

ABSORPTION COLUMN WITH CO₂ BALANCE

Introduction

The purpose of the Sour Gas Processing is to remove H₂S from natural gas and to avoid of CO₂ absorption in the solution of MDEA with H₂O. Absorption of H₂S with solution of MDEA is so fast that it could be driven by equilibrium on every stage. On the other hand, CO₂ absorption is driven by mass transfer coefficients and kinetics. Mass transfer coefficients are calculated by article which is discussed below. The reaction **1** of CO₂ with water is reversible reaction and kinetic constant of backward reaction is faster than the forward.



Transfer of CO₂ from gaseous phase to liquid phase is unwanted effect for gas purification – our project. When CO₂ is presented in liquid it is more difficult for H₂S to transfer into the liquid phase and react with MDEA. The reaction is selective due to hindered nitrogen atom. Also, CO₂ could interact with MDEA and this interaction would be considered ineffective – “a few” molecules could stay like ions and... Whole problem is simplified for three components – CO₂, CH₄, H₂O. CH₄ and H₂O are inert component – they do not interact with each other.

In the figure **1** it could be seen the sketch of CO₂ transfer from gas to liquid phase through phase boundary. Lines in films phase are not same oriented. On the phase boundary mole fractions, in gas and liquid phase, are in equilibrium. Bulk is marked “b” and surface is “s”.

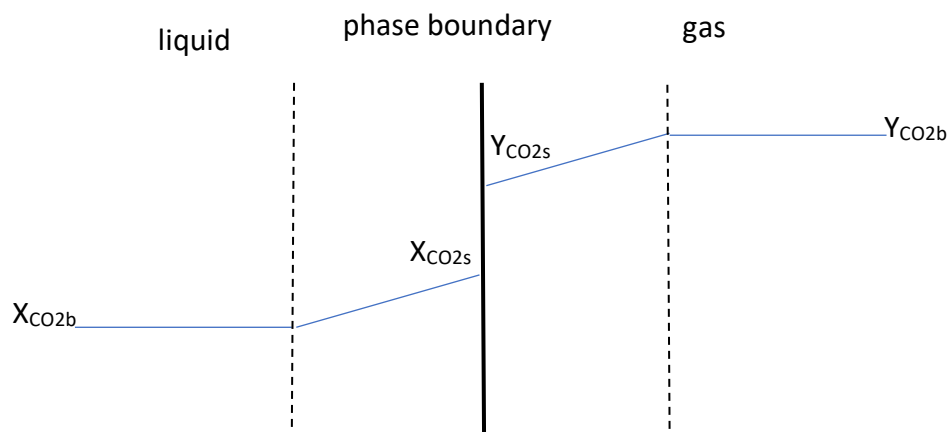


Figure 1 – Sketch of mass transfer from gas to liquid phase through phase boundary.

Balance of Limiting Example

Introduction into Balance

In the previous report is total balance of absorption column and it is calculated mole flows, mole fractions, superficial gas velocity, ... These values are taken and it is calculated with them in this report. Rest of the values are taken from scientific articles. This overview it is seen in the table 1 where by green color are marked values which were taken from total balance from previous report, orange is significant for articles, blue is for known values and black is for calculated values in this report.

Mark	Value	Description	Unit	Source
T	313,15	Constant temp. in column	K	Given by Bryan
p	$7,1 \cdot 10^6$	Const. pressure in column	Pa	Given by Bryan
yCO ₂	0,05	Mole fraction of CO ₂ in gas phase	-	Given by Bryan
wMDEA	0,5	Weight fract. In liquid	-	Calc. in previous report
u	0,1436	Superficial gas velocity	m/s	Calc. in previous report
s	0,1	Submergence of liquid on the tray	m	Guess (based on article)
nL	52,8249	Liquid flow considered const.	mol/s	Calc. in previous report
A	0,8855	Surface	m ²	Calc. in previous report
nyCO ₂	$26,9 \cdot 10^{-6}$	Molar volume of CO ₂	m ³ /mol	"skripta"
nyCH ₄	$25,14 \cdot 10^{-6}$	Molar volume of CH ₄	m ³ /mol	"skripta"
MCO ₂	0,044	Molar weight of CO ₂	kg/mol	-
MCH ₄	0,016	Molar weight of CH ₄	kg/mol	-
Dg	$2,7622 \cdot 10^{-7}$	Diffusion coef. in gas phase	cm ² /s	"skripta"
kg	$0,151 \cdot 10^{-4}$	Mass transfer coef. in gas ph.	mol/cm ² /s/atm	1
DI	$1,214 \cdot 10^{-9}$	Diffusion coef. in liquid phase	cm ² /s	2
kl	0,0278	Mass transfer coef. in liquid ph.	cm/s	1
AA	-8,55445	Parameter for calc. Henry of CO ₂	-	3

