process of removing the Carbon dioxide (CO_2) gas away from the atmosphere. South Africa is responsible for 1.5% of the global greenhouse gases emissions because of its dependant on coal for energy [1]. The absorption-based processes are believed to be appropriate for large-scale Post-combustion CCP from coal-fired power plants [2]. Post-combustion theories based on absorption of CO_2 in aqueous amine solutions are considered the most mature technologies for CO_2 capture from power plants [3]. The most commercially applied amine is Monoethanolamine (MEA) due to its high absorptive capacity [4]. Since these theories exist, they need to be advanced in order to increase the gas-liquid contact in the absorption column due to the increase in energy demand globally and the fact that coal is a major source of energy more especially in South Africa. The country is a fast-developing nation with an energy economy that is highly dependent on coal [5].

II. MODELLING

The principal equation was based on the concentration balance of the flue gas and solvent absorbent around the absorption column. The numerical method of lines technique was used to reduce the Partial Differential Equation (PDE) to the Ordinary Differential Equation (ODE). Similar models were applied by [6; 7]. The difference between the solvent absorbent model and Carbon dioxide gas model is the reaction rate term as seen in equation (1) and (2). A transfer of Ions occurs during the process. Ions in the liquid phase attract the Carbon dioxide ions. The output concentration on the left-hand side is equivalent to the right-hand side whereby the first term is the change in concentration of Carbon dioxide in equation (1) and solvent

absorbent in equation (2). The second term is the concentration due to the mass transfer whereby it is denoted by the molar flux and mass transfer area. The last term equation (2) is the second order rate of reaction, first order due to Carbon dioxide and first order due to solvent absorbent.

$$\frac{\partial C_i^v}{\partial t} = -\frac{\partial (C_i^v U_i^v)}{\partial z} + A_\varepsilon N_i \tag{1}$$

$$\frac{\partial C_i^l}{\partial t} = -\frac{\partial (C_i^l U_i^l)}{\partial z} - A_\varepsilon N_i + N_R \tag{2}$$

C_i, U_i, A_ε, N_i, N_R, z and t are Concentration (kmol/m^3), velocity (m/s), mass transfer are (m^2/m^3), molar flux (Kmol/m^{2}s), rate of reaction (Kmol/m^3.s for second order), Column height (m) and time (s).

2.1. Reduction of the equations
l is the liquid phase symbol for specie i and v is the gas phase symbol for specie i.

$$\frac{dC_i^l}{dt} = -C_i^l \frac{d(U_i^l)}{dz} - U_i^l \frac{d(C_i^l)}{dz} - a_e N_i + N_R \tag{3}$$

$$\frac{dC_i^v}{dt} = C_i^v \frac{d(U_i^v)}{dz} - U_i^l \frac{d(C_i^v)}{dz} - + a_e N_i \tag{4}$$

$$\frac{d(U_i)}{dz} = 0 \tag{5}$$

Equations (3) and (4) are the results of differentiating equation (1) and (2) . (3) and (4) formed equation (6) and (7) when substituted with (5).

$$\frac{dC_i^l}{dt} = -U_i^l \frac{d(C_i^l)}{dz} - a_e N_i + N_R \tag{6}$$

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$$\frac{dC_i^v}{dt} = -U_i^v \frac{d(C_i^v)}{dz} + a_e N_i \tag{7}$$

$$\frac{dC_{i,n}^l}{dt} = -U_i^l \frac{d(C_{i,n}^l - C_{i,n-1}^l)}{dz} - a_e N_i + N_R \tag{8}$$

$$\frac{dC_{i,n}^v}{dt} = -U_i^v \frac{d(C_{i,n}^v - C_{i,n-1}^v)}{dz} + a_e N_i \tag{9}$$

2.2. Reaction rate model

The overall reaction rate is second-order, first-order with respect to both CO_2 and the solvent absorbent, and is expressed in terms of the molar concentrations of CO_2 and MEA as:

$$N_R = K_R [CO_2][Solvent\ Absorbent] \tag{10}$$

K_R is the reaction rate constant [2]. The reaction CO_2-Solvent absorbent is second order.

2.3. Reaction rate constant

The rate constant is defined by equation (11) below.

$$K_R = Ae^{\left(-\frac{E}{RT}\right)} \tag{11}$$

Where by A is the Arrhenius constant, E is the Activation energy (kJ), R is the gas constant (Kmol/kJ. K) and T temperature of the system (K). The following equations defined the rate constant for the solvent absorbent investigated:

$$K_{R,MEA} = 2.83 \times 10^8\ e^{\left(-\frac{5900}{T}\right)} \tag{12}$$

$$K_{R,K_2CO_3} = 0.22 \times 10^{-7}\ e^{\left(\frac{5200}{T}\right)} \tag{13}$$

$$K_{R,chilled\ NH_3} = 04.79 \times 10^5\ e^{\left(-\frac{3500}{T}\right)} \tag{14}$$

