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MASS TRANSFER COEFFICIENTS IN AN ABSORBER RECTOR IN THE UNIT OPERATIONS LABORATORY, THE TEMPERATURE PROFILE (2)

Mariano Pérez Camacho[1]
[1]Departamento de Ingeniería Química,
UNAM, Facultad de Estudios Superiores
Zaragoza,
Ciudad de México C.P. 09230

Antonio Valiente Barderas[2]
[2]Departamento de Ingeniería Química,
UNAM, Facultad de Química,
Ciudad de México C.P. 04510

Ricardo Pérez Camacho[3]
[3]Departamento de Ingeniería Química,
UNAM, Facultad de Química,
Ciudad de México C.P. 04510

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ABSTRACT

In the first article Mass Transfer Coefficients in an Absorber Reactor in the Unit Operations Laboratory (1) reference [4], it was developed by students of the Faculty of Chemistry of the National Autonomous University of Mexico, UNAM. Students now obtain the temperature profile along the column by posing and solving the differential equation of energy balance (heat) that is a function of the temperatures of the liquid with the position TL = TL (z) and compare the results with experimental values that were obtained with thermocouples distributed every 22 cm throughout the top of the column. To solve the energy equation numerically, it is necessary to use the matter balance program developed in reference [4], to calculate the value of the individual coefficient of mass transfer on the liquid side kL and with this value obtain the absorption speed in the presence of a chemical reaction at the interface using successive iterations of calculation and thus numerically solving the temperature profile of the liquid vs. the position in the column.

With this type of experimentation, the teaching by competences is reinforced, a necessary teaching that a chemical engineer must possess.

KEYWORDS: ***Balances of matter and energy in absorption with chemical reaction. MEA-H2O / CO_2-air reaction system. Thermodynamic balance between phases in the presence of chemical reaction. Teaching by competencies.***

1. INTRODUCTION

Chemical engineering education today is based on so-called competencies. Professional competencies are those that are learned during the career and that include the specific knowledge of the same, as well as the professional skills and attitudes of the students. The UNAM Chemical Engineering Laboratory is one of the places where these skills can be developed and refined through the development of laboratory experimentations, since during these apprenticeships' students must use their knowledge and apply it, as well as develop your personal skills and attitudes. In this laboratory unit operations are studied among other disciplines. There chemical engineering students experiment in various equipment, one of which is the absorption tower. In it, students are asked to experimentally find the individual gas-transfer and liquid-side mass transfer coefficients in the presence of a chemical reaction and to compare the temperature profiles of the theoretical models and experimental temperature data throughout the column.

2.- THEORETICAL FOUNDATIONS

It was mentioned in the first article **[4]** the system (MEA-H2O / CO2-AIR) that has a reaction mechanism made up of consecutive reversible reactions, but when adding and canceling the partial terms they generate the following 2nd order reaction and exothermic.

$$CO_2 + 2\,R_1NH_2 \longleftrightarrow R_1NHCOO^- + R_1NH3^+,\quad T°C\ MEA = 24°C,\quad k_2 := 10^{\left(10.99 - \frac{2152}{T°K}\right)}$$

= 5 595.854 L/gmol s, see reference [6].

To study now the proposed model of heat as a function of liquid temperatures and the position TL = TL (z) within the column, the students of the Faculty of Chemistry used an absorption tower located in the Chemical Engineering Laboratory of the Faculty of Chemistry of the National Autonomous University of Mexico, UNAM. To do this, it was necessary to vary the experimental operating conditions to make observations and consider possible theoretical and practical simplifications.

For example:
a) The reaction is fast enough to develop in the film of the liquid. This study is contemplated in the first article **[4].**
b) The reaction is exothermic and increases the internal temperature in the column with increasing liquid phase feed flow.

2.1 To propose the models of the balance of matter [4] and now that of energy (heat), use Fig. (1)

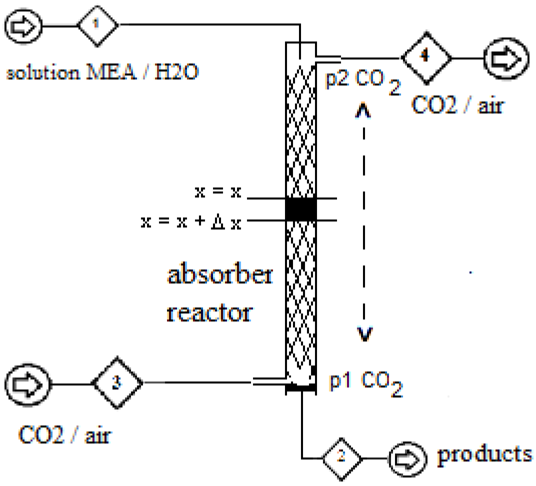


Fig. (1) Absorber Reactor

Assumptions:
(1) When using high mass flows of MEA / H2O, the reaction behaves like a pseudo-primer order with respect to solute A (CO2), [4].
(2) The longitudinal speed of the liquid is constant, there is no radial or angular speed, [4].
(3) Radial mixing is perfect, there are no radial concentration gradients.
(4) Axial diffusion is negligible, compared to convective axial effects.
(5) The density of the system is practically constant.
(6) The molar volumetric concentration of the soluble gas in the liquid in the column = 0, all CO2 reacts in the liquid film.
(7) The partial pressures along the column have values very close to the values of equilibrium pressures at the interface.
(8) There are no radial or angular molar fluxes in the absorber-reactor, only longitudinal and temporary.
(9) Control of mass transfer resides in the film of the liquid phase.

COMMENTARY. - The changes in the z positions along the absorber-reactor of Fig. (1) are obtained by the following differential equation by solving for the z position, for this the partial pressures at the inlet and outlet of the column of known height h.

$$\frac{d^2 p_{CO2}}{dz^2} = 0$$

$$\text{border conditions} \qquad (1)$$

$$\left.\begin{array}{l} p_{CO2} = p_{1\,CO2} \quad to \quad z = 0 \\ p_{CO2} = p_{2\,CO2} \quad to \quad z = h \end{array}\right\} \; solution \rightarrow p_{CO2} = \left(\frac{p_{2\,CO2} - p_{1\,CO2}}{h}\right) z + p_{1\,CO2}$$

2.2- The following differential mass balance can be proposed for CO_2 in the liquid phase in the absorber reactor [4]:

$$-D_L\,\varepsilon\,A_T \left.\frac{\partial[A_0]}{\partial z}\right|_Z + \varepsilon\,A_T\,L[A_0]\big|_Z + R_A\,a\,\Delta z\,A_T = -D_L\,\varepsilon\,A_T \left.\frac{\partial[A_0]}{\partial Z}\right|_{Z+\Delta Z} + \varepsilon\,A_T\,L[A_0]\big|_{Z+\Delta Z} + \varepsilon\,A_T\,\Delta_Z \frac{\partial[A_0]}{\partial t} - r\,\varepsilon\,A_T\,\Delta_Z \qquad (2)$$

Dividing between the control volume ($\varepsilon\,A_T\,\Delta z$) and taking limits equation (4) is obtained

$$\lim_{\Delta z \to 0}\left\{ D_L \left.\frac{\partial[A_0]}{\partial z}\right|_{z+\Delta z} - D_L \left.\frac{\partial[A_0]}{\partial z}\right|_{z} - \frac{L[A_0]\big|_{z+\Delta z} - L[A_0]\big|_{z}}{\Delta z}\right\} = \frac{\partial[A_0]}{\partial t} - \frac{R_A\,a}{\varepsilon} - r \qquad (3)$$

If there is no accumulation in the permanent regime, and disregarding the convective and diffusive terms of the absorbed CO2, compared to the reaction in the film, and if also the absorption speed with reaction is appreciably greater than the physical absorption speed, we obtain:

$$\underbrace{L\,\cancel{\frac{\partial[A_0]}{\partial z}}}_{convection} + \underbrace{\cancel{\frac{\partial[A_0]}{\partial t}}}_{accumulation} - \underbrace{\frac{R_A\,a}{\varepsilon}}_{\text{Absorption with reaction}} - \underbrace{r}_{\text{raction}} = \underbrace{D_L\,\cancel{\frac{\partial^2[A_0]}{\partial z^2}}}_{\cancel{diffusion}} \qquad (4)$$

$$\boxed{-\frac{R_A\,a}{\varepsilon} - r = 0} \qquad (5)$$

2.3.- The following differential mass balance can also be proposed for the monoethanolamine in the liquid phase in the absorber reactor:

$$\varepsilon\,A_T\,L[B_0]\big|_Z = \varepsilon\,A_T\,L[B_0]\big|_{Z+\Delta Z} - r\,\varepsilon\,A_T\,\Delta z \qquad (6)$$

Dividing by the control volume ($\varepsilon\,A_T\,\Delta z$) and taking limits to equation (6) is obtained

$$\text{lím}\left\{\frac{L[B_0]\big|_{Z+\Delta Z} - L[B_0]\big|_Z}{\Delta z}\right\} = r$$

$$\Delta z \rightarrow 0$$

The differential balance for amine is:

$$\boxed{L\frac{d\left[B_0\right]}{dz}=r} \tag{7}$$

By equating (5) and (7) we arrive at

$$-\frac{R_A\ a}{\varepsilon}=L\frac{d\left[B_0\right]}{dz}$$

$$L\ d\left[B_0\right]=-\frac{R_A\ a}{\varepsilon}\,d\,z \tag{8}$$

Integrating equation (8) from the top to the bottom of the column we obtain:

$$\boxed{h=-\frac{L\ \varepsilon}{a}\int_{B_0\ top}^{B_0\,bottom}\frac{d\left[B_0\right]}{R_A}} \quad \text{Ó} \quad \boxed{h=\frac{L\ \varepsilon}{a}\int_{B_0\ bottom}^{B_0\,top}\frac{d\left[B_0\right]}{R_A}} \tag{9}$$