BB	4,01195	Parameter for calc. Henry of CO ₂	-	3
CC	9,52345	Parameter for calc. Henry of CO ₂	-	3
pH₂O	7386,34	Vapour pressure of H ₂ O	Pa	Calc. by Aspen (NRTL)
TC	647	Critic temp. of solvent (H ₂ O)	K	-
TR	0,484	Reduced temp of solvent (H ₂ O)	-	-
tau	0,5159		K	3
kHCO₂	2,3384*10 ⁽⁸⁾	Calc. Henry of CO ₂	Pa	3
KCO₂	32,9364	Distributing coef. of CO ₂	-	-
a	6,2349	Effective interfacial area	m ² (recalc. to change the unit)	
aa	7,0411	Effective interfacial area	cm ² /cm ² (floor area of plate)	1
k2	6*10 ⁽⁻²⁾	Const. of reaction rating	s ⁻¹ (at 25°C 1 atm)	4
Ha	0,9368*10 ⁽⁻³⁾	Hatta number	-	-
cTOT	32247	Total conc. in liquid	mole/m ³	-
rho_l	1008,555	Density of the liquid phase	kg/m ³	-
yCO₂s	0,04900283286	Mole fraction of CO ₂ on phase boundary	-	-
xCO₂b	0,0002975399603	Mole fraction of CO ₂ in liquid phase	-	-
xCO₂s	0,001487799339	Mole fraction of CO ₂ on phase boundary	-	-
nCO₂	0,06669573447	Mole flow of transferred CO ₂	mol/s	-

Table 1 – The overview of all values which were used for further calculations in this report.

Total Balance

According to the article¹ there is described how to evaluate diffusion coefficient in the liquid phase. To obtain the diffusion coefficient it is needed to calculate the viscosity of the solution. Equations for viscosity are correct but when diffusion coefficient of N₂O is evaluate the value is too low. In comparing with the source, where the data was obtain to create the equation to evaluate the diffusion coefficient of N₂O, are different. In order to the mistake diffusion coefficient is taken from the original article². Then mass transfer coefficient in liquid phase¹ is calculated with using the correct diffusion coefficient which it could be seen in the equation **1**. Unit is *cm/s* and it needs to be recalculated to obtain basic unit which it is shown below. The number of the equation has own units – *cm^{0,25}/s^{0,25}*.

$$k_l = 13 \cdot u^{0,25} \cdot S^{-0,5} \cdot D_l^{0,5} \quad \mathbf{1}$$

It is needed to calculate Hatta's number to figure out where the reaction **1** acts. The reaction is the first order and the number is modified based on the order. Evaluation of Hatta's number is shown in the equation **2**. The number is so small and this tell us that the reaction occurs in the bulk of the liquid phase.

$$Ha = \frac{k_2 \cdot D_l}{k_l^2} \quad \mathbf{2}$$

To balance how much amount of CO₂ transfer from gas to liquid phase the below it is needed to calculate and balance.

Diffusion coefficient in gas phase is calculated by equation **3** – Fuller's equation. All variables have to have basic units.

$$D_g = \frac{3,2 \cdot 10^{-8} \cdot T^{1,75}}{p \cdot (v_{CO_2}^{\frac{1}{3}} + v_{CH_4}^{\frac{1}{3}})^2} \cdot \left(\frac{1}{M_{CO_2}} + \frac{1}{M_{CH_4}} \right)^{0,5} \quad \mathbf{3}$$

Mass transfer coefficient in gas phase is calculated in the equation **4** according to the article¹. Units of the coefficient are *mole/cm²/s/atm* and they need to be recalculated to obtain basic units, which it is shown below. The number in the equation has own units – *mole/cm^{2,75}/s^{0,25}/atm*.

$$k_g = 0,000467 \cdot u^{0,25} \cdot S^{-0,25} \cdot D_g^{0,5} \quad \mathbf{4}$$

Effective interfacial area is calculated by article¹ with units unit floor area of the plate (*cm²/cm²*). These units have to be recalculated to obtain basic units, which it is shown below. The number in the equation has own units – *cm^{0,58}/s^{0,25}*. The equation is shown in the equation **5**.

