

## OPTIMIZATION OF A STRIPPER UNIT FOR THE DESORPTION OF MEA FROM (MEA-H<sub>2</sub>O-CO<sub>2</sub>) SYSTEM

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**Abstract.** The aim of this paper is to develop an optimization NLP mathematical model to determine the best operating conditions for the amine regeneration unit of the CO<sub>2</sub> post-combustion process. The amine regeneration is an energy intensive process and its optimization is the most important key to obtain cost-effective designs. Thus, an objective function defined as the ratio between the heating duty and the mass of CO<sub>2</sub> captured is proposed for minimization. The resulting model involves a high number of non-linear constraints given by the mass and energy balances and the specific correlations used to compute physical-chemical properties. In addition, bilinear terms are also considered which lead to non-convex constraints.

Also, an initialization phase is proposed to solve the model with the aim of dealing with convergence difficulties. In this way, the model and the initialization strategy resulted to be robust and flexible enough to allowing perform all optimization cases without computational problems. Optimization results including a sensitive analysis are discussed through different case studies.

## 1 INTRODUCTION

In the amine-based CO<sub>2</sub> post-combustion capture, the absorber and regenerator units are the main process-components. In the absorber, the CO<sub>2</sub> of the flue-gas is chemically absorbed by an amine solution. During the CO<sub>2</sub> absorption, the CO<sub>2</sub> reacts rapidly to form stable carbamates. Thus, the resulting solution stream, which is mainly composed by carbamates (MEA-CO<sub>2</sub>), MEA, CO<sub>2</sub> H<sub>2</sub>O, is regenerated in a stripper unit (Figure 1) in order to capture the CO<sub>2</sub> and to recover the initial amine to be used again in the absorption process. However, the solvent regeneration is energy-intensive (reboiler heat duty) and consequently its energy cost is particularly high.

The reboiler heat duty ( $Q_R$ ) is strongly influenced by the operating conditions and type and concentration of the MEA solution. For instance, at higher stripper pressure the reboiler heat duty decreases while the amine degradation rate increases. On the other hand, the reboiler duty increases with the CO<sub>2</sub> removal (lower lean loadings at a defined rich loading) due to increases of solvent rate. Moreover, higher rich loadings and/or higher feed solvent temperatures reduces the amount of stripping steam required to regenerate de amine at a defined stripper recovery.

The main goal of this work is to optimize the regenerator unit shown in Figure 1 employing mathematical programming. Thus, a deterministic mathematical model which takes into account the trade-off between the main variables previously mentioned is presented. A high-level algebraic modeling system for large scale optimization GAMS (General Algebraic Modeling System) is used for implementation and solving the resulting mathematical model. In general, mathematical programming environments such as GAMS, have shown to be powerful tools, especially when the optimization problem is large, combinatorial and highly non-linear. In addition, an initialization procedure is implemented in order to solve the proposed NLP model successfully. An efficient initialization strategy is required because a local optimization algorithm based on the generalized reduced gradient is used.

The work is outlined as follows. Section 2 introduces the problem formulation. Section 3 summarizes the assumptions and the mathematical model. Obtained results and initialization strategy are discussed in Sections 4 and 5 respectively. Finally, section 6 presents the conclusions.

## 2 PROBLEM FORMULATION

The proposed optimization problem can be stated as follows. Given the column dimensions and flow rate and composition of the rich solvent, the goal is to obtain the optimal operating conditions in order to minimize the ratio between the reboiler duty ( $Q_R$ ) and the amount of CO<sub>2</sub> leaving the condenser  $[(GC)_{out} y_{CO_2}]$ . In this way, optimal pressure, temperature, composition and flow rate profiles along the desorber unit and optimal cooling and heating requirements at minimum reboiler duty and maximum stripper recovery are simultaneously obtained.

In order to evaluate several operating conditions, the influence of temperature ( $T_{RH}$ ) and CO<sub>2</sub> loading ( $\alpha_{rich}$ ) of the rich amine solution, reboiler pressure ( $P_R$ ) and water composition into the stream giving the condenser ( $y_{H_2O}$ ) are also investigated.