2.4- Energy balance on the volume differential element located in some arbitrary distance z of Fig. (1), See reference [1].

$$\begin{array}{lllll} \text{Rapid flow} & \text{Rapid flow} & \text{Accumulated} & \text{Generated} & \text{Exchanged} \\ \text{of incoming} = & \textit{of exiting} \ + & \textit{energy} \ - & \textit{energy} \ - & \textit{energy} \\ \text{energy} & \text{energy} & & & \end{array}$$

If the total energy flux in z is defined as the sum of the diffusive and convective fluxes

$$e_z=q_z+\rho_L\ Cp_L\ v_z\ \left(T_L-T_R\right) \tag{10}$$

Where is the reference temperature (for example, that of the environment)

$$q_z=\frac{Q_Z}{A_T}=-k_{axial}\ \frac{dT_L}{dz} \tag{11}$$

The heat generated by the reaction is:

$\Phi_H=r\ (-\Delta H_r)$, where ΔH_r is the enthalpy change due to the reaction and r is the reaction speed = - $k_{Am}\left[Am\right]\left[CO_2\right]$

An equivalent form of this term is to use the diffusive absorption-reaction flux through the interface, where the speed of reaction in the liquid phase does not occur in the bulk of the liquid but in the interfacial region [5], since It is a fast reaction that depends on the diffusive absorption flux.

$$\Phi_H=R_A\,a\ (\Delta H_{abs}) \tag{12}$$

Where the heat of absorption $\Delta H_{abs}=(84.68-0.1135\times T_L+0.0027\times T_L^2)$ in [kjoules / gmol] reported by Hanne M. Kvamsdal and Magne Hillestad [2], [3]. TL is the temperature of the liquid in the absorber reactor in [° C] and ***a*** is the specific gas-liquid interface area [m^2/m^3]

The volumetric heat loss to the neighborhoods of the column is calculated as:

$$Q_V=-h_{walls}\,a\left(T_L-T_{amb}\right)$$

Where $h_{walls}=1000\times 4.05\times 10^{-3}\times\left(\frac{\rho_g\ V_g}{D_{hyd}}\right)^{0.5}\left(Cp_g\right)^{0.33}$ in [$W/m^2\ K$] (13)

$$\rho_g=\left[kg/m^3\right],\quad V_g=[m/s],\quad D_{hyd}=[m],\quad Cp_g=[j/m^3\,K]$$

The foundations of this coefficient are found in the work of Hanne M. Kvamsdal and Magne Hillestad **[2]**, **[3]**, TL is the temperature of the liquid in the tower and T_{amb} is the ambient temperature.

Substituting the previous equations in the general energy balance described above, the following is obtained:

$$\begin{aligned} A_T\ q_Z\big|_z+A_T\ \rho_L\ Cp_L\ v_z\left(T_L-T_R\right)\big|_z &= A_T\,q_Z\big|_{z+\Delta z}+A_T\ \rho_L\ Cp_L\ v_z\left(T_L-T_R\right)\big|_{z+\Delta z} \\ &+\Delta z\ A_T\ \rho_L\ Cp_L\ \frac{dT_L}{dt}-\Delta z\ A_T\ \Theta_H-\Delta z\ A_T\ Q_V \end{aligned} \tag{14}$$

Dividing equation (14) by the control volume $\left(A_T\ \Delta z\right)$ and taking the limit when $\Delta z \rightarrow 0$, the following differential equation is obtained:

$$\underbrace{-k_{axial}\frac{\partial^2 T}{\partial z^2}}_{\substack{\text{diffusion } o\\ \text{conducction}}} + \underbrace{\rho_L\ Cp_L\ v_z\frac{\partial T}{\partial z}}_{\text{convection}} + \underbrace{\rho_L\ Cp_L\frac{\partial T}{\partial t}}_{\text{accumulation}} - \underbrace{\Phi_H}_{\text{generation}} - \underbrace{Q_V}_{\substack{\text{energy}\\ \text{exchange}}} = 0 \qquad (15)$$

If in equation (15) the term axial conduction is neglected and if this reactor operates continuously in a stable state, then there is no accumulation of energy, it also operates as non-adiabatic and non-isothermal. The following model is obtained:

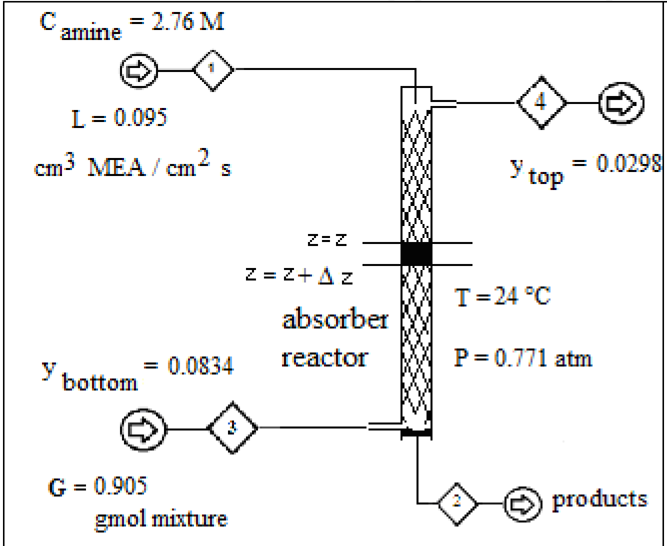
$$\underbrace{-k_{axial}\cancel{\frac{\partial^2 T}{\partial z^2}}}_{\substack{\text{diffusion } o\\ \text{conducction}}} + \underbrace{\rho_L\ Cp_L\ v_z\frac{\partial T}{\partial z}}_{\text{convection}} + \underbrace{\cancel{\rho_L\ Cp_L}\frac{\partial T}{\partial t}}_{\text{acumulation}} - \underbrace{\Phi_H}_{\text{generation}} - \underbrace{Q_V}_{\substack{\text{energy}\\ \text{exchange}}} = 0$$

$$\boxed{\frac{d\,T}{d\,z} = \frac{\Phi_H + Q_V}{V_Z\ \rho_L\ Cp_L}} \qquad (16)$$

where $v_z = \dfrac{volumeric\ \ flow}{cross\ \ flow\ area\ beetwen\ \ packages}$, ρ_L is the density of the liquid and Cp_L is the specific heat at constant pressure of the liquid.

3.- EXPERIMENTAL DATA AND CALCULATIONS

The equipment used for experimentation was as follows



The equipment has the following specifications:
Internal column diameter: 5.08 cm
Flow cross-sectional area (ATF): 14.66 cm^2
Packed height: 106 cm
Construction material: Glass
Packaging: External diameter, internal diameter and length glass Raschig rings0.703 cm0.545 cm0.854 cm
Chromatograph: Gow-Mac electrical conductivity
Fraction of hollows $\varepsilon = 0.70$
a = 0.839 cm^2/cm^3
a_t = 7.169 cm^2/cm^3
Six thermocouples installed each through the column22 cm

Absorption tower brand PIGNAT in the Chemical Engineering Laboratory

Fig. (2) Absorber Reactor

3.1 In experimentation the students obtained the following results shown in the Table (1)

Table (1). Experimental Temperature Data

The experimental values of the temperatures were obtained by means of six thermocouples distributed every 22 cm throughout the column, these are interconnected to a MODEM located in the right corner of the equipment and then to the central computer of the Chemical Engineering Laboratory.

Position z (cm)	Temperatures (°C)		
	5 L / h	**8 L / h**	**10 L /h**
0	24.1	24.2	24.2
22	28.1	28.5	29.0
44	31.2	32.0	32.4
66	33.2	33.7	35.2
88	34.4	34.6	38.0
110	34.4	36.4	38.9

Table (1). Experimental Data of Flows and Concentrations

Feeding air temperature = 24 ºC. Temperature of the fed CO2 = 23 ºC. Hollow fraction $\varepsilon = 0.70$. Inlet air density = 1.204 10^{-3} g / cm^3. Cross flow area between packages = 14.66 cm^2. Inlet CO_2 density = 1.885 10 $^{-3}$ g / cm3 Density of the liquid mixture fed 1.004 g / cm^3

Feed flow (L / h)	**Concentration MEA N = gmol / Lsol**		**Concentration MEA (% in mass) % mass = 6.064 (N) + 0.0231 (g MEA / g solution)**		**Q $_{air}$ (m^3 / h)**	**Q CO_2 (L / h)**
	entrance	**exit**	**entrance**	**exit**		
5	2.76 N	1. 28 N	16.76 %	7.78 %	2.606	257.127
8		1. 35 N		8.20 %		
10		1. 70 N		10.33 %		

3.2 Evaluation of the terms of the heat balance of the Eq. (16) using the experimental data in Table (1).

$$\frac{\partial T}{\partial z} = \frac{\Phi_H + Q_V}{v_z \ \rho_L \ Cp_L}$$

$$\frac{°C}{cm} = \frac{\frac{cal}{s \cdot cm^3} + \frac{cal}{s \cdot cm^3}}{\frac{cm}{s} \cdot \frac{gmol}{cm^3} \cdot \frac{cal}{gmol \cdot °C}}$$