$$aa = 0,535 \cdot u^{0,25} \cdot S^{0,83} \quad \mathbf{5}$$

For description of equilibrium between x_{CO2s} and y_{CO2s} (see figure 1) it is needed to use Henry's law because CO_2 is over the Critic Point. According to article³ it is general equation for several components to evaluate Henry's law. It is a function of temperature and vapour pressure of the solvent - in this case it is H_2O . The equation 7 for Henry's law is shown below. A , B and C are parameters which depends on the transfer component, tau is shown in the equation 6 and T_R is reduced temperature.

$$tau = 1 - T_R \quad 6$$

$$\ln\left(\frac{k_{HCO2}}{p_{H2O}}\right) = \frac{A}{T_R} + \frac{B \cdot tau^{0,355}}{T_R} + C \cdot T_R^{-0,41} \cdot e^{tau} \quad 7$$

To evaluate equilibrium it is used Dalton-Henry's equation 8 which is shown below. K_{CO2} is a distributing coefficient obtained by dividing Henry's number by total pressure in the column.

$$p \cdot y_{CO2s} = k_{HCO2} \cdot x_{CO2s} \quad 8$$

The last variable for the model is a total concentration in the liquid – c_{TOT} (molar concentration). The derivation could be seen in the 9 equation. Total amount of moles is simplified to moles of H_2O and MDEA. Moles of H_2S and CO_2 is not needed because their amount is too low. The final equation is function of density of the liquid, which is a constant in this case, weight fraction and molar weight.

$$c_{TOT} = \frac{n_{H2O} + n_{MDEA}}{V_l} = \frac{w_{H2O} \cdot \frac{m_l}{M_{H2O}} + w_{MDEA} \cdot \frac{m_l}{M_{MDEA}}}{V_l} \quad 9$$

$$c_{TOT} = \rho_l \cdot \left(\frac{w_{H2O}}{M_{H2O}} + \frac{w_{MDEA}}{M_{MDEA}} \right)$$

To balance whole problem it is needed to describe the mass transfer from bulk of the gas phase to the phase boundary (10 equation), then through phase boundary where CO_2 amounts are in equilibrium (11 equation) and from phase boundary to the bulk of the liquid phase (12 equation). The last step is the balance the CO_2 with the reaction. To describe the reaction with absorbed amount is used CSTR balance (13 equation) and the problem is sketched in the figure 2. The equations 10 and 12 use the intensity of the mass flow j_{CO2} .

$$j_{CO2} = k_g \cdot (y_{CO2b} - y_{CO2s}) \cdot a \quad 10$$

$$y_{CO2s} = K_{CO2} \cdot x_{CO2s} \quad 11$$

$$j_{CO2} = k_l \cdot (x_{CO2s} - x_{CO2b}) \cdot a \quad 12$$

$$n_{CO2} - k_2 \cdot c_{TOT} \cdot x_{CO2b} \cdot S \cdot A = n_l \cdot x_{CO2b} \quad 13$$

According to the article¹ it is shown all variables and their units. It is needed to use their units and then to convert them to the general units. Equation 10 the mass transfer coefficient has

$\text{mole}/\text{cm}^2/\text{s}/\text{atm}$ and it has to be multiplied by total pressure (in atm) to obtain general units – original equation for mass flow uses motive force of partial pressure of the component. Recalculation could be seen in the equation **14**.

$$j_{\text{CO}_2} = k_g \cdot p \cdot 10^{-5} \cdot (y_{\text{CO}_2b} - y_{\text{CO}_2s}) \quad \mathbf{14}$$

Original equation for mass flow in liquid phase is derived from flow of weight concentration. It needs to be modified to use motive force of mole fraction. It is shown in the equation **15**. Density of liquid and molar mass have to be in kg .

$$j_{\text{CO}_2} = k_l \cdot \frac{\rho_l \cdot 10^{-6}}{M_l} (x_{\text{CO}_2s} - x_{\text{CO}_2b}) \quad \mathbf{15}$$

Density of the liquid is obtained by summation of multiplying weight fraction with the density of the all components. Units of the density are kg/cm^3 . The molar weight of the liquid is obtained by summation of multiplying molar fraction with the molar weight of the all components. Units of the molar weight are kg/mol . For both examples are considered H_2O and MDEA.

Equations **14** and **15** are equal which it leads to the equation **16**. The CSTR balance is the overall balance of the absorption column. It means that inlet concentration of CO_2 in liquid is zero.