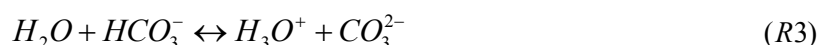
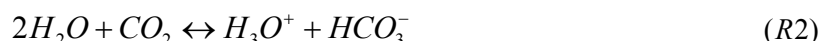
## 3 HYPOTHESIS AND MATHEMATICAL MODEL

### 3.1 Assumptions

The following are the main hypothesis assumed. The packing is divided into N stages (known value). MEA concentration and CO<sub>2</sub> loading of the rich solvent stream as well as the height and the diameter of the column are specified.

The liquid and gas phases are considered to be well-mixed and consequently there is no concentration and temperature gradients in single liquid and gas phases.

Non-ideal behavior in the gas phase is assumed and the fugacity coefficients are computed by using Peng-Robinson equations of state (multi-component mixture). In contrast to this, ideal behavior is assumed for the liquid phase. Pressure drop along the packing height is considered. It is assumed that the following chemical reactions take place at the liquid and vapor interface:



The condenser and reboiler are modeled as equilibrium stages. The condenser reflux and stripping gas are fed in the top and the bottom stages respectively.

Upper bounds for the water molar fraction of gas stream leaving the condenser ( $y_{H_2O}$ ), and reboiler pressure ( $P_R$ ) are taken into account. Similarly, lower and upper bounds for the difference between the lean solvent temperature and the rich solvent temperature ( $\Delta T = T_{lean} - T_{rich}$ ) are defined.

A pressure drop of 81.7 kPa per meter of packing is defined as lower bound. This value is suggested in the literature to ensure a minimum vapor rate to avoid laminar vapor flow and vapor mal-distribution.

### 3.2 Mathematical model

Figure 1 shows a schematic view of the stripper and the main process variables nomenclature. Figure 2 schematically shows a non-equilibrium stage “z” used to model the stripper unit. In this figure, z ( $z = 1, \dots, N$ ), j ( $j = CO_2, MEA, H_2O$ ) and i ( $i = CO_2, MEA, H_2O, MEAH^+, MEACOO^-, HCO_3^-, CO_3^{2-}, H_3O^+, HO^-$ ) denote each stage and either gas and liquid component respectively. As shown, the vapor goes up into stage z from stage z-1 and the liquid flows down into stage z from stage z+1.