2.4. Velocity definition

Fig.1 present the velocity against the amount of carbon dioxide absorbed. The graph assists in determining the velocity of the flue gas that corresponds to the velocity of the solvent absorbent in order to obtain the absorption rate of the process.
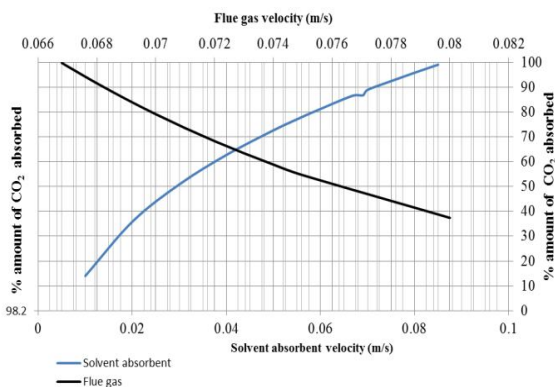

Fig.1. Relation between the velocity of the flue gas and the solvent absorbent to the amount of carbon dioxide absorbed

The solvent absorbent velocity was plotted as a primary plot and the flue gas velocity was plotted as a secondary plot. Since the mother equation was modeled using the gas phase conditions, the determination of the velocity starts on the flue gas side then corresponded with the solvent absorbent velocity. To prove this concept, the estimated data was simulated to compare the absorption rate and the results are listed in Table 1.

Table 1: data validating the correlation on figure 1.

Estimated Absorption rate (%)	Simulated Absorption rate results (%)	Error analysis (%)
100	98.75963	1.378184
95	92.79909	2.316745
90	89.55756	0.491596
85	84.12852	1.025265
80	79.43097	0.711292
75	73.86613	1.511822
70	69.37396	0.894339

The results correspond well with each other with an error less 2.5%.

III. RESULTS AND DISCUSSION

The solvent absorbent flows from the top of the column to the bottom of the column and the flue gas flow from the bottom of the column.
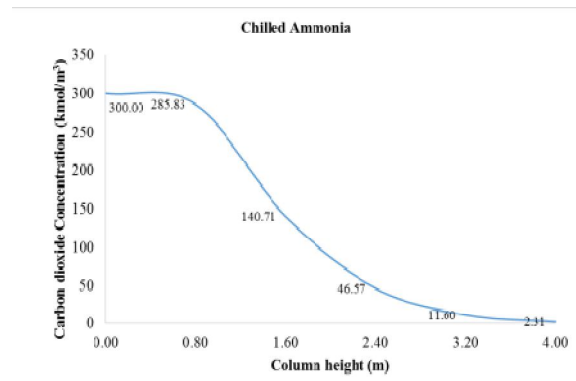

Fig.2. Concentration of Carbon dioxide profile: Chilled Ammonia system.

The concentration profile of Carbon dioxide when the chilled Ammonia is used as an absorbent has been illustrated by Fig.2. The amount of Carbon dioxide that remained with the flue gas is 2.31 Kmol/m³. This amount to 99.23% of the Carbon dioxide absorbed. The highest amount of Carbon dioxide was capture at the second and third segment of the column. There was a minimal absorption activity taking place at the first segment of the column. Stabilization of the capturing was reached at the final segment of the column.
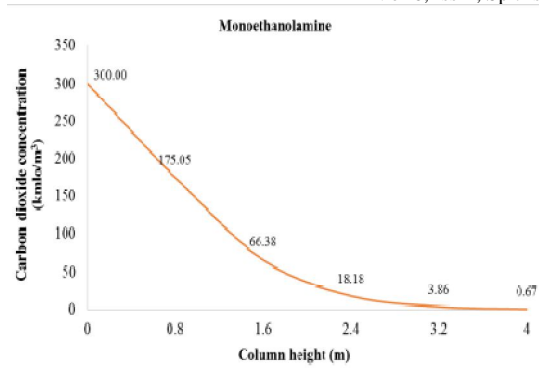
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Fig.3. Concentration of Carbon dioxide profile: MEA system.

The amount of Carbon dioxide in concentration that remained in the flue gas for the MEA system is lower compared to the Chilled Ammonia system. The amount is 1.61 Kmol/m^3 lower than the Chilled ammonia system results. Fig.3 illustrated the concentration profile of Carbon dioxide when MEA was used as an absorbent. The amount of Carbon dioxide in concentration remaining in the flue gas is 0.67 Kmol/m^3 which amounts to 99.78% Carbon dioxide captured. With the MEA system, there is a very high absorption activity from the first segment to the third segment. The process starts to stabilise from the fourth segment to the last segment.

The concentrate profile of Carbon dioxide for the Potassium Carbonate system is shown by fig.4. The amount of Carbon dioxide absorbed by the Potassium Carbonate is higher than the amount absorbed by the chilled Ammonia.