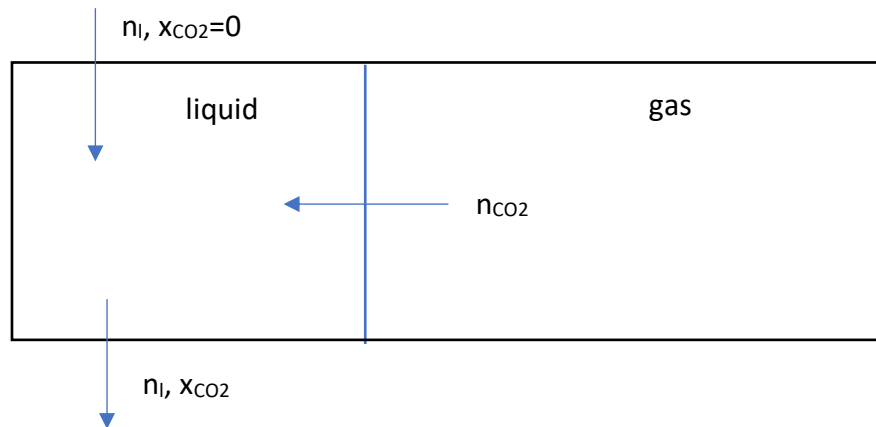


Figure 2 – Scheme of the CSTR balance for all absorption column.

The final equations are **16**, **17**, **18**, **19**. It does not matter if it is used equation **18** with flow in liquid or gas phase – they are same. Unknown variables are y_{CO_2s} , x_{CO_2s} , x_{CO_2b} and A .

$$k_g \cdot p \cdot 10^{-5} \cdot (y_{\text{CO}_2b} - y_{\text{CO}_2s}) = k_l \cdot \frac{\rho_l \cdot 10^{-6}}{M_l} (x_{\text{CO}_2s} - x_{\text{CO}_2b}) \quad \mathbf{16}$$

$$y_{\text{CO}_2s} = K_{\text{CO}_2} \cdot x_{\text{CO}_2s} \quad \mathbf{17}$$

$$n_{\text{CO}_2} = k_l \cdot (x_{\text{CO}_2s} - x_{\text{CO}_2b}) \cdot a \cdot 10^4 \quad \mathbf{18}$$

$$n_A - k_2 \cdot c_{TOT} \cdot x_{CO2b} \cdot S \cdot A = n_l \cdot x_{CO2b}$$

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From the results – y_{CO2b} and y_{CO2s} it is seen that the resistance in mass transfer is neglecting for gas phase. It could be assumed that y_{CO2b} is same as y_{CO2s} . The mass transfer in liquid phase has to be calculated like it is mentioned above.

Balance on Every Stage of Absorption Column – Written Generally

How it was mentioned above, to calculate mass transfer of CO₂ with reaction in the bulk of liquid phase, it is needed four equations (16, 17, 18, 19). In the figure 3 is a sketch of absorption column with unknown variables – on the outlet from stages (outlet streams). Column is numbered from top to bottom and the calculation of the first and bottom stage has to be done separately – the MatLAB code is written generally (it is needed to input the number of stages) the matrix is for the middle stages.

The variables with zero are inlet parameters to the column, “s” is for surface (=phase boundary), “b” for bulk and the number is for the stage. It means that y_{CO_2s1} – it is CO₂ concentration on the surface (=phase boundary) for first stage. For “ n_{CO_21} ” the last number is for the number of stage and it is the amount of CO₂ which goes through the phase boundary – from bulk of gas phase to the bulk of liquid phase.