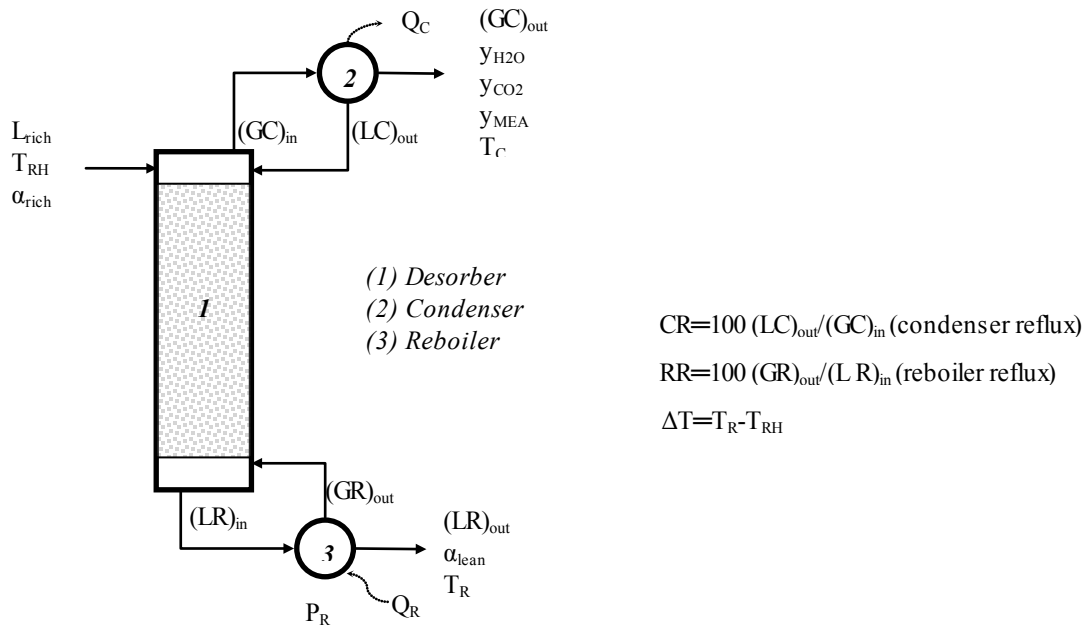


Figure 1: Schematic view of stripper unit

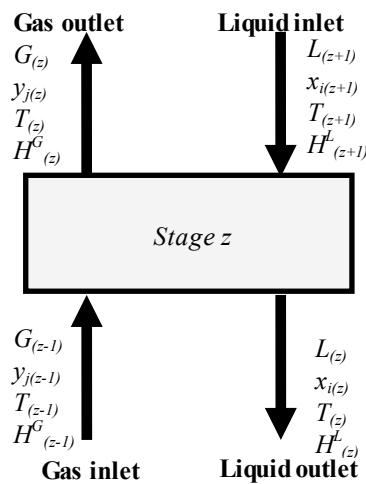


Figure 2: Generic stage

where  $L$ ,  $G$ ,  $H^L$  and  $H^G$  refer to the liquid and vapor flow-rates and enthalpies,  $x_i$  and  $y_j$  refer to the mole fraction of component “i” or “j” in liquid and vapor phases respectively.

By considering the assumptions presented in section 3.1, the following mode I was derived.

- *Mass and energy balances in stage “z”*

$$L_{z+1} - L_z + G_{z-1} - G_z = 0 \tag{1}$$

$$L_{z+1} x_{iz+1} - L_z x_{iz} + G_{z-1} y_{jz-1} - G_z y_{jz} = 0 \quad (2)$$

$$L_{z+1} H_{z+1}^L - L_z H_z^L + G_{z-1} H_{z-1}^G - G_z H_z^G + (\Delta H_R)_z - (\Delta H_{H_2O})_z = 0 \quad (3)$$

$$[MEAH^+]_z + [H_3O^+]_z = [MEACOO^-]_z + [HCO_3^+]_z + 2[CO_3^{2-}]_z + [OH^-]_z \quad (4)$$

$[i]_z$  is the molar concentration of specie “i” in stage “z”;  $\Delta H_R$  and  $\Delta H_{H_2O}$  are the heat released by the reaction and vaporization heat of water and the corresponding correlations (equations 5 to 6) are taken from Oyenekan et al. (2007) and Hilliard et al. (2008).

$$-\frac{\Delta \dot{H}_R [KJ / mol \text{ of } CO_2 \text{ absorbed}]}{R} = \left[ 1.428 \times 10^4 + 1.093 \times 10^6 \frac{\alpha_z^2}{T_z} + 6.801 \times 10^6 \frac{\alpha_z}{T_z} - 3.267 \times 10^4 \alpha_z \right] \quad (5)$$

$$\Delta \dot{H}_{H_2O} [KJ/mol \text{ of } H_2O \text{ vaporized}] = 40.628 \left[ \frac{(T_{c_{H_2O}} - T_z)}{(T_{c_{H_2O}} - 373.15)} \right]^{0.38} \quad (6)$$

where  $T_{c_{H_2O}}$  is the water critical temperature [K] and  $\alpha$  is the  $CO_2$  loading, defined as the ratio between total  $CO_2$  and total amine (eq. 7).

$$\alpha ([MEACOO^-]_z + [MEAH^+]_z + [MEA]_z) = ([MEACOO^-]_z + [CO_2]_z + [HCO_3^-]_z + [CO_3^{2-}]_z) \quad (7)$$