The speed of the liquid v_z

$$V_z := \frac{Le \cdot \frac{1}{3600} \cdot \frac{1000}{1}}{ATF}$$

$$\frac{cm}{s} = \frac{\frac{L}{h} \cdot \frac{1h}{3600 \cdot s} \cdot \frac{1000cm^3}{L}}{cm^2}$$

$$V_z = 0.095 \quad \frac{cm}{s}$$

The heat capacity of the constant pressure-fed liquid CPL

$$TLe := 24 \quad °C$$

$$TLe°K := TLe + 273.15$$

$$Cp_{H2O} := \left(92.053 - 3.9953 \cdot 10^{-2} \cdot TLe°K - 2.1103 \cdot 10^{-4} \cdot TLe°K^2 + 5.3469 \cdot 10^{-7} \cdot TLe°K^3\right) \cdot 0.2369$$

$$\frac{cal}{gmol \cdot °C} = \frac{Joule}{gmol \cdot °K} \cdot \frac{0.23901 \cdot cal}{1 \cdot Joule}$$

$$Cp_{H2O} = 17.904 \quad \frac{cal}{gmol \cdot °C}$$

$$\text{TLe} := 24 \quad °\text{C}$$

$$\text{TLe°K} := \text{TLe} + 273.15$$

$$Cp_{H2O} := \left(92.053 - 3.995310^{-2}\cdot\text{TLe°K} - 2.110310^{-4}\cdot\text{TLe°K}^{2} + 5.346910^{-7}\cdot\text{TLe°K}^{3}\right)\cdot 0.2369$$

$$\frac{\text{cal}}{\text{gmol}\cdot°\text{C}} = \frac{\text{Joule}}{\text{gmol}\cdot°\text{K}}\cdot\frac{0.23901\cdot\text{cal}}{1\cdot\text{Joule}}$$

$$Cp_{H2O} = 17.904 \quad \frac{\text{cal}}{\text{gmol}\cdot°\text{C}}$$

$$Cp_{MEA} := \left(23.11 + 1.2283\text{TLe°K} - 3.121810^{-3}\cdot\text{TLe°K}^{2} + 3.071410^{-6}\cdot\text{TLe°K}^{3}\right)\cdot 0.23901$$

$$Cp_{MEA} = 46.138 \quad \frac{\text{cal}}{\text{gmol}\cdot°\text{C}}$$

$$\text{CpL} := \left[Cp_{MEA}\cdot\text{xMolarMEAE} + Cp_{H2O}\cdot(1 - \text{xMolarMEAE})\right]$$

$$\text{CPL} = 19.486 \, \frac{\text{cal}}{\text{gmol}\cdot°\text{C}}$$

The density of the fed liquid ρ_L

$$\rho\text{L} := \rho_{L}\cdot\frac{1}{PM_{MEA.H2O}}$$

$$\frac{\text{gmol}\cdot\text{mezcla}}{\text{cm}^{3}} = \frac{\text{g}\cdot\text{mezcla}}{\text{cm}^{3}}\cdot\frac{\text{gmol}\cdot\text{mezcla}}{\text{g}\cdot\text{mezcla}}$$

$$\rho L = 0.049\frac{gmol\ mezcla}{cm^{3}\ mezcla}$$

Volumetric heat flow through the walls of the column Qv

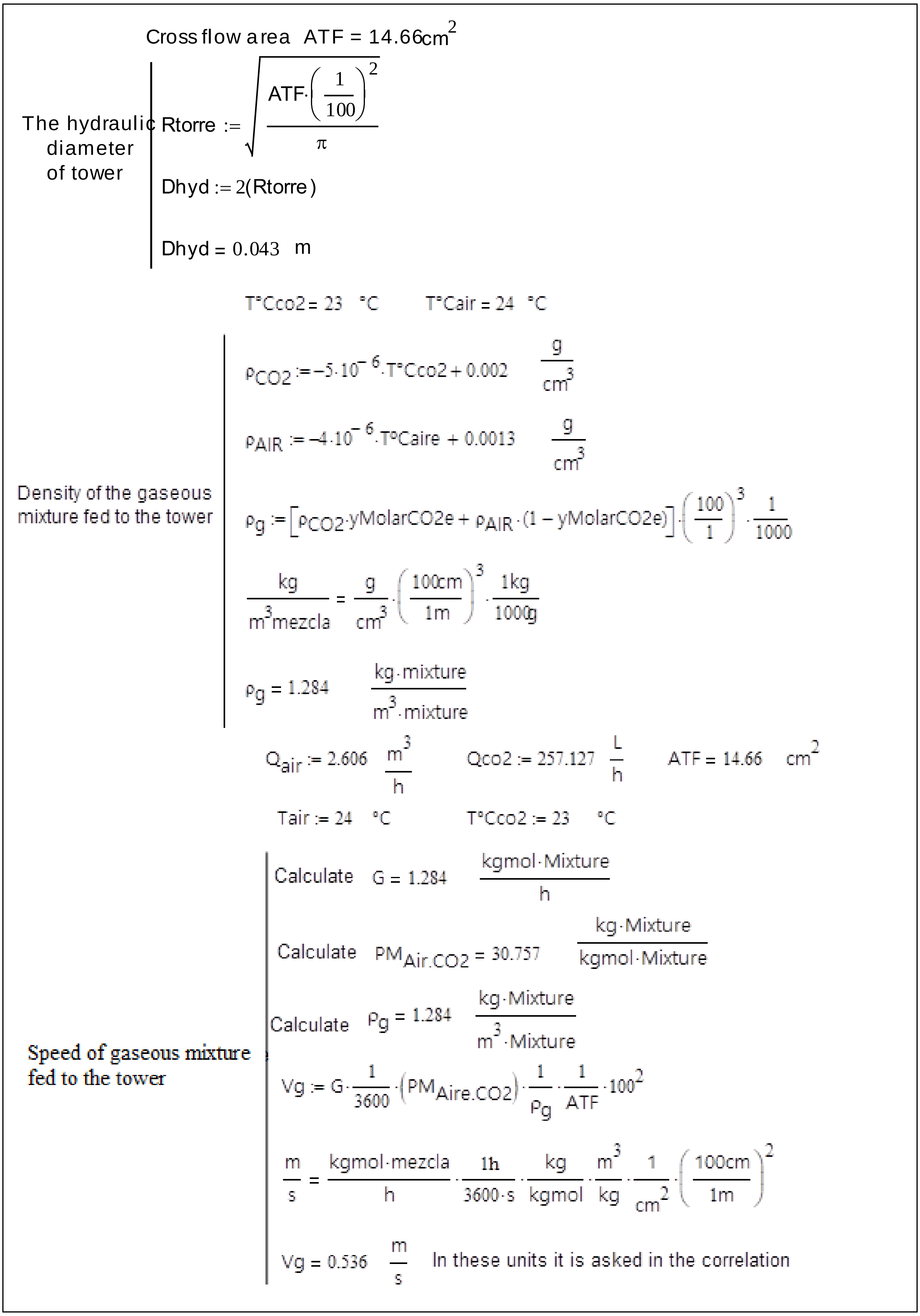
$$\text{Qv} = -h_{walls}\cdot a\cdot(\text{TL} - \text{TAmb})$$

TL= Variable temperature along the function column (z)
Tamb = 24 °C

$$a = 0.839 \ \frac{cm^{2}}{cm^{3}}$$

The heat transfer coefficient

$$h_{walls} = 1000\times 4.05\times 10^{-3}\times\left(\frac{\rho_{g}\ V_{g}}{D_{hyd}}\right)^{0.5}\left(Cp_{g}\right)^{0.33}$$



Cross flow area $ATF = 14.66 cm^2$

The hydraulic diameter of tower

$$Rtorre := \sqrt{\frac{ATF\cdot\left(\frac{1}{100}\right)^2}{\pi}}$$

$$Dhyd := 2(Rtorre)$$

$Dhyd = 0.043$ m

$T°Cco2 = 23$ °C $\quad T°Cair = 24$ °C

Density of the gaseous mixture fed to the tower

$$\rho_{CO2} := -5\cdot10^{-6}\cdot T°Cco2 + 0.002 \quad \frac{g}{cm^3}$$

$$\rho_{AIR} := -4\cdot10^{-6}\cdot T°Caire + 0.0013 \quad \frac{g}{cm^3}$$

$$\rho_g := \left[\rho_{CO2}\cdot yMolarCO2e + \rho_{AIR}\cdot(1 - yMolarCO2e)\right]\cdot\left(\frac{100}{1}\right)^3\cdot\frac{1}{1000}$$

$$\frac{kg}{m^3 mezcla} = \frac{g}{cm^3}\cdot\left(\frac{100cm}{1m}\right)^3\cdot\frac{1kg}{1000g}$$

$$\rho_g = 1.284 \quad \frac{kg\cdot mixture}{m^3\cdot mixture}$$

$Q_{air} := 2.606 \ \frac{m^3}{h}$ $\quad Qco2 := 257.127 \ \frac{L}{h}$ $\quad ATF = 14.66 \ cm^2$

$Tair := 24$ °C $\quad T°Cco2 := 23$ °C

Speed of gaseous mixture fed to the tower

Calculate $G = 1.284 \quad \frac{kgmol\cdot Mixture}{h}$

Calculate $PM_{Air.CO2} = 30.757 \quad \frac{kg\cdot Mixture}{kgmol\cdot Mixture}$

Calculate $\rho_g = 1.284 \quad \frac{kg\cdot Mixture}{m^3\cdot Mixture}$

$$Vg := G\cdot\frac{1}{3600}\cdot\left(PM_{Aire.CO2}\right)\cdot\frac{1}{\rho_g}\cdot\frac{1}{ATF}\cdot100^2$$

$$\frac{m}{s} = \frac{kgmol\cdot mezcla}{h}\cdot\frac{1h}{3600\cdot s}\cdot\frac{kg}{kgmol}\cdot\frac{m^3}{kg}\cdot\frac{1}{cm^2}\cdot\left(\frac{100cm}{1m}\right)^2$$

$Vg = 0.536 \ \frac{m}{s}$ In these units it is asked in the correlation

$T°Cair := 24$ °C

Heating capacity at constant pressure of the inlet gas to the tower

Calculate $Cp_{CO2} := 38.387 \dfrac{joule}{gmol\cdot °C}$

Calculate $CP_{AIR} := 29.138 \dfrac{joule}{gmolAIRE\cdot °C}$

$$Cp_g := \left[Cp_{CO2}\cdot yMolarCO2e + CP_{AIR}\cdot(1 - yMolarCO2e)\right]$$

$$\left(\frac{1}{PM_{Aire.CO2}}\cdot\rho_g\cdot 1000\right)\left(\frac{1}{PM_{Aire.CO2}}\cdot\rho_g\cdot 1000\right)$$

$$\frac{Joules}{m^3\cdot °K} = \left(\frac{joule}{gmolCO2\cdot °C}\cdot\frac{gmolCO2}{gmolmezcla} + \frac{joule}{gmolAIRE\cdot °C}\cdot\frac{gmolAIRE}{gmolmezcla}\right)\cdot x$$

$$\left(\frac{gmolmezcla}{gmezcla}\cdot\frac{kg\cdot mezcla}{m^3\cdot mezcla}\cdot\frac{1000g}{1kg}\right)$$

$Cp_g = 1261.403 \dfrac{Joules}{m^3\cdot °K}$ are required in these units, see article from Hanne M. Kvmsdal, page 15

Substituting

$$h\ walls := \left[1000\cdot 4.05\cdot 10^{-3}\cdot\left(\frac{\rho_g\cdot Vg}{Dhyd}\right)^{0.5}\cdot\left(Cp_g\right)^{0.33}\right]\cdot\frac{1}{(1000)}\cdot 239.006\cdot\frac{1}{100^2}$$

$$\frac{cal}{s\cdot cm^2\cdot °C} = \frac{W}{m^2 °K}\cdot\frac{1kw}{1000W}\cdot\frac{239.006\cdot\frac{cal}{s}}{1kw}\cdot\left(\frac{1m}{100cm}\right)^2$$

$$h\ walls = 0.0041 \frac{cal}{s\cdot cm^2\cdot °C}$$

$a = 0.839$ cm²/cm³

Heat generated by the reaction

$\Phi_H = R_A\, a\, (-\Delta Hr)$ Hanne M. Kvmsdal Correlation, page 15 is used

$\Delta Hr = \Delta H$ absorption Hanne M. Kvmsdal Correlation, page 14 is used

$$\Delta Habs = \left(84.68 - 0.1135\cdot T + 0.0027\cdot T^2\right)\cdot 1000\cdot 0.23901$$

$$\frac{cal}{gmol} = \frac{kj}{gmol}\cdot\frac{1000J}{1kj}\cdot\frac{0.23901cal}{1J}$$

$$R_A := -1\cdot 10^{-12}\cdot z^3 + 3\cdot 10^{-11}\cdot z^2 + 2\cdot 10^{-8}\cdot z + 1\cdot 10^{-6} \quad \frac{gmolCO2}{s\cdot cm^2}$$

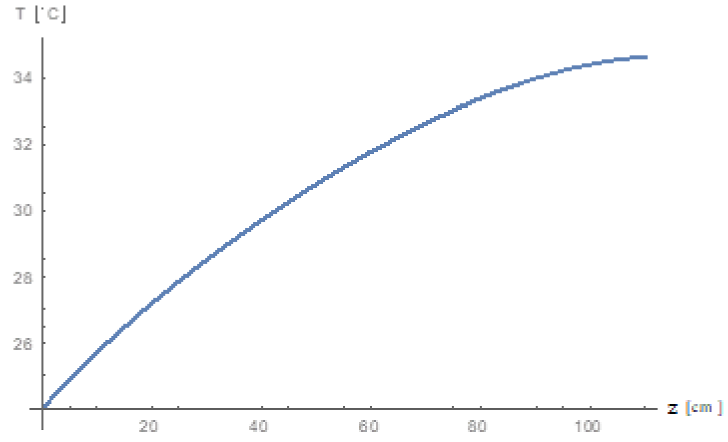
Relationship obtained with the Appendix A program

4.- RESULTS

4.1 The theoretical and experimental temperature profiles obtained by students

It was resolved Eq. (16) $\frac{dT}{dz} = \frac{\Phi_H + Q_V}{v_z \ \rho_L \ Cp_L}$ numerically using the "Mathematica-Wolfram Research" program to find the functionality of the temperatures of the liquid phase within the column Vs. the position z the entire length of the reactor-absorber for each experiment of 5, 8 and 10 L / h of fed MEA / H2O solution. The program with the theoretical results of the first experimentation is attached in Fig. (3).

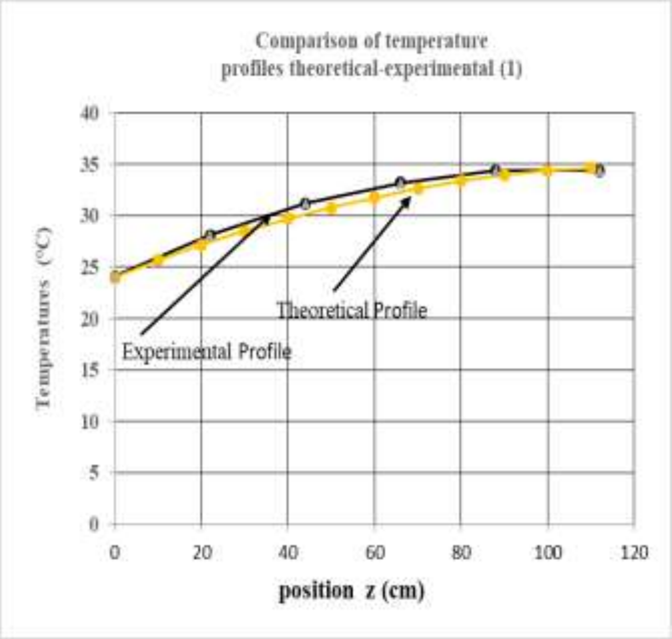
Δ Habs = (84.68 - 0.1135 ∗ T[z] + 0.0027∗T[z]^{2}) ∗ 1000 ∗ 0.23901;
RA = -1∗10^{-12} ∗ z^{3} + 3∗10^{-11} ∗ z^{2} + 2 ∗10^{-8} ∗ z + 1∗10^{-6};
a = 0.839;
hwall = 0.0041;
Tamb = 24;
Qv = - hwall ∗ a ∗ (T[z] - Tamb);
Vz = 0.095;
ρL = 0.049;
CpL = 19.486;
sol = NDSolve [{T' [z] == (Δ Habs ∗ RA∗ a + Qv) / (Vz∗ ρL ∗CpL), T[0]==Tamb}, T, {z, 0, 110}]
Plot [Evaluate [T[z] /. %], { z, 0, 110 }, AxesLabel -> { "Z [cm]", "T [°C]" }]
TableForm [{{ "z"   cm, T °C } }, TableDepth -> 2]
Table [{z, T[z] /.sol}, {z, 0, 110, 10}] // TableForm
{{T->InterpolatingFunction}}



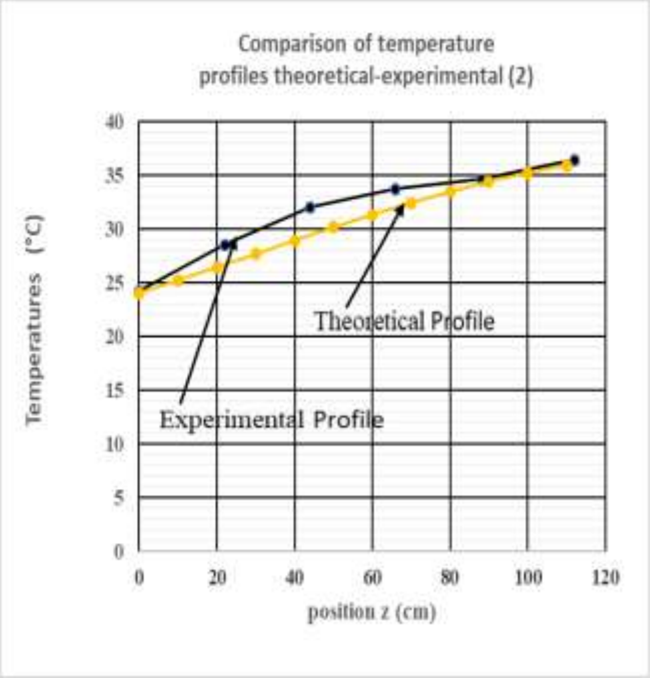
Z (cm)	T °C
0	24.0000
10	25.7015
20	27.1781
30	28.4964
40	29.6927
50	30.7826
60	31.7673
70	32.6384
80	33.3807
90	33.9742
100	34.3957
110	34.6199