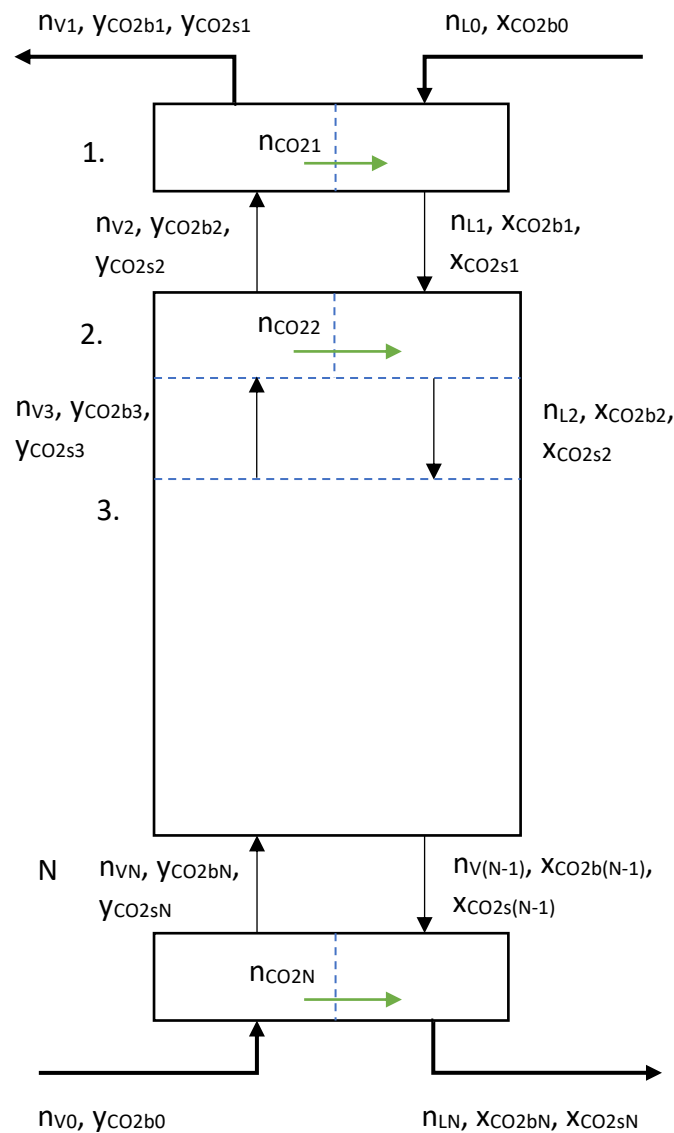


Figure 3 – The sketch of absorption column with streams which leads to the balance on every stage.

For the balance of the absorption column the inlet characteristics (gas and liquid) are something like “initial conditions” and everything could be calculated from that.

Balance of the First Stage

The balance of the first stage have to be done separately due to numbering of absorption column (in the matrix does not exist zeroth element).

$$n_{L0} \cdot x_{CO2b} + n_{CO2(1)} - k_2 \cdot c_{TOT} \cdot x_{CO2b(1)} \cdot S \cdot A = n_{L(1)} \cdot x_{CO2b(1)} \quad 20$$

$$n_{V(2)} \cdot y_{CO2b(2)} = n_{V(1)} \cdot y_{CO2b(1)} + n_{CO2(1)} \quad 21$$

$$n_{CO2(1)} = k_l \cdot \frac{\rho_L \cdot 10^{-6}}{M_L} (x_{CO2s(1)} - x_{CO2b(1)}) \cdot a \cdot 10^4 \quad 22$$

$$k_g \cdot p \cdot 10^{-5} \cdot (y_{CO2b(1)} - y_{CO2s(1)}) = k_l \cdot \frac{\rho_L \cdot 10^{-6}}{M_L} (x_{CO2s(1)} - x_{CO2b(1)}) \quad 23$$

$$y_{CO2s(1)} = K_{CO2} \cdot x_{CO2s(1)} \quad 24$$

$$n_{L(1)} = n_{L0} + n_{CO2(1)} \quad 25$$

$$n_{V(2)} = n_{CO2(1)} + n_{V(1)} \quad 26$$

In the table 2 it is shown the unknown variables for the first stage. It is also seen that there are more unknown parameters than in table 2 – they are inlet parameters of the gas, but they are already calculated because the calculation goes against of the it.

Overview of the Unknown Variables of the First Stage
$n_{L(1)}$
$n_{V(1)}$
$n_{CO2(1)}$
$y_{CO2s(1)}$
$y_{CO2b(1)}$
$x_{CO2s(1)}$
$x_{CO2b(1)}$

Table 2 – Overview of the unknown variables of the first stage.

The principal of balance of the rest column is same, but the middle stages are written generally and the bottom stage is written same like first stage.