▪ *Chemical reactions and phase equilibrium relationship:*

The relationships of the equilibrium constants of reactions R1 to R5 and Henry's coefficient ( $H_{CO_2}$ ) with the temperature and composition are as below:

$$(K_m)_z = \prod_i (a_{iz})^{v_i} = \prod_i (x_{iz} \gamma_{iz})^{v_i} \quad \forall m, \quad m = R_1, R_2, R_3, R_4, R_5 \quad (8)$$

$$(K_m)_z = \exp \left( A + \left( \frac{B}{T_z} \right) + C \ln (T_z) \right) \quad \forall m, \quad m = R_1, R_2, R_3, R_4, R_5 \quad (9)$$

$$H_{CO_2-iz} = \exp \left( A + \left( \frac{B}{T_z} \right) + C \ln (T_z) + D T_z \right) \quad \forall i, \quad i = MEA, H_2O \quad (10)$$

T is absolute temperature (K) and  $a_{iz}$ ,  $\gamma_{iz}$ ,  $v_i$  are activity, coefficient activity and stoichiometric coefficient to component “i” in reaction “m” respectively. The coefficients used in eq. (8) to (10) are taken from Aboudheir et al. (2003) and Liu et al. (1999).

▪ *Phase equilibrium relationship:*

$$y_{CO_2,z} \varphi_{CO_2,z} P_z = H_{CO_2,z} [CO_2]_z \quad (11)$$

$$y_{H_2O,z} \varphi_{H_2O,z} P_z = p_{H_2O,z} x_{H_2O,z} \quad (12)$$

where  $\varphi_z$ ,  $P_z$  and  $p_{H_2O,z}$  refer to fugacity coefficient, total pressure and partial pressure of water, respectively.

Solubility of CO<sub>2</sub> in MEA solution (H<sub>CO<sub>2</sub></sub>), which is corrected for solution ionic strength, is calculated as follow (Greer et al. (2008)):

$$H_{CO_2 z} = \left(10^{0.152 I_z}\right) \left[ \frac{x_{H_2O z} H_{CO_2 MEA z} + x_{CO_2 z} H_{CO_2 H_2O z}}{\rho_z^L} \right] \quad (13)$$

$$I_z = \frac{1}{2} \sum_i \psi_i [i]_z \quad \forall i, \quad i = MEAH^+, MEACOO^-, H_3O^+, OH^-, CO_3^{2-}, HCO_3^- \quad (14)$$

where  $\psi_i$  is the ion charge.

Fugacity coefficients are computed by using Peng-Robinson equations of state for multi-components (Peng and Robinson (1976)).

▪ *Dependence of stage efficiency with the column height and process variables:*

Non-equilibrium stage is considered by incorporating an effectiveness term for the stage ( $\eta$ ) through Murphree's equation.

$$\eta_z = \frac{G_z y_{iz} - G_{z-1} y_{i z-1}}{G_z y_{iz}^* - G_{z-1} y_{i z-1}} \quad (15)$$

where  $y_{i z}^*$  is the equilibrium composition of molecular specie considered leaving the stage z.

The following constraint can be formulated by assuming that the liquid and vapor phases are well-mixed and point efficiency is equivalent to Murphree's efficiency:

$$\eta_z = 1 - \exp\left(-\frac{HTU_z}{h_z}\right) = 1 - \exp\left\{-\frac{\left[\frac{G'_z}{RT_z a_z k_z^G \rho_z^G}\right] + \lambda_z \left[\frac{L'_z}{k_z^L a_z \rho_z^L E_z}\right]}{h_z}\right\} \quad (16)$$

$$h_z = HTU_z \times NTU_z \quad (17)$$

NTU<sub>z</sub> and HTU<sub>z</sub> are the number of transfer units based in the total mass transfer coefficient and the transfer unit height, respectively. G' and L' are the gas and liquid mass velocities (Kg/m<sup>2</sup> s),  $\rho^{G}$  and  $\rho^{L}$  are gas and liquid mass densities (Kg/m<sup>3</sup>);  $\lambda$  is the stripping factor ( $\lambda=m/(L/G)$ );  $k^G$  (Kmol/Pa s m<sup>2</sup>) and  $k^L$  (m/s) are the mass transfer coefficient;  $a$  is the effective interfacial area for mass transfer (m<sup>2</sup>/m<sup>3</sup>),  $h$  is the height of the stage (m); and  $E$  is the dimensionless Enhancement factor.