Fig. (3) Theoretical results of the model

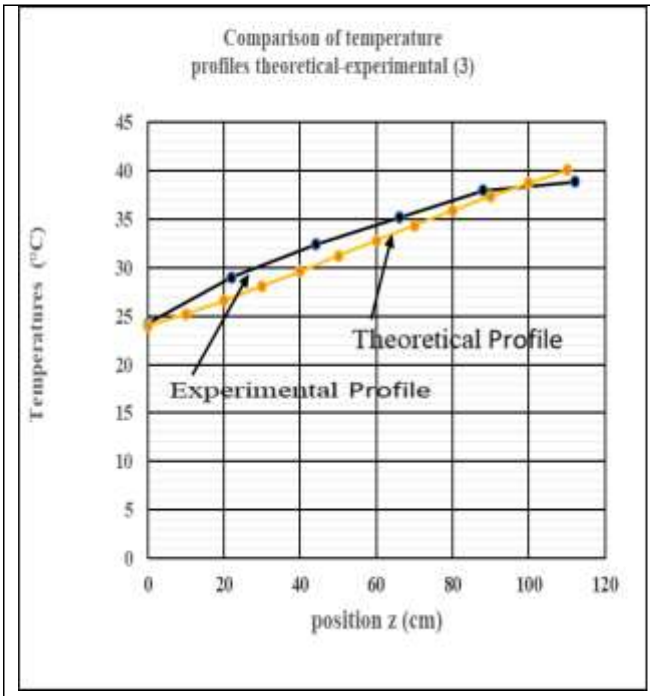
In the Fig. (4) the graphical profiles of comparisons of the theoretical and experimental liquid temperatures are shown.



z (cm)	TL (°C)	
0	24.1	
22	28.1	
44	31.2	
66	33.2	
88	34.4	
112	34.4	
0		24
10		25.7015
20		27.1781
30		28.4964
40		29.6927
50		30.7826
60		31.7673
70		32.6384
80		33.3807
90		33.9742
100		34
110		34.6199



z (cm)	TL (°C)	
0	24.2	
22	28.5	
44	32	
66	33.7	
88	34.6	
112	36.4	
0		24
10		25.1878
20		26.4221
30		27.6743
40		28.92
50		30.1379
60		31.3093
70		32.4174
80		33.447
90		34.3839
100		35
110		35.9247



z (cm)	TL (°C)	
0	24.2	
22	29	
44	32.4	
66	35.2	
88	38	
112	38.9	
0		24
10		25.2421
20		26.6267
30		28.11
40		29.6552
50		31.2317
60		32.8133
70		34.3774
80		35.9043
90		37.3764
100		39
110		40.0929

Fig. (4) Comparison of theoretical and experimental curves of liquid temperatures in the column TL (°C) Vs. position z (cm)

5.- CONCLUSIONS

In this experimental study, the students of the Faculty of Chemistry obtained the temperature profiles as shown in Fig. (4), they compare the values in the steady state of temperatures Vs. position of both the model and the values experimental.

It can be seen that increasing the flow of the MEA / H2O (5, 8, 10) L / h solution increases the temperatures of the phases within the column, this is because initially any element of the interfacial surface is exposed to the penetration of the solute for a time t, but by increasing the flows of liquid fed Le residence times decrease $\tau = ATF \times h/Le$ and the surface elements are replaced faster and faster by fresh CO_2 from the gaseous phase, causing an increase in the diffusive flux R_A at the interface and that as the amount of CO_2 in the liquid phase increases, the reaction that is exothermic is It will be favored by the limiting reagent transferred, increasing the temperatures inside the column more and more.

6.- NOMENCLATURA

$[A_0]$ = CO_2 concentration in the liquid phase bulk: gmol CO_2 /L solution
a = Effective interfacial area per unit of volume packed: cm^2/cm^3
a_t = Area of total packing surface per unit volume packed: cm^2/cm^3
A_T = Cross area of the column: cm^2
ATF = Cross-sectional area of flow between packaging: cm^2
[A*] = CO_2 interfacial concentration in the film model: gmol CO_2 / L solution
[Bo] = MEA concentration in bulk within the liquid phase: gmol MEA /L solution
BPS = Amina free without reacting at the selected point in the column: gmol MEA/L solution
C* = Concentración del equilibrio termodinámico: gmol MEA /cm^3 solution
Cp_g = Specific heat at constant gas pressure: joules/m^3 °K; Note. - These are the units required by the correlation (13). **[2]**
Cp_L = Specific heat at constant pressure from the liquid mixture: cal / gmol mezcla °C
D_L = CO_2 diffusion coefficient in the liquid phase: cm^2/s
D_{hyd} = Hydraulic column diameter: cm
E = Enhancement factor
E1 = Enhancement factor formula parameter
Ei = Enhancement factor formula parameter assessed at the interface

GPS = Mass speed at the selected point: gmol mixture /s cm^2
G's = Mass feed air speed: gmol aire /s cm^2
G_{CO2} = Mass feeded CO_2 speed: gmol CO2 /s cm^2
h = Absorption-reaction column height: cm
h walls = Interfacial heat transfer film coefficient on the walls of the column: watts/m^2 K
k_G a = Individual and temporal volumetric coefficient on the gas phase side: gmolCO_2 /s cm^3 atm
k_L a = Individual and temporal volumetric coefficient on the liquid phase side: 1/ s
***Le* =** Flow of the liquid flow fed: L/ s
L = Mass liquid speed: cm^3 solution/ cm^2 s
m = Thermodynamic equilibrium ratio: cm^3 atm / gmol CO_2
Pop = Operating pressure in Mexico City: (0.771) atm
PM = Molecular mass: g A/gmol A
p_{CO2} = Partial CO_2 pressure: atm
p* = Thermodynamic equilibrium pressure: atm
Q_{CO2} = Carbon dioxide flow: L/h
Q_{AIR} = Airflow: m^3 / h
Q_V = Volumetric heat to column neighborhoods: cal/ s cm^3
r = Rapid reaction: $(cm^3/gmol)^{-1+n}/s$
R_A= Rapid absorption with chemical reaction through the interface: gmol A/ s cm^2
t = Operating time: s
Tamb = Environmental temperature: °C
TL = Temperature of the liquid in the column: °C
V_g = Speed of the gas mixture in the column: m/s
V_Z = Speed of liquid mixing in the columna: cm/s
$X_{Molar\ MEA}$ = Molar fraction of MEA: gmol MEA / gmol mezcla líquida
W_{MEA} = MEA mass fraction: g MEA /g mezcla
Z= Arbitrary position in the absorption column: cm
z = Stochiometric reaction factor
ΔH_r = Change of enthalpy due to reaction: cal/gmol
ΔH_{abs}= Change of enthalpy due to absorption with chemical reaction: cal/gmol
Φ_H = Volumetric heat generated by the reaction: cal/s cm^3
ε = fraction of gaps between the absorption column packaging
ρ_G = Density of the gas phase: g/cm^3
ρ_L = Liquid mixture density: gmol/cm^3

7.- BIBLIOGRAFÍA

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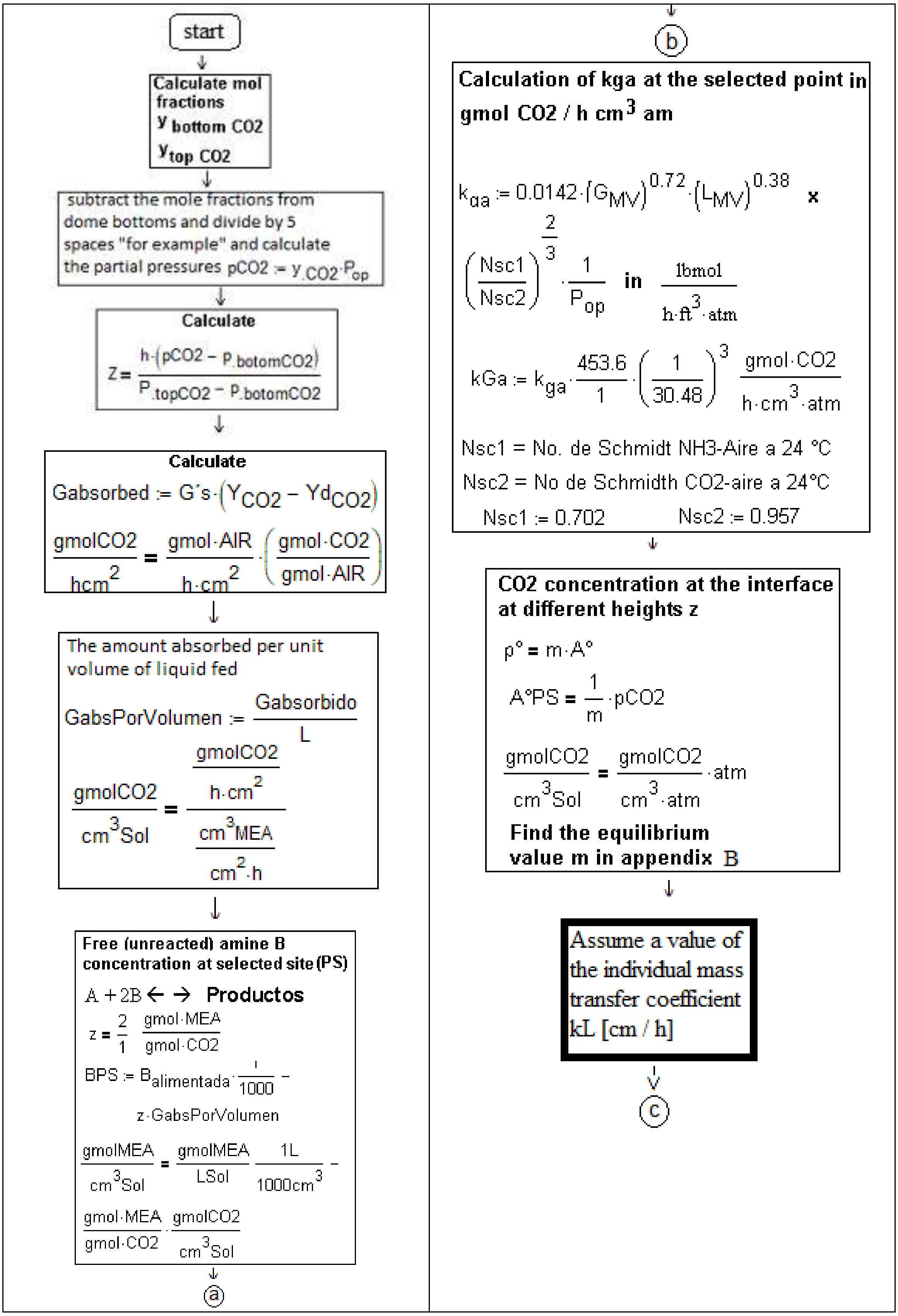
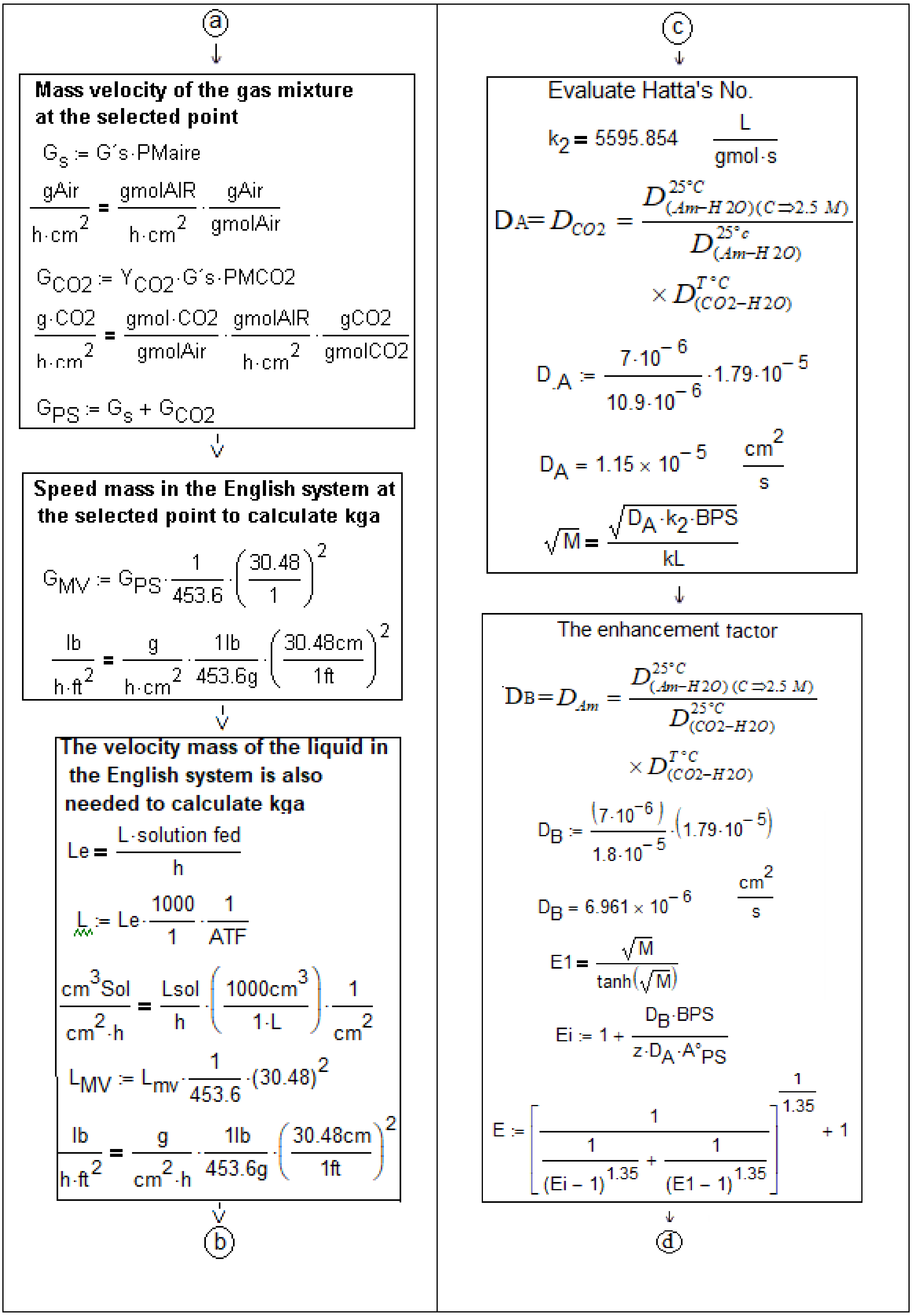
APPENDIX A

To determine quantitatively $\Phi_H = R_A\, a\ (\Delta H_{abs})$ it is necessary to calculate the ratio of the diffusive absorption flux with chemical reaction as a function of the z position along the tower and the individual coefficient of mass transfer on the liquid side kL. For this, students used the experimental information from Table (1) and the next program used in reference **[4]**.





Mass velocity of the gas mixture at the selected point

$G_s := G's \cdot PMaire$

$$\frac{gAir}{h\cdot cm^2} = \frac{gmolAIR}{h\cdot cm^2}\cdot\frac{gAir}{gmolAir}$$

$G_{CO2} := Y_{CO2}\cdot G's\cdot PMCO2$

$$\frac{g\cdot CO2}{h\cdot cm^2} = \frac{gmol\cdot CO2}{gmolAir}\cdot\frac{gmolAIR}{h\cdot cm^2}\cdot\frac{gCO2}{gmolCO2}$$

$G_{PS} := G_s + G_{CO2}$

Speed mass in the English system at the selected point to calculate kga

$$G_{MV} := G_{PS}\cdot\frac{1}{453.6}\cdot\left(\frac{30.48}{1}\right)^2$$

$$\frac{lb}{h\cdot ft^2} = \frac{g}{h\cdot cm^2}\cdot\frac{1lb}{453.6g}\cdot\left(\frac{30.48cm}{1ft}\right)^2$$

The velocity mass of the liquid in the English system is also needed to calculate kga

$$Le = \frac{L\cdot solution\ fed}{h}$$

$$L := Le\cdot\frac{1000}{1}\cdot\frac{1}{ATF}$$

$$\frac{cm^3Sol}{cm^2\cdot h} = \frac{Lsol}{h}\cdot\left(\frac{1000cm^3}{1\cdot L}\right)\cdot\frac{1}{cm^2}$$

$$L_{MV} := L_{mv}\cdot\frac{1}{453.6}\cdot(30.48)^2$$

$$\frac{lb}{h\cdot ft^2} = \frac{g}{cm^2\cdot h}\cdot\frac{1lb}{453.6g}\cdot\left(\frac{30.48cm}{1ft}\right)^2$$

Evaluate Hatta's No.

$$k_2 = 5595.854\ \frac{L}{gmol\cdot s}$$

$$D_A = D_{CO2} = \frac{D^{25°C}_{(Am-H2O)(C\Rightarrow 2.5\ M)}}{D^{25°c}_{(Am-H2O)}}\times D^{T°C}_{(CO2-H2O)}$$

$$D_A := \frac{7\cdot10^{-6}}{10.9\cdot10^{-6}}\cdot1.79\cdot10^{-5}$$

$$D_A = 1.15\times10^{-5}\ \frac{cm^2}{s}$$

$$\sqrt{M} = \frac{\sqrt{D_A\cdot k_2\cdot BPS}}{kL}$$

The enhancement factor

$$D_B = D_{Am} = \frac{D^{25°C}_{(Am-H2O)(C\Rightarrow 2.5\ M)}}{D^{25°C}_{(CO2-H2O)}}\times D^{T°C}_{(CO2-H2O)}$$

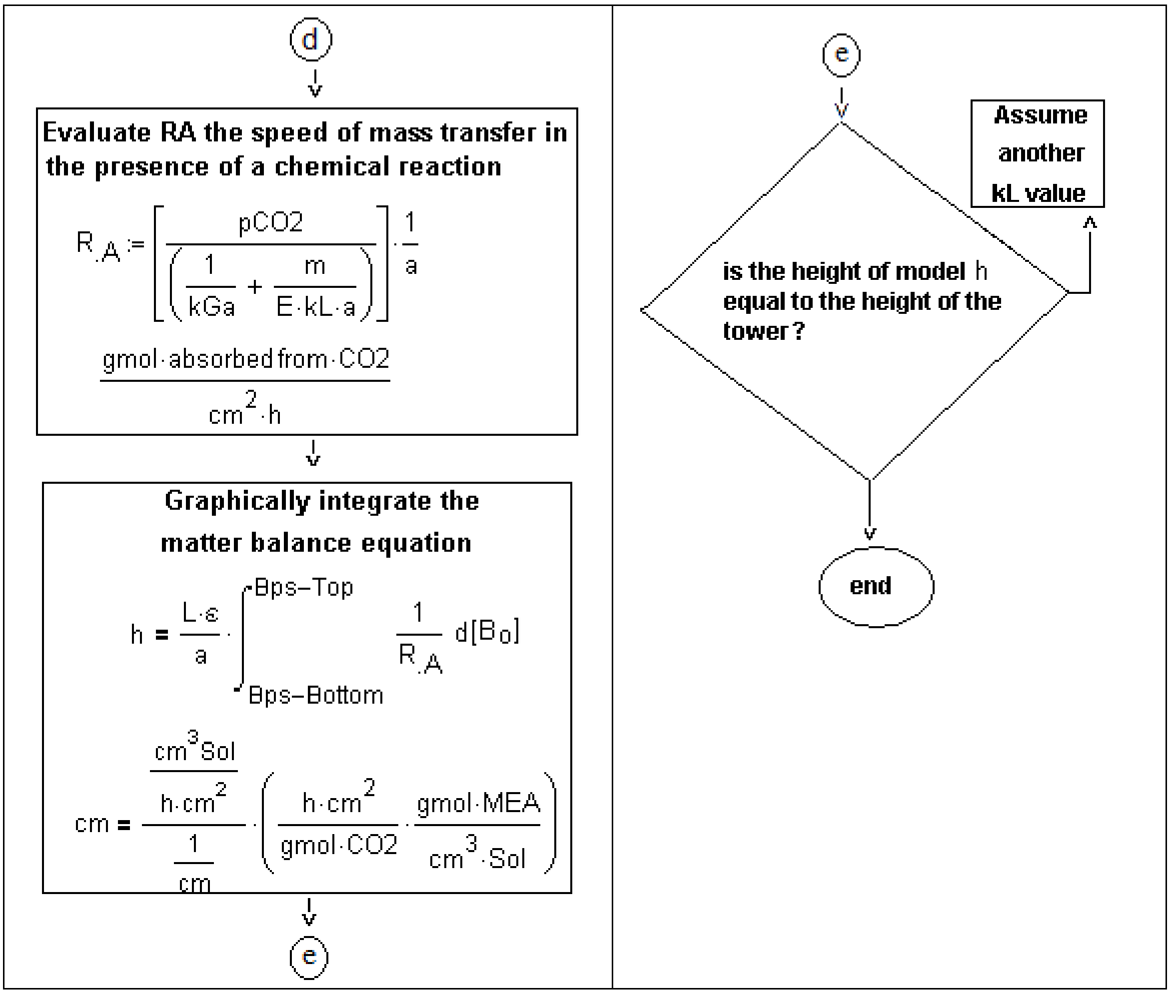
$$D_B := \frac{(7\cdot10^{-6})}{1.8\cdot10^{-5}}\cdot(1.79\cdot10^{-5})$$

$$D_B = 6.961\times10^{-6}\ \frac{cm^2}{s}$$

$$E1 = \frac{\sqrt{M}}{\tanh(\sqrt{M})}$$

$$Ei := 1 + \frac{D_B\cdot BPS}{z\cdot D_A\cdot A°_{PS}}$$

$$E := \left[\frac{1}{\frac{1}{(Ei-1)^{1.35}}+\frac{1}{(E1-1)^{1.35}}}\right]^{\frac{1}{1.35}} + 1$$



When the above program equates the height **h** of the mass balance model with the height of the absorption column, students complete the program and report the values of the individual liquid-side mass transfer coefficient kL and the fluxes of mass transfer in the presence of chemical reaction at the R_A interface to different positions z along the column.

5 L/h	
kL = 48.7 cm / h	$z = \begin{pmatrix} 0 \\ 21.16 \\ 42.321 \\ 63.679 \\ 84.84 \\ 106 \end{pmatrix}$ cm $R_A = \begin{pmatrix} 1.347\times10^{-6} \\ 1.744\times10^{-6} \\ 2.053\times10^{-6} \\ 2.233\times10^{-6} \\ 2.203\times10^{-6} \\ 1.828\times10^{-6} \end{pmatrix}$ $gmolCO_2$ / s cm^2 $R_A := -1\cdot10^{-12}\cdot z^3 + 3\cdot10^{-11}\cdot z^2 + 2\cdot10^{-8}\cdot z + 1\cdot10^{-6}$

8 L/h	
	$z = \begin{pmatrix} 0 \\ 21.16 \\ 42.321 \\ 63.679 \\ 84.84 \\ 106 \end{pmatrix}$ $R_A = \begin{pmatrix} 1.247\times10^{-6} \\ 1.769\times10^{-6} \\ 2.2\times10^{-6} \\ 2.519\times10^{-6} \\ 2.714\times10^{-6} \\ 2.758\times10^{-6} \end{pmatrix}$

kL = 40.8 cm / h	cm gmolCO$_2$ / s cm^2 $R_A := -7\cdot 10^{-14}\cdot z^3 - 1\cdot 10^{-10}\cdot z^2 + 2\cdot 10^{-8}\cdot z + 1\cdot 10^{-6}$

.

10 L/h	$z = \begin{pmatrix} 0 \\ 21.16 \\ 42.321 \\ 63.679 \\ 84.84 \\ 106 \end{pmatrix}$ $R_A = \begin{pmatrix} 1.069\times 10^{-6} \\ 1.792\times 10^{-6} \\ 2.447\times 10^{-6} \\ 3.022\times 10^{-6} \\ 3.494\times 10^{-6} \\ 3.847\times 10^{-6} \end{pmatrix}$ cm gmolCO$_2$ / s cm^2 $R_A := 9\cdot 10^{-14}\cdot z^3 - 1\cdot 10^{-10}\cdot z^2 + 2\cdot 10^{-8}\cdot z + 1\cdot 10^{-6}$
kL = 66.8 cm / h	

APENDICE B

B.1 Thermodynamic equilibrium data for the system (monoethanolamine/water) - (carbon dioxide / air), in the presence of chemical reaction, reports it **Donal L. Katz [5]**.

T = 37.77 ºC = 100 ºF	
$X^* = \dfrac{gmol\, CO_2}{gmol\, MEA}$	$p^* = mm\ Hg$
0	0
0.05	0
0.10	0
0.15	0
0.20	0
0.25	0
0.30	0
0.35	0
0.4	0
0.43908	0
0.46951	3.2785
0.49885	9.9449
0.53994	34.728
0.56128	56.058
0.57409	70.811
0.58262	85.535
0.58902	103.50
0.59756	126.37
0.60183	142.7
0.61037	162.31
0.61677	180.27
0.62424	200.05
0.62843	214.74
0.63261	231.05
0.63676	253.88
0.64304	276.72
0.64934	294.67
0.65562	317.51
0.66383	379.47
0.66587	397.4
0.67212	425.12
0.67408	457.72
0.68032	488.71
0.68447	509.91
0.6865	531.1
0.690	555.56
0.69687	576.54

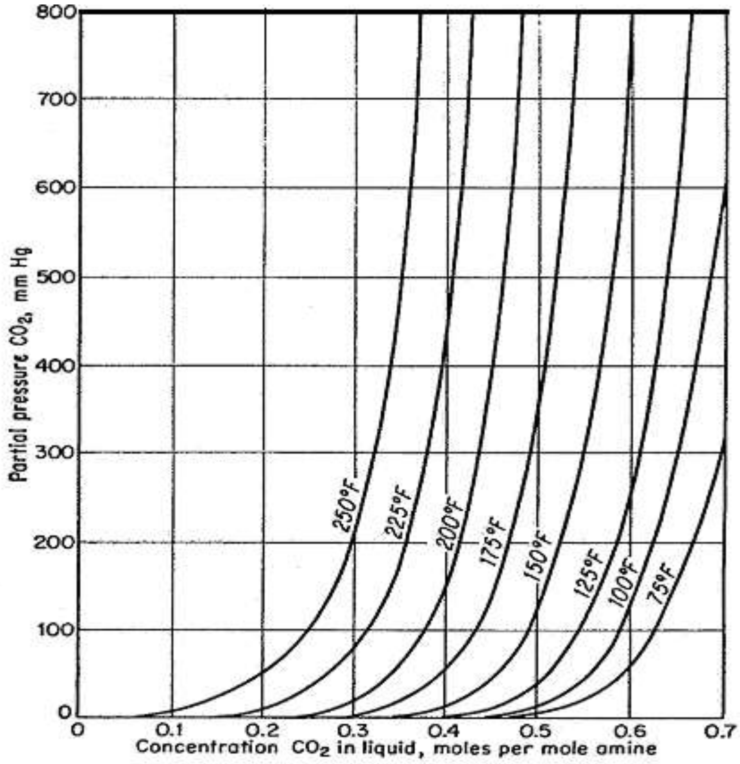


Fig. 16-36. Equilibrium pressure of CO_2 from 15 wt % monoethanolamine solution. *(Kohl, 16-45; Mason and Dodge, 16-52. Courtesy AIChE.)*

Fig. (5)

The students of the Chemical Engineering Laboratory of the Faculty of Chemistry used the experimental temperature data from the Experimental Data Table (1) and selected the curve at 100 ° F in Fig. (5) to obtain the equilibrium relationship for this experimentation. This requires changing the units of the coordinate axes according to the following diagram in Fig. (6).

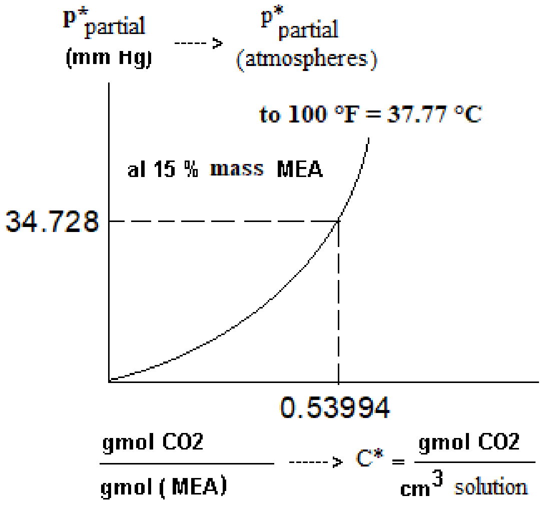


Fig. (6)

As the solution reported by Donal L. Katz [5]. it is 15% by mass, 0.15 g MEA / g solution the students took a base of 100 g solution.