MatLAB code

The Function – Calculating Software

```
function [res] = abs_react(yvec,pars)
% ABS_REACT
% CH4+CO2 (g), MDEA+H2O (l), transfer of CO2 with reaction in liquid bulk

T      = pars(1); % K
p      = pars(2); % Pa
wMDEA  = pars(3); % weight fract of MDEA in liq
u      = pars(4); % superficial velo. m/s
S      = pars(5); % submergence of the liquid m
nLin   = pars(6); % inlet liquid flow mol/s
nVin   = pars(7); % inlet gas flow mol/s
xC02in = pars(8); % inlet conc of CO2 in liq
yC02in = pars(9); % inlet conc of CO2 in gas
A      = pars(10); % area of the tray
k2     = pars(11); % const of velocity rating
rhoMDEA = pars(12); % kg/m3
rhoH2O  = pars(13); % kg/m3
MH2O    = pars(14); % kg/mol
MMDEA   = pars(15); % kg/mol
xMDEA   = pars(16); % inlet conc of MDEA in liq
N       = pars(17); % number of MEZIPATER stages

j=1;
for i=1:N
    nC02(i) = yvec(j+0);
    yC02b(i) = yvec(j+1);
    yC02s(i) = yvec(j+2);
    xC02s(i) = yvec(j+3);
    xC02b(i) = yvec(j+4);
    nV(i)    = yvec(j+5);
    nL(i)    = yvec(j+6);
    j = j+7;
end

% mass transfer in the gas phase
nyC02 = 26.9*10^(-6); % molar volume
m3/mol
nyCH4 = (15.9+2.31*4)*10^(-6);
MC02 = (12+2*16)*10^(-3); % molar weight
kg/mol
MCH4 = (12+4*1)*10^(-3);
Dg = 3.2*10^(-8)*T^(1.75) / (p*(nyC02^(1/3)+nyCH4^(1/3))^2) * ... % m2/s
    (1/MC02 + 1/MCH4)^(0.5);
kg = 0.000467 * (u*100)^(0.25) * (S*100)^(-0.5) * ... % mol/cm2/s/atm
    (Dg*10000)^(0.5);

% mass transfer in the liquid phase
DL = 1.214*10^(-9); % m2/s
kl = 13 * (u*100)^(0.25) * (S*100)^(-0.5) * (DL*10000)^(0.5); % cm/s

% equilibrium
AA = -8.55445; BB = 4.01195; CC = 9.52345; % param for Henry's law
pH2O = 7386.34; % vapour pressure Pa
TC = 647; % critic temp of solvent = H2O
TR = T/TC;
tau = 1-TR;
kHC02 = pH2O*exp(AA/TR + BB*tau^(0.355)/TR + ... % Henry Pa
    CC*TR^(-0.41)*exp(tau)); % distributing coef Pa/Pa
KC02 = kHC02/p;
```

```

% effective interfacial area
a = 0.535 * (u*100)^(0.25) * (S*100)^(0.83); % cm2/cm2
a = a*A; % m2

% total conc of liquid
rhoL = wMDEA*rhoMDEA + (1-wMDEA)*rhoH2O; % density of liq kg/m3
Ml = xMDEA*MMDEA + (1-xMDEA)*MH2O; % molar weight of liq kg/mol
cTOT = rhoL * ((1-wMDEA)/MH2O + wMDEA/MMDEA); % mol/m3

% inlet conditions
nL0 = nLin;
nV0 = nVIn;
xC02b0 = xC02in;
yC02b0 = yC02in;

j=1;
% first stage
res(j+0) = nL0*xC02b0 + nC02(1) - k2*cTOT*xC02b(1)*S*A - (nL(1)*xC02b(1)); % C02 bal✓
in liq
res(j+1) = nV(2)*yC02b(2) - (nV(1)*yC02b(1) + nC02(1)); % C02 bal✓
in gas
res(j+2) = nC02(1) - (kl*rhoL*10^(-6)/Ml * (xC02s(1) - ... % flow C02✓
xC02b(1))*a*10^(4));
balance
res(j+3) = kl*rhoL*10^(-6)/Ml * (xC02s(1) - xC02b(1)) - ... % flow of✓
kg*p*10^(-5)*(yC02b(1) - yC02s(1));
C02 through phases
res(j+4) = yC02s(1) - (KC02*xC02s(1)); % eq on✓
phase boundary
res(j+5) = nL(1) - (nL0 + nC02(1)); % liq bal
res(j+6) = nV(2) - (nC02(1) + nV(1)); % gas bal

j=8; % number of place in res vector
for i=2:N-1
res(j+0) = nL(i-1)*xC02b(i-1) + nC02(i) - k2*cTOT*xC02b(i)*S*A - ... % C02 bal✓
(nL(i)*xC02b(i));
in liq
res(j+1) = nV(i+1)*yC02b(i+1) - (nC02(i) + nV(i)*yC02b(i)); % C02 bal✓
in gas
res(j+2) = nC02(i) - (kl*rhoL*10^(-6)/Ml * (xC02s(i) - ... % flow C02✓
xC02b(i))*a*10^(4));
bal
res(j+3) = kl*rhoL*10^(-6)/Ml * (xC02s(i) - xC02b(i)) - ... % flow of✓
(kg*p*10^(-5) * (yC02b(i) - yC02s(i)));
C02 through phases
res(j+4) = yC02s(i) - (KC02*xC02s(i)); % eq on✓
phase boundary
res(j+5) = nL(i) - (nL(i-1) + nC02(i)); % liq bal
res(j+6) = nV(i+1) - (nC02(i) + nV(i)); % gas bal
j = j+7;
end

j = N*7-6; % number of place in res vector
% bottom stage (the last one)
res(j+0) = nL(N-1)*xC02b(N-1) + nC02(N) - k2*cTOT*xC02b(N)*S*A - ...
nL(N)*xC02b(N);
res(j+1) = nV0*yC02b0 - (nC02(N) + nV(N)*yC02b(N));
res(j+2) = nC02(N) - (kl*rhoL*10^(-6)/Ml * (xC02s(N) - ...
xC02b(N))*a*10^(4));
res(j+3) = kl*rhoL*10^(-6)/Ml * (xC02s(N) - xC02b(N)) - ...
kg*p*10^(-5) * (yC02b(N) - yC02s(N));
res(j+4) = yC02s(N) - KC02*xC02s(N);
res(j+5) = nL(N) - (nL(N-1) + nC02(N));
res(j+6) = nV0 - (nC02(N) + nV(N));

res = res';
end