$k^G$ ;  $k^L$  and  $a$  are computed as follows (Onda et al. (1968)):

$$k_z^L \left(\frac{\rho_z^L}{\mu_z^L g}\right)^{1/3} = 0.0051 \left(\frac{L_z}{a_z \mu_z^L}\right)^{2/3} \left(\frac{\mu_z^L}{\rho_z^L (D_{CO_2})_z}\right)^{-1/2} (a_t D_p)^{0.4} \quad (18)$$

$$k_z^G \left(\frac{RT_z}{a_t D_z^G}\right) = 5.23 \left(\frac{G}{a_t \mu_z^G}\right)^{0.7} \left(\frac{\mu_z^G}{\rho_z^G D_z^G}\right)^{1/3} (a_t D_p)^{-2} \quad (19)$$

$$a_z = a_t \left( 1 - \exp \left( -1.45 \left( \frac{\sigma_c}{\sigma_z} \right)^{0.75} \left( \frac{L'_z}{a_t \mu_z^L} \right)^{0.1} \left( \frac{(L'_z)^2 a_t}{(\rho_z^L)^2 g} \right)^{-0.05} \left( \frac{(L'_z)^2}{\rho_z^L \sigma_z a_t} \right)^{0.2} \right) \right) \quad (20)$$

The enhancement factor (E) is defined as follows:

$$E_z = \frac{\sqrt{(D_{CO_2}^L)_z [(k_{r,CO_2-MEA})_z [MEA]_z + (k_{r,CO_2-OH})_z [CO_2]_z]}}{k_z^L} \quad (21)$$

The forward constants ( $k_{r, CO_2-MEA}$  and  $k_{r, CO_2-OH}$ ) of the parallel and kinetically controlled reactions (R6-R7) are taken from Kucka et al. (2002) and Aboudheir et al. (2003) and are computed as follows:

$$(k_{r,CO_2-MEA})_z = 4.495 \times 10^{11} \exp \left( -\frac{44940}{R T_z} \right) \quad (22)$$

$$(k_{r,CO_2-OH})_z = \exp \left( 31.396 - \frac{6658}{T_z} \right) \quad (23)$$

#### ▪ Column pressure drop

The total pressure drop along the packing column is given by:

$$\Delta P = \sum_z \Delta P_z h_z \quad (24)$$

Pressure drop (kPa/m) in each stage is estimated by using Robbins et al. (1990) correlation. It takes into account the pressure drop due to the dry packing and due to the liquid presence. It depends on liquid and gas flow rates, liquid and gas densities, liquid viscosity, gas velocity, dry packing factor and operative pressure.

Finally, the model includes correlations to compute fluid properties (vapor pressure, density, viscosity, enthalpies and diffusivity) which are taken from different specialized literature (Austgen (1989), Freguia et al. (2002), Dugas (2006), Greer et al. (2008)) and are valid for a wide range of operating conditions.

The optimization model involves approximately 1500 variables and constraints. As mentioned earlier the model was implemented in General Algebraic Modeling System GAMS (Brooke et al. (1996)). The generalized reduced gradient algorithm CONOPT 2.041 was here used as a local NLP solver (Drud (1992)).

As previously shown, the model includes many high non-linear constraints. Moreover, the model includes bilinear terms (equations 2, 3, 5, 8, 11, 16, 18, 21, among others) which lead to non convex constraints. It is well known that these types of models are difficult to solve and good starting points and lower-upper bounds are essential to guarantee the model's convergence towards finding optimal solutions. After the discussion of results, the developed initialization procedure to overcome convergence difficulties is described in detail.