For the monoetanolamina

$$gmol\ MEA = 100\ \frac{15}{100}\ \frac{1}{61.084}$$

$$gmol\ MEA = g\ solution\left(\frac{g\ MEA}{g\ solution}\right)\frac{gmol\ MEA}{g\ MEA}$$

$$gmol\ MEA = 0.246$$

b) For the water

$$gmol\ water = 100\frac{85}{100}\frac{1}{18}$$

$$gmol\ water = 4.722$$

.

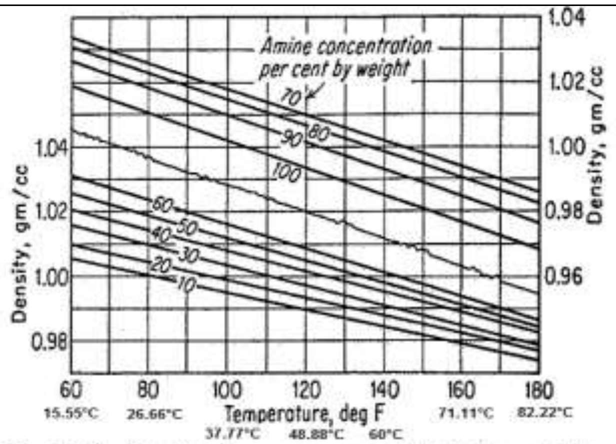


Fig. 16-40. Density of aqueous monoethanolamine solutions. (16-38, Courtesy Dow Chemical Co.)

Fig. (7)

Data

$PM\ mea = 61.084$

$PM\ water = 18$

$\%W\ mea = 15$

$T°C\ mea = 24°C$

From the graph in Fig. (7) **[5]** you can read solution density

$$\rho\, solution = 1.005 \frac{g\ solution}{cm^3\ solution}$$

Calculations

$$x\ Molar\ mea = 0.0494 \frac{gmol\ mea}{gmol\ solution}$$

$$PM\ solution = x\ Molar\ mea \times PM\ mea + (1 - x\ Molar\ mea) \times PM\ water$$

$$PM\ solution = 20.13 \frac{g\ solution}{gmol\ solution}$$

$$\rho Molar\ Solution = \rho\, solution \times \frac{1}{PM\ solution}$$

$$\rho Molar\ Solution = 0.05\ \frac{gmol\ solution}{cm^3\ solution} = \frac{gmol\ water}{cm^3\ water}$$

Changes in the abscisas

$$0.53994\ \frac{gmol\ CO_2}{\cancel{gmol\ MEA}}\ \frac{0.246\ \cancel{gmol\ MEA}}{4.722\ \cancel{gmol\ H_2O}}\ \frac{0.5\ \cancel{gmol\ solution}}{cm^3\ \ solution} = 0.0014\ \frac{gmol\ CO_2}{cm^3\ solution}$$

Changes in the ordinates

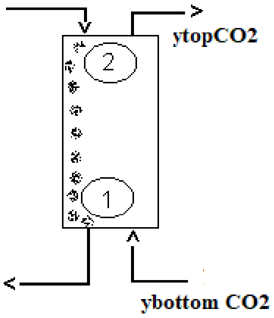
$$p^*\ atm\ = p^*\ \cancel{mm}\ Hg\ \ \frac{1\ atm}{760\ \cancel{mm}\ Hg}$$

Table of Results (1) shows the unit changes for the ordinates and the abscissa

T = 37.77 °C = 100 °F			T = 37.77 °C = 100 °F	
$X^* = \frac{gmol\ CO_2}{gmol\ MEA}$	$p^* = mm\ Hg$		$c^* = \frac{gmolCO_2}{cm^3\ solución}$	$p^* = atm$
0	0		0	0
0.05	0		0.00013	0
0.10	0		0.00026	0
0.15	0		0.00039	0
0.20	0		0.00052	0
0.25	0		0.00065	0
0.30	0		0.00078	0
0.35	0		0.00091	0

0.4	0	0.00104	0
0.43908	0	0.00114	0
0.46951	3.2785	0.00122	0.00431
0.49885	9.9449	0.0013	0.01309
0.51433	18.255	0.00134	0.02402
0.525	24.847	0.00137	0.03269
0.53994	34.728	0.0014	0.04569
0.56128	56.058	0.00146	0.07376
0.57409	70.811	0.00149	0.09317
0.58262	85.535	0.00152	0.11255
0.58902	103.50	0.00153	0.13618
0.59756	126.37	0.00155	0.16628
0.60183	142.7	0.00157	0.18776
0.61037	162.31	0.00159	0.21357
0.61677	180.27	0.0016	0.2372
0.62424	200.05	0.00162	0.26322
0.62843	214.74	0.00163	0.28255
0.63261	231.05	0.00165	0.30401
0.63676	253.88	0.00166	0.33405
0.64304	276.72	0.00167	0.36411
0.64934	294.67	0.00169	0.38772
0.65562	317.51	0.00171	0.41778
0.66383	379.47	0.00173	0.4993
0.66587	397.4	0.00173	0.52289
0.67212	425.12	0.00175	0.55937
0.67408	457.72	0.00175	0.60226
0.68032	488.71	0.00177	0.64304
0.68447	509.91	0.00178	0.67093
0.6865	531.1	0.00179	0.69882
0.690	555.56	0.00179	0.731
0.69687	576.54	0.00181	0.75861

B.2 Cálculo de la equilibrium relationships **m** $\left[atm/(gmol\,CO_2/cm^3\,sol)\right]$



h = 106 cm
Pop = 0.771 atm
P1 = 0.0643 atm
P2 = 0.023 atm
Pop ≡ pCO2 atm

Molar fractions were calculated in the tower y_{top} = 0.02998 and y_{bottom} = 0.0834 using Table (1) of Experimental Data, and were divided into five spaces, with these values the partial pCO_2 pressures were calculated

$$yTopCO2 = 0.02998 \qquad \text{Top}\ \ p2 = 0.023\ \ \text{atm}$$

$$y_{CO2} := \begin{pmatrix} 0.0298 \\ 0.0405 \\ 0.0512 \\ 0.062 \\ 0.0727 \\ 0.0834 \end{pmatrix} \qquad y_{CO2} \cdot P_{op} := pCO2 \qquad pCO2 = \begin{pmatrix} 0.023 \\ 0.0312 \\ 0.0395 \\ 0.0478 \\ 0.0561 \\ 0.0643 \end{pmatrix}$$

$$ybottomCO2 = 0.0834 \qquad \text{bottom}\ \ p1 = 0.0643\ \ \text{atm}$$

Appliying Eq. (1)

$$P_{op} = p1 + \frac{p2 - p1}{h} \cdot Z$$

$$Z = \frac{h \cdot (pCO2 - p1)}{p2 - p1} \qquad Z = \begin{pmatrix} 0 \\ 21.16 \\ 42.321 \\ 63.679 \\ 84.84 \\ 106 \end{pmatrix} \text{cm}$$

The students of the Chemical Engineering Laboratory found that the potential model adjusts the curvilinear data of the equilibrium

$c^* = \frac{gmolCO_2}{cm^3\ solución}$	$p^* = atm$
0.00122	0.00431
. . .	. . .
0.00181	0.75861

In the potential model they substituted the values of the partial pressures

$$\text{Top} \quad p2 = 0.023 \quad \text{atm}$$

$$pCO2 = \begin{pmatrix} 0.023 \\ 0.0312 \\ 0.0395 \\ 0.0478 \\ 0.0561 \\ 0.0643 \end{pmatrix}$$

$$\text{bottom} \quad p1 = 0.0643 \quad \text{atm}$$

and found the corresponding concentration values $c^*=(p^*/a)^{1/b}$.

Finally, the students represented these values as in Fig. (8) with ordinates (pCO2 = p *) vs. abscissa C * obtaining a practically linear profile from which the equilibrium relations **m** were calculated for the three experiments as shown in the Results Table (2).

Linear model : y = m x +b

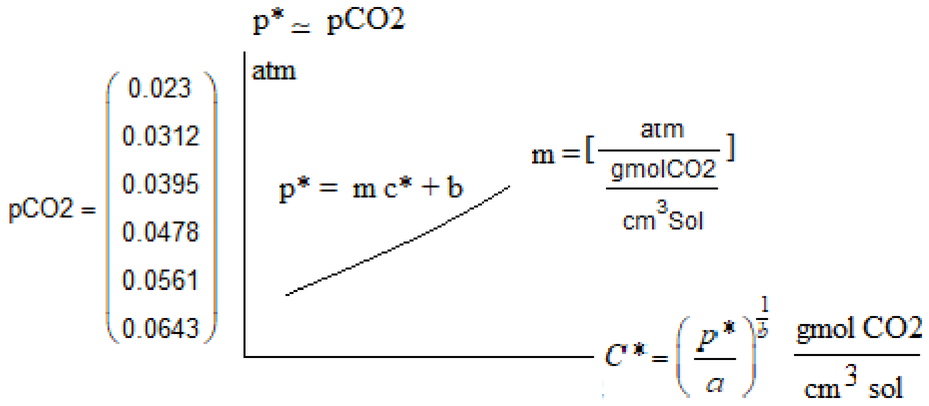


Fig. (8)

Results Table (2)

Flow of feeding (L / h)	**Equilibrium relationships m** $\left[atm / (gmol\,CO_2 / cm^3\,sol) \right]$
5	404.141
8	371.312
10	335.176