```

The Main – Controlling Software

```
% ABS_REACT
% CH4+CO2 (g), MDEA+H2O (l), CO2 transfer with reaction in liquid bulk
clear all; clc;
T      = 40+273.15;      % K
p      = 7.1*10^(6);     % Pa
wMDEA  = 0.5;            % weight fract of MDEA in liq
u      = 0.1436;         % superficial velo. m/s
S      = 0.1;            % submergence of the liquid m
nLin   = 52.82493556;    % inlet liquid flow mol/s
nVin   = 347.0251241;    % inlet gas flow mol/s
xC02in = 0;              % inlet conc of CO2 in liq
yC02in = 0.05;           % inlet conc of CO2 in gas
A      = 0.8855109225;   % area of the tray
k2     = 0.06;           % const of velocity rating
rhoMDEA = 1024.9;        % kg/m3
rhoH2O  = 992.21;        % kg/m3
MH2O    = 0.018;         % kg/mol
MMDEA   = 0.11916;       % kg/mol
xMDEA   = 0.1313868613;  % inlet conc of MDEA in liq
N       = 6;             % number of stages

pars = [T p wMDEA u S nLin nVin xC02in yC02in A k2 rhoMDEA rhoH2O MH2O MMDEA xMDEA
N];

yguess = 0.5;
yguess = ones(N*7,1)*yguess;

ysol = mmfsolve(@(y) abs_react(y,pars), yguess);

% 1col=nC02; 2col=xC02b; 3col=xC02s; 4col=yC02s; 5col=yC02b; 6col=nV; 7col=nL

% converting calculating vector to matrix
NN=7; % number of unknown variables
ysoll = v2a(ysol,N,NN); disp(ysoll);

nC02  = ysoll(:,1); yC02b = ysoll(:,2); yC02s = ysoll(:,3);
xC02s = ysoll(:,4); xC02b = ysoll(:,5); nV   = ysoll(:,6); nL = ysoll(:,7);

aa = zeros(N,1);
j=1;
for i=1:N
    aa(i) = j;
    j=j+1;
end

figure(1);
subplot(2,2,1);
plot(nC02,aa,'g'); title('Molar Flow of CO2');
xlabel('nC02 [mol/s]'); ylabel('Stages [-]');

subplot(2,2,3);
plot(nV,aa,'k'); title('Gas Flow [mol/s]');
xlabel('Gas Flow [mol/s]'); ylabel('Stages [-]');

subplot(2,2,4);
plot(nL,aa,'b'); title('Liquid Flow [mol/s]');
xlabel('Liquid Flow [mol/s]'); ylabel('Stages [-]');

figure(2);
subplot(2,2,1);
plot(yC02b,aa,'m'); title('Mol. Frac. of CO2 in Bulk of Gas Phase');
```

```
xlabel('yC02b [-]'); ylabel('Stages [-]');

subplot(2,2,2);
plot(yC02s,aa,'c'); title('Mol. Frac. of C02 on Surface in Gas Phase');
xlabel('yC02s [-]'); ylabel('Stages [-]');

subplot(2,2,3);
plot(xC02s,aa,'r'); title('Mol. Frac. of C02 on Surface in Liquid Phase');
xlabel('xC02s [-]'); ylabel('Stages [-]');

subplot(2,2,4);
plot(xC02b,aa,'g'); title('Mol. Frac. of C02 in Bulk of Liquid Phase');
xlabel('xC02b [-]'); ylabel('Stages [-]');
```