## 4 RESULTS AND DISCUSSION

In this section the optimal solutions obtained by the proposed optimization mathematical model are presented.

The packing was modeled with 10 segments. Column specifications are presented in Table 1.

<b>Column Type</b>	Packed
Diameter (m)	5
Total packing height (m)	12
Stages number	10
<b>Packing specifications</b>	
Type of packed	IMTP#40
Specific area (m <sup>2</sup> /m <sup>3</sup> )	154
Nominal packing size (m)	0.04
Void fraction	0.97
Dry packing factor (m <sup>2</sup> /m <sup>3</sup> )	85

Table 1: Column specifications.

The following specifications were used as model parameters:

- Rich amine flow rate ( $L_{rich}=8000$  mol/s)
- Rich solvent composition ( $0.43 \leq \alpha_{rich} \leq 0.55$ ; 30% w/w of MEA).

In order to consider some technological constraints, the following sets of lower and upper bounds have been considered:

- 1)  $P_R \leq 150$  kPa,  $y_{H_2O} \leq 0.1$  and  $\Delta T \geq 10$  and
- 2)  $P_R \leq 180$  kPa,  $y_{H_2O} \leq 0.05$  and  $\Delta T \geq 5$ .

As mentioned in the introduction, in all cases the variables reached, as expected, its defined bounds.

The effect of the main process variables on the stripper performance is discussed as follows.

Figures 3 to 7 show optimal solution families for the main process variables which strongly influence the process performance: 1) specific reboiler duty (OF); 2) mass rate of CO<sub>2</sub> captured; 3) CO<sub>2</sub> lean loading; 4) % of stripping gas produced in the reboiler; 5) % of liquid reflux to the stripper; 6) column pressure drop; 7) condenser and reboiler duties.

Figure 3 and Figure 4 show the objective function, mass of CO<sub>2</sub> captured and reboiler duty for the range of rich CO<sub>2</sub> loading adopted as model parameter.

The condenser duty and the liquid reflux versus the mass of CO<sub>2</sub> captured are shown in Figure 5. Figure 6 shows optimal values of CO<sub>2</sub> recovery (%) versus optimal values of lean CO<sub>2</sub> loading. Finally, in Figure 7 is shown the relationship between the percentages of gas refluxed to the stripper and the column pressure drop.



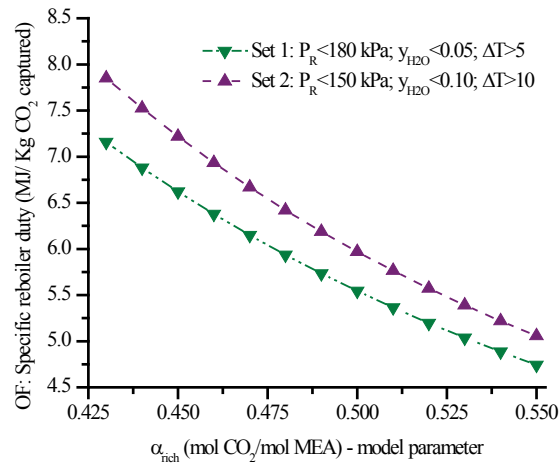


Figure 3: Optimal Objective function vs. rich CO<sub>2</sub> loading

From Figure 3 it can be easily observed that same trends are obtained for both sets of bounds. That is the specific reboiler duty decreases as  $\alpha_{rich}$  increases. The specific heat reboiler for Set 2 is 8.5 % greater than to that required by Set1.

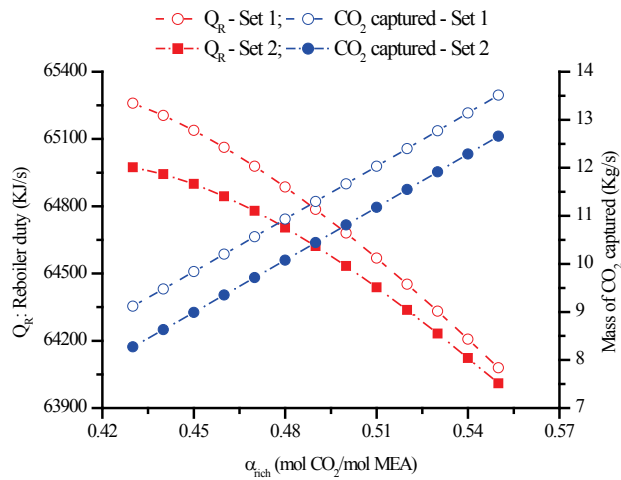


Figure 4: Optimal reboiler heat duty and mass of CO<sub>2</sub> captured vs. rich CO<sub>2</sub> loading

In Figure 4 is shown that the mass of CO<sub>2</sub> captured increases with the increasing of  $\alpha_{rich}$  while the reboiler duty decreases. For both cases the mass of CO<sub>2</sub> absorbed increases faster than the reboiler duty.

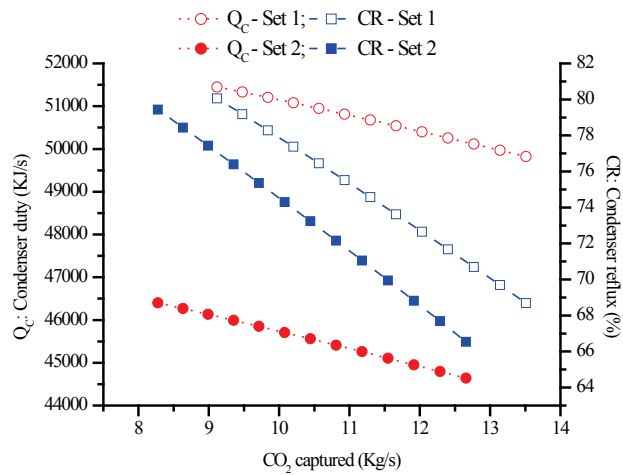


Figure 5: Optimal condenser heat duty and condenser reflux to the stripper vs. mass of CO<sub>2</sub> captured.

In Figure 5 is shown a linear relationship between the mass of CO<sub>2</sub> captured and the condenser duty. Moreover, cooling utilities requirements are higher for case 1 where higher amounts of liquid are refluxed to the stripper.

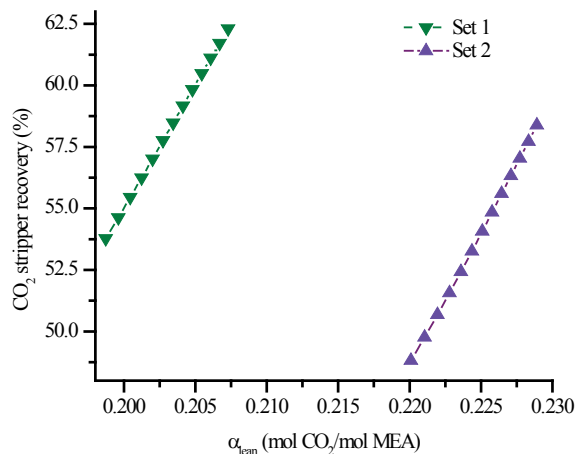


Figure 6: Optimal lean CO<sub>2</sub> loading vs. stripper recovery

In Figure 6 is shown that for set 1, the optimal values of lean CO<sub>2</sub> loading range between 0.199 and 0.207 while for case 2,  $0.220 \leq \alpha_{lean} \leq 0.229$ . For the same recovery, for instance 57%, in case 1  $\alpha_{rich}=0.47$  and  $\alpha_{lean}=0.202$  while in case 2,  $\alpha_{rich}=0.53$  and  $\alpha_{lean}=0.228$ .

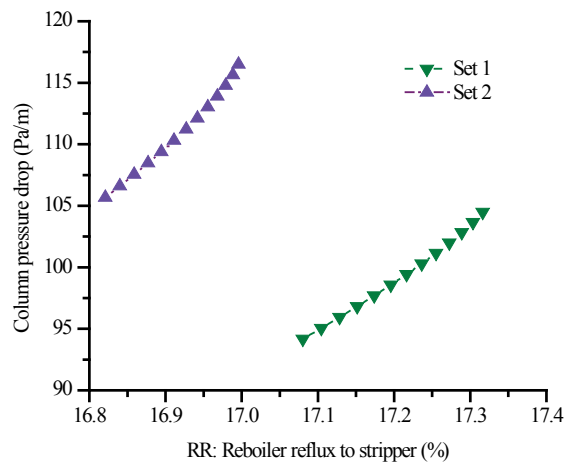


Figure 7: Optimal column pressure drop vs. reboiler reflux

Finally, Figure 7 shows that in set 1 lower amounts of stripping gas are produced and higher column pressure drops are obtained.

To sum up, from the figures can be observed that a better performance is obtained for the set 1 and higher  $\alpha_{rich}$ . The figures show the numerical values of the main operating process for preliminary designs. It should be mention however, that other aspects such as, the rate of amine degradation, the compression and pumping works, among others should be consider for a final design.

## 5 INITIALIZATION STRATEGY

As mentioned, the resulting mathematical model involves non-linear and non-convex constraints. It is well known that the models with these characteristics are difficult to solve and require good solution strategies especially when local optimization algorithms are used instead of global search methods. Certainly, local optimization techniques require feasible initial solutions to guarantee the convergence of the model. Thus, the following initialization strategy for all model variables was used in this paper:

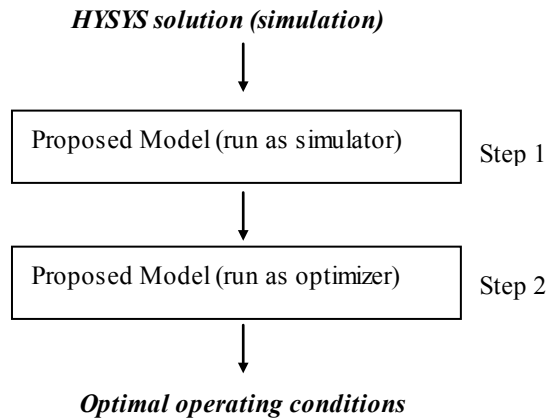


Figure 8: Initialization strategy

As shown in Figure 8, a simulation solution obtained by the HYSYS process simulator and reported in the literature (Lars (2007)) is used as initialization to solve the developed model in a simulation step. Thus, in Step 1, the proposed model is solved as simulator because the values corresponding to the main process variables are fixed according to the HYSYS solution. In other words, the degree of freedom of the total equation system is zero; the main objective in Step 1 is to find a feasible solution of the model in few iterations. Then, the solution obtained in Step 1 is used as initialization to solve the optimization problem involved in Step 2 and the optimal operating conditions of the regenerator unit is obtained as solution. It should be mentioned that scaling on variables and equations has been also implemented in order to also facilitate the model convergence.

Finally, it is important to mention that several tests using different random initialization settings have been also considered. In some cases, same solutions reported in the paper have been obtained but in other cases, the optimization algorithm failed. However, despite that same solutions were obtained in all converged cases, global solutions can not be guaranteed due to the non-convex constraints.

## CONCLUSIONS

A deterministic NLP mathematical model for the reactive CO<sub>2</sub> desorption into aqueous MEA amine solutions is presented. Temperatures, compositions, flow-rates and pressures drops through the length of the stripper as well as CO<sub>2</sub> recovery, condenser and reboiler duties were the main optimization variables. The proposed model is a valuable tool not only to optimize the process but also to simulate the regeneration process if the degrees of freedom of the equation system are zero. Also, an initialization procedure has been implemented which guarantee the convergence of the high non-linear mathematical model. Thus, the resulting mathematical model and the proposed initialization strategy are robust and flexible enough to allowing perform simulations and optimizations without computational problems. The influence of main process operating conditions (composition, temperature, pressure and flow-rate) on desorption performance has been investigated.

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