



CH 3522: Unit Operations Lab

Batch Absorption

Batch - R, Group - 05

Date of Experiment: 22nd January, 2025

Date of Submission: 29th January, 2025

Roll Numbers	Group Members
CH22B019	N. Pranavi
CH22B020	Deepanjhan Das
CH22B021	Siddhartha R
CH22B022	P. Ganesh

1. Objective

- To study gas absorption of CO_2 in water and ethanol solvents.
- To calculate solubility and bulk mass transfer coefficient at room temperature for the absorption of CO_2 gas in water and ethanol solvents.

2. Introduction

Absorption is a mass transfer process where atoms, molecules, or ions from one phase (gas, liquid, or solid) enter another phase. It can be classified as physical (no chemical reaction) or chemical (involving chemical reactions). Gas absorption involves dissolving a gas into a liquid, with mass transfer occurring from the gas phase to the liquid phase. The reverse process, gas desorption, transfers mass from the liquid to the gas phase.

Gas-liquid absorption is a critical process in many chemical and environmental engineering applications, such as carbon capture, beverage carbonation, and chemical synthesis. The batch absorption of CO_2 in ethanol and water provides an opportunity to study solubility and mass transfer phenomena. Understanding the solubility of CO_2 in solvents like ethanol and water is essential for optimizing industrial processes. Factors such as temperature, pressure, and solvent composition significantly influence the absorption efficiency. By analyzing the pressure drop of CO_2 in a closed system containing these solvents, researchers can estimate parameters like Henry's Law constant and absorption rate, which are crucial for designing efficient gas absorption systems. This knowledge aids in developing effective methods for carbon capture and utilization, contributing to environmental sustainability.

3. Theory

In this experiment we use CO₂ and ethanol & water to perform the absorption process. For each of them, we take the solvent in the reaction container (vessel) and insert CO₂ in the container through a supply line. The gas starts to dissolve in the solvent and there is a pressure change due to this reason. We note the pressure change and the time spent for experimental use.

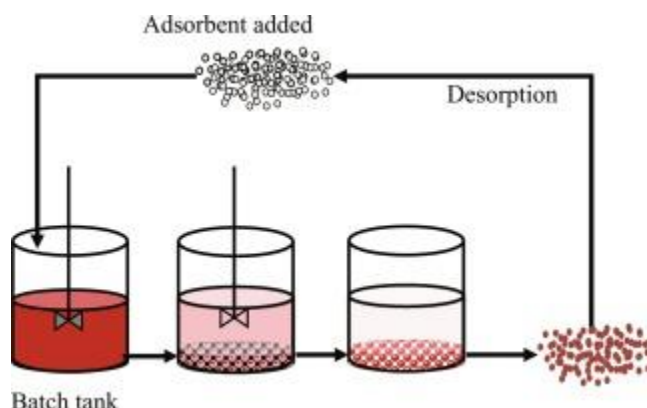


Figure 1: Batch Absorption process in water treatment

We use the Ideal gas law to fit the data. It is the equation of state of a hypothetical ideal gas. It is a good approximation of the behavior of many gases under many conditions, although it may have its limitations. It was first stated by Emile Clapeyron in 1834 as a combination of Boyle's law, Charles's law and Avogadro's law. It (used to calculate C from P data) is given as

$$PV = nRT \Rightarrow C = n/V = P/RT \quad (1)$$

Where P is the pressure of the gas,

V is the volume of the gas,

n is the amount of gas (in moles),

R is the universal gas constant,

T is the absolute temperature of the gas.

We also used the Peng–Robinson equation of state to fit the data for our experiment by calculating the C values. This equation of state is used for real gases and it is represented as follows:

$$P = \frac{RT}{V_m - b} - \frac{a \times \alpha}{(V_m^2 + 2bV_m - b^2)} \quad (2)$$

Where V_m is the molar volume of the gas and it is given by $V_m = V/n$,

P is the pressure,

T is the absolute temperature,

n is the number of moles,

R is the universal gas constant,

a, b and α are gas constants.