Comparing it with the MEA, Potassium Carbonate absorbed the lowest amount of Carbon dioxide. Potassium Carbonate performs better than Chilled Ammonia. 1.93 Kmol/m^3 of Carbon dioxide remained in the flue gas for the Potassium Carbonate system. The process is much faster than the chilled Ammonia system, but it is slower when comparison it to the MEA system. Stability is reached at the final segment of the column. High absorption activity occurred from the first segment of the column to the third segment.
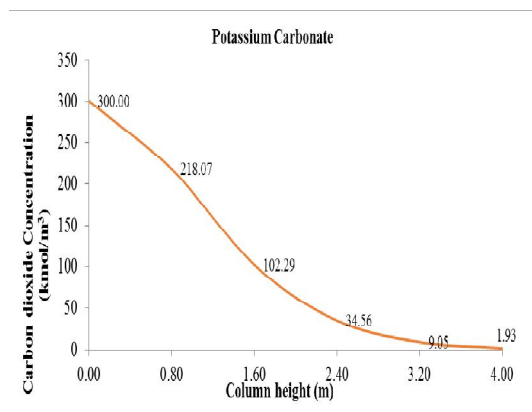

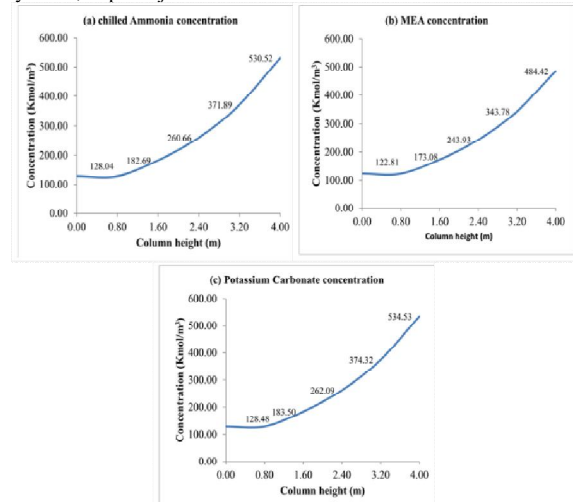**Fig.4. Concentration of Carbon dioxide profile: Potassium Carbonate system.**

Fig.5. Concentration profiling of the solvent absorbent. (a) chilled Ammonia (b) MEA (c0 Potassium Carbonate.

The concentration of the solvent absorbents was high at the top of the absorption column. The top of the column is the entry point of the solvent absorbents. The distribution of the solvent absorbent across the column is shown by Fig. 5a, 5b and 5c. Concentration of the solvent absorbent was low at the bottom of the absorption column. The flue gas flow rate should be inversely proportional to absorbent flow rate to keep a constant gas-liquid contact time [9]. At the bottom of the column, there was a high concentration of the flue gas which meant that a low concentration of the solvent absorbent was expected.

The amount of Carbon dioxide lost in the gas phase should be equivalent to the amount of Carbon dioxide absorbed by the absorbent. The concentration profile of the chilled Ammonia behaved the same way as the Potassium carbonate. Low concentration of MEA was observed.
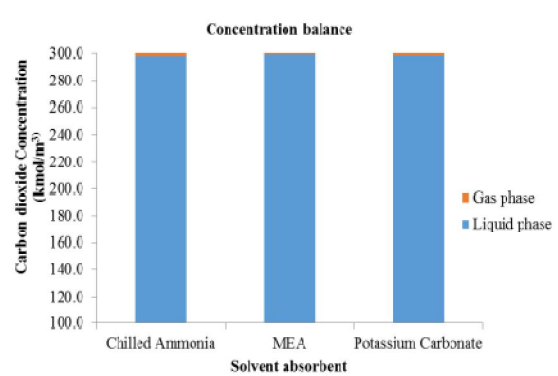

Fig.6. Carbon dioxide Concentration balance

Fig.6 shows the concentration balance of Carbon dioxide. The graph has presented the amount of Carbon dioxide absorbed by the solvent absorbents in the liquid phase and the amount of Carbon dioxide lost by the flue gas in the gas phase. The ratio of the volume flow rate of the solvent absorbents to the concentration of Carbon dioxide was calculated by equation 15. The absorption efficiency is determined

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by the ratio of the solvent absorbent's concentration to the amount of carbon dioxide absorbed in concentration.

$$molar\ volume = \frac{F^l}{C^v_{CO_2}} \qquad (15)$$

$$MEA = 0.63\, m^3 / kg_{co_2}$$

$$Potassium\ Carbonate = 0.22\, m^3 / kg_{co_2}$$

$$Chilled\ Ammonia - 0.18\, m^3 / kg_{co_2}$$

$$Absorption\ effeciency\ ratio = \frac{C^v_{CO_2}}{C^v_{solvent\ absorbent}}$$

(12)

MEA - 0.62
Potassium Carbonate - 0.56
Chilled Ammonia - 0.57

CONCLUSIONS

A graphical correlation for predicting the velocity of the flue gas and solvent absorbent was created. The results were validated by simulating the flue gas volume and calculating the amount of Carbon dioxide absorbed. The simulated results compared with the graphical estimation, corresponded well with each other.

The highest amount of Carbon dioxide will be captured with a lesser concentration of MEA. This makes MEA to be economically efficient than chilled Ammonia and Potassium Carbonate. This validates that MEA is the best absorbent in Carbon dioxide capture process with comparison to the two absorbents investigated. The Python programme was able to execute the Numerical Method of Lines equations.

ACKNOWLEDGMENTS

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