Overview of Used Symbols with Their Characteristics

Mark	Value	Description	Unit	Source
T	313,15	Constant temp. in column	K	Given by Bryan
p	$7,1 \cdot 10^6$	Const. pressure in column	Pa	Given by Bryan
yCO₂	0,05	Mole fraction of CO ₂ in gas phase	-	Given by Bryan
wMDEA	0,5	Weight fract. In liquid	-	Calc. in previous report
u	0,1436	Superficial gas velocity	m/s	Calc. in previous report
s	0,1	Submergence of liquid on the tray	m	Guess (based on article)
nL	52,8249	Liquid flow considered const.	mol/s	Calc. in previous report
A	0,8855	Surface	m ²	Calc. in previous report
nyCO₂	$26,9 \cdot 10^{-6}$	Molar volume of CO ₂	m ³ /mol	"skripta"
nyCH₄	$25,14 \cdot 10^{-6}$	Molar volume of CH ₄	m ³ /mol	"skripta"
MCO₂	0,044	Molar weight of CO ₂	kg/mol	-
MCH₄	0,016	Molar weight of CH ₄	kg/mol	-
Dg	$2,7622 \cdot 10^{-7}$	Diffusion coef. in gas phase	cm ² /s	"skripta"
kg	$0,151 \cdot 10^{-4}$	Mass transfer coef. in gas ph.	mol/cm ² /s/atm	1
DI	$1,214 \cdot 10^{-9}$	Diffusion coef. in liquid phase	cm ² /s	2
kl	0,0278	Mass transfer coef. in liquid ph.	cm/s	1
AA	-8,55445	Parameter for calc. Henry of CO ₂	-	3
BB	4,01195	Parameter for calc. Henry of CO ₂	-	3
CC	9,52345	Parameter for calc. Henry of CO ₂	-	3
pH₂O	7386,34	Vapour pressure of H ₂ O	Pa	Calc. by Aspen (NRTL)

TC	647	Critic temp. of solvent (H ₂ O)	K	-
TR	0,484	Reduced temp of solvent (H ₂ O)	-	-
tau	0,5159		K	3
kHCO₂	2,3384*10 ⁽⁸⁾	Calc. Henry of CO ₂	Pa	3
KCO₂	32,9364	Distributing coef. of CO ₂	-	-
a	6,2349	Effective interfacial area	m ² (recalc. to change the unit)	
aa	7,0411	Effective interfacial area	cm ² /cm ² (floor area of plate)	1
k2	6*10 ⁽⁻²⁾	Const. of reaction rating	s ⁻¹ (at 25°C 1 atm)	4
Ha	0,9368*10 ⁽⁻³⁾	Hatta number	-	-
cTOT	32247	Total conc. in liquid	mole/m ³	-
rhoL	1008,555	Density of the liquid phase	kg/m ³	-
yCO₂s	0,04900283286	Mole fraction of CO ₂ on phase boundary	-	-
xCO₂b	0,0002975399603	Mole fraction of CO ₂ in liquid phase	-	-
xCO₂s	0,001487799339	Mole fraction of CO ₂ on phase boundary	-	-
nCO₂	0,06669573447	Mole flow of transferred CO ₂	mol/s	-

References

1. Carey, T. R.; Hermes, J. E.; Rochelle, G. T., A model of acid gas absorption/stripping using methyldiethanolamine with added acid. *Gas Separation & Purification* **1991**, 5 (2), 95-109.
2. Al-Ghawas, H. A.; Hagewiesche, D. P.; Ruiz-Ibanez, G.; Sandall, O. C., Physicochemical properties important for carbon dioxide absorption in aqueous methyldiethanolamine. *Journal of Chemical & Engineering Data* **1989**, 34 (4), 385-391.
3. Roberto Fernández-Prini, J. L. A., Allan H. Harvey, Henry's Constants and Vapor-Liquid Distribution Constants for Gaseous Solutes in H₂O and D₂O at High Temperatures. *J. Phys. Chem. Ref. Data* **2003**, 32 (2).
4. Mitchell, M. J.; Jensen, O. E.; Cliffe, K. A.; Maroto-Valer, M. M., A model of carbon dioxide dissolution and mineral carbonation kinetics. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science* **2010**, 466 (2117), 1265-1290.