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We got the expressions for the constants from literature and they are provided below

$$a = \frac{0.45724 R^2 T_c^2}{P_c} \quad (3)$$

$$b = \frac{0.07780 R T_c}{P_c} \quad (4)$$

$$\alpha = (1 + \kappa(1 - T_r^{0.5}))^2 \quad (5)$$

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2, \text{ when } \omega \leq 0.49 \quad (6)$$

$$\kappa = 0.379642 + 1.48503\omega - 0.164423\omega^3 + 0.016666\omega^4, \text{ when } \omega > 0.49 \quad (7)$$

$$T_r = \frac{T}{T_c} \quad (8)$$

Where T_c is the critical temperature of the gas,

P_c is the critical pressure of the gas and ω is acentric factor.

Also, we know the following relation for mass transfer process,

$$\frac{dc}{dt} = k_a(C^* - C) \quad (9)$$

Where C is the concentration of the gas,

C^* (or C^{sat}) is the solubility of the gas (concentration at saturation) in the liquid,

k_a is the volumetric mass transfer coefficient.

By integrating equation (8) we obtain the following equation,

$$C = C^{sat} + (C^{ini} - C^{sat})\exp(-k_a t) \quad (10)$$

And by multiplying with RT we get (this conversion is possible only for the ideal case)

$$P = P^{sat} + (P^{ini} - P^{sat})\exp(-k_a t) \quad (11)$$

Where P is the pressure of the gas,

P^{sat} is the saturation pressure,

P^{ini} is the initial pressure & t is the time.

We can use the equation (11) to find the volumetric mass transfer coefficient only for the ideal case since in the real scenario the interconversion between C & P is not straightforward (coming from PR equation, eq(2)). Hence rather than using P to fit a model, we will calculate the C from each of ideal & real equations (eq 1 & 2) and then using equation 10, we will fit a non-linear model to obtain the estimated C values. And these values will further be used to perform model adequacy checking.



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4. Apparatus Required

- Infinite source of CO₂ (supplied from cylinder; as the reaction container is small enough)
- Reaction container,
- Pressure Gauge attached to container,
- Heating plate, Magnetic stirrer,
- Measuring cylinder,
- Thermocouple, Stopwatch
- Distilled water, Ethanol, Gasket,
- Clamp & Stands, PVC tubing, Soap Solution

5. Schematic of Experimental Setup

Experimental setup includes the following components:

- Batch reactor (sealed container/vessel)
- Pressure gauge connected to the reactor
- Inlet valve for CO₂ gas
- Magnetic stirrer below the reactor
- Temperature control unit

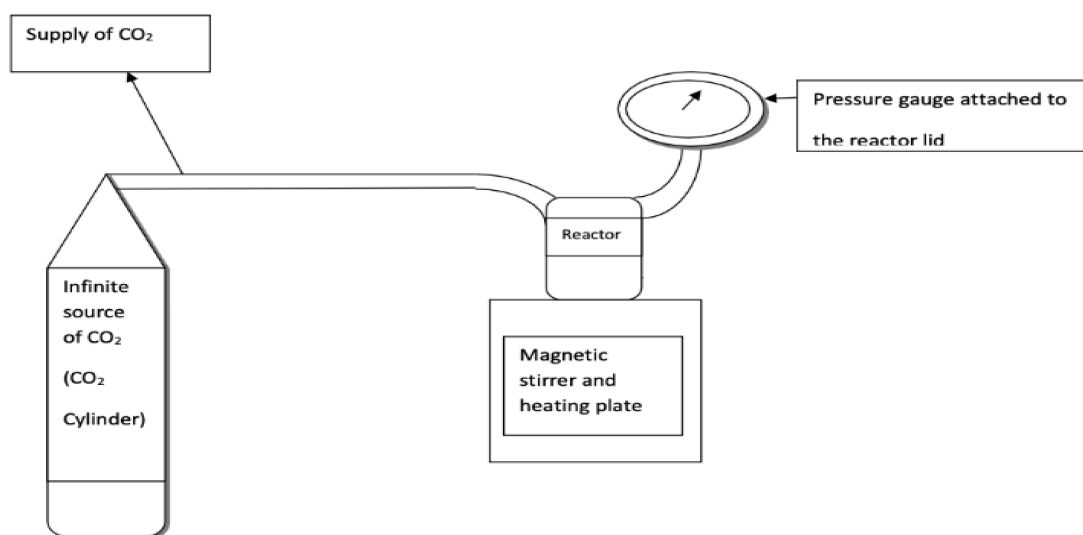


Figure 2: Line Diagram of Experimental Setup

We also show the set-up used while performing the experiment in the laboratory. All the components provided above can easily be found in the following figure (figure 3) too.

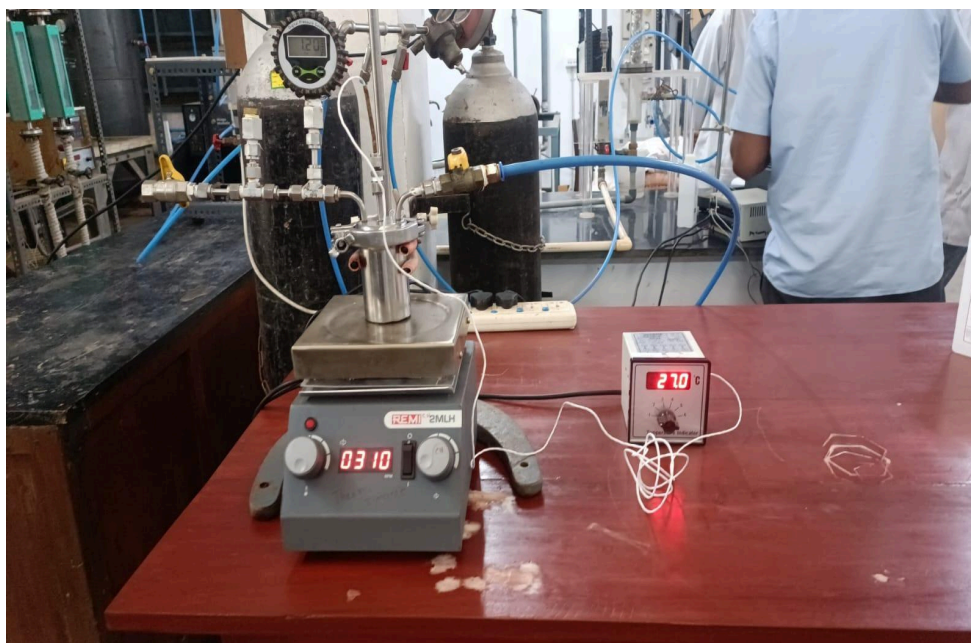


Figure 3: Setup used in Laboratory

6. Procedure

Reactor volume measurement:

1. First, we measure the volume of the absorption vessel by filling it completely with water, and measuring the volume of water.
2. Volume of the vessel is found to be 135 mL.

Solvent (H_2O /Ethanol) + Gas (CO_2):

1. Now fill the vessel with 67.5 mL (half the container) of solvent.
2. The vessel is kept at room temperature of around 26.7°C while performing the absorption of CO_2 in water and it was around 27°C during the absorption experiment of CO_2 in ethanol.
3. We close the container and clamp the lid so that it does not move during the experiment after placing a magnetic palette into the vessel for uniform mixing of the reactants.
4. We use a magnetic stirrer at 300-330 rpm for uniform mixing of reactants.
5. We also use a silicone gasket to seal the vessel and, using a bracket, close the vessel tightly to prevent leakage.
6. We attach the source of gas to the valve on the lid of the container and open the gas cylinder and let the CO_2 enter the container.
7. We operate at around 3 bar pressure and the pressure decreases with time.
8. After the gas enters the container, we detach the valve and observe the pressure readings.
9. We take the pressure readings and the time readings corresponding to it till pressure becomes constant and note them down for calculations.



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7. Experimental Observations

In both cases the RPM was around 300-310 and the vessel volume was 135 mL. All the experimental observations that were tabulated during the laboratory session are included in order at the end.

In the following two tables, the data for the pressure of CO₂ in the vessel (batch system) containing CO₂ & a solvent is provided with the corresponding time it was measured. In the case of CO₂ absorption in ethanol the room temperature was set to be 27°C.

CO ₂ and EtOH		CO ₂ and EtOH	
Time (min)	Pressure (Bar)	Time (min)	Pressure (Bar)
0	3.15	16	1.15
1	2.30	17	1.15
2	1.90	18	1.15
3	1.70	19	1.15
4	1.55	20	1.10
5	1.45	21	1.10
6	1.40	22	1.10
7	1.30	23	1.10
8	1.30	24	1.10
9	1.25	25	1.10
10	1.20	26	1.10
11	1.15	27	1.10
12	1.15	28	1.10
13	1.15	29	1.10
14	1.15	30	1.10
15	1.15	31	1.10

Table 1: Data for CO₂ absorption in Ethanol



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Now, in the case of CO₂ absorption in water, the room temperature was around 26.7 °C.

CO ₂ and H ₂ O		CO ₂ and H ₂ O		CO ₂ and H ₂ O	
Time (min)	Pressure (Bar)	Time (min)	Pressure (Bar)	Time (min)	Pressure (Bar)
0	3.10	18	2.35	39	1.95
0.5	2.95	19	2.30	40	1.95
1	2.95	20	2.30	41	1.95
1.5	2.90	21	2.30	42	1.95
2	2.85	22	2.25	43	1.95
2.5	2.85	23	2.25	44	1.95
3	2.85	24	2.20	45	1.90
4	2.80	25	2.15	46	1.90
5	2.75	26	2.15	47	1.90
6	2.70	27	2.15	48	1.85
7	2.70	28	2.15	49	1.85
8	2.60	29	2.15	50	1.85
9	2.60	30	2.10	51	1.85
10	2.55	31	2.10	52	1.85
11	2.50	32	2.05	53	1.85
12	2.50	33	2.05	54	1.85
13	2.50	34	2.05	55	1.85
14	2.45	35	2.05	56	1.85
15	2.40	36	2.05	57	1.85
16	2.40	37	2.0	58	1.85
17	2.40	38	2.0		



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Table 2: Data for CO₂ absorption in Water

8. Sample Calculations

Since the model estimation requires all the data points we have, it's insignificant to show sample calculation for a single tabulation. Rather we will demonstrate the flow of calculations done in MATLAB to obtain each of the results described and presented in the “Results” section.

We obtain the values of several constants corresponding to CO₂ from literature & these are

$$T_c = 304.25 \text{ K}; P_c = 7.39 \text{ MPa}; \omega = 0.228$$

Using these values the gas constants are calculated which are coming out to be

$$a = 0.395895 \text{ kg} \cdot \text{m}^5 \cdot \text{s}^{-2} \cdot \text{mol}^{-2}; b = 2.663028 \times 10^{-5} \text{ m}^3$$

Since for CO₂, the ω is less than 0.49, thus using equation 6, we get

$\kappa = 0.712243$ and α is a function of T which we have to take differently for the two different cases since the room temperature was set to two slightly different values.

Thereafter using the corresponding equations we calculated $C \text{ (mol/m}^3\text{)}$ from the experimental P values. For ideal state assumption, the equation is straightforward unlike the case of the real state assumption, where we have used a numerical method *fsolve* to find the experimental values of C corresponding to the P (pressure) data. Then we have used a concise form of equation (10) in order to perform the regression on it, which is as follows:

$$C = C^{sat} + (C^{ini} - C^{sat}) \exp(-k_a t) \Rightarrow y = A + B \times \exp(-D \times t) \quad (12)$$

Since the above equation can not be expressed in linear form, a non-linear regression is performed using MATLAB's in-built optimization function *lsqnonlin* which requires some initial values for A, B & D and therefore they are chosen randomly but keeping in mind of their respective orders for better convergence of the objective function. Each model thus obtained, is presented in the latter section along with proper case descriptions.

After this step, respective models are used to calculate the estimated concentration values and these are further used to recalculate the pressure. And for each of C & P the time-dependent plots are shown in the latter section too.

Since we know that $C = n / V$, an alternate representation of PR equation (eq 2) is used to calculate the P using estimated C, which is as follows:

$$P = \frac{RT}{(1/C) - b} - \frac{a \times \alpha}{(1/C)^2 + (2b/C) - b^2} \quad (13)$$

And at the end the in order to perform “model adequacy checking”, the R^2 score of each model is computed. The result section ends with providing the amount of moles of CO₂ that got absorbed in the experiment, estimated from each of these models.



9. Results & Discussions

Absorption of CO₂ in Ethanol:

This sub-experiment is modelled using two different equations, one being ideal and the other is the real equation of state, discussed in “Theory” section of this report. Each of them is discussed below.

Case 1: Ideal behaviour is assumed

The resulting plot we obtained is shown below:

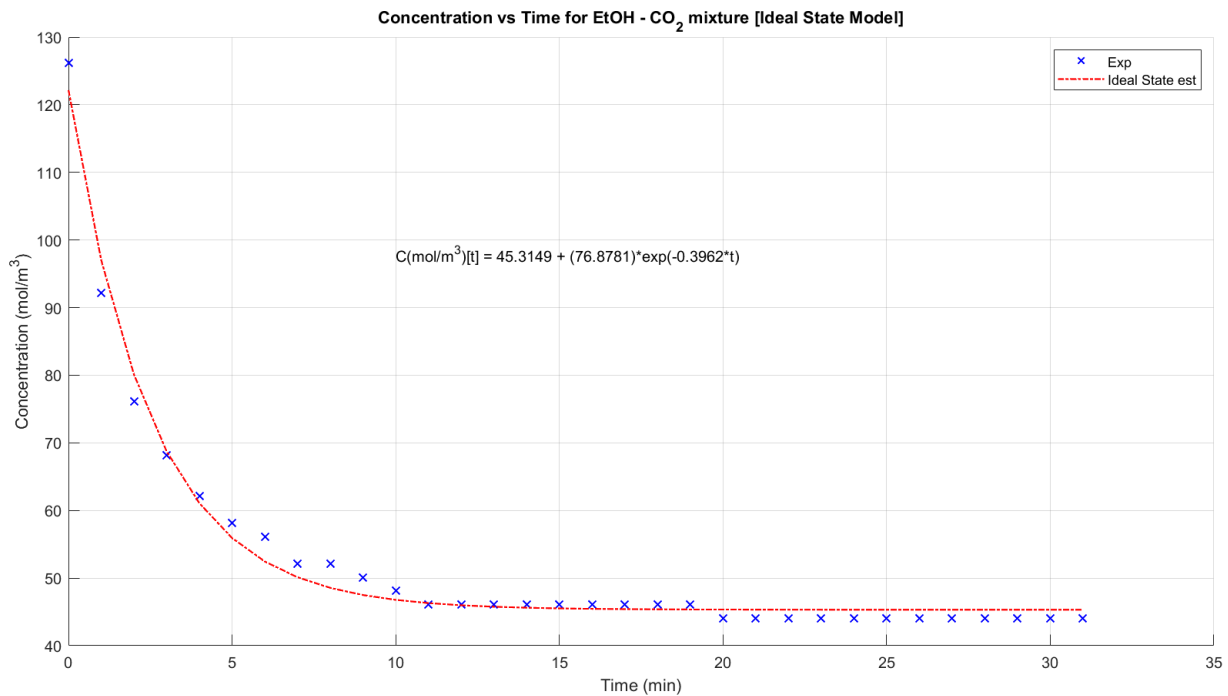


Figure 4: CO₂ absorption in Ethanol estimated using Ideal Equation of State

In the legend the terms “Exp” implies that data to be obtained from experiment and “Ideal State est” implies the estimation is performed using the ideal equation of state respectively. And further figures will also have such explanatory legends. The following are the results of concern:

$$\text{model: } C(t) = 45.3149 + (76.8781) \exp(-0.3962 \times t)$$

$$\text{parameters: } C^{\text{sat}} = 45.3149 \text{ mol/m}^3; (C^{\text{ini}} - C^{\text{sat}}) = 76.8781 \text{ mol/m}^3$$

$$\text{mass transfer coefficient: } k_a = 0.3962 \text{ s}^{-1}$$

$$\text{moles of CO}_2 \text{ being absorbed: } n_{\text{absorbed}} = (C^{\text{ini}} - C^{\text{sat}}) * V = 0.00518927 \text{ moles.}$$

$$\text{model accuracy: } R^2 = 0.986774$$



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Case 2: Real behaviour is assumed

The resulting plot we obtained is shown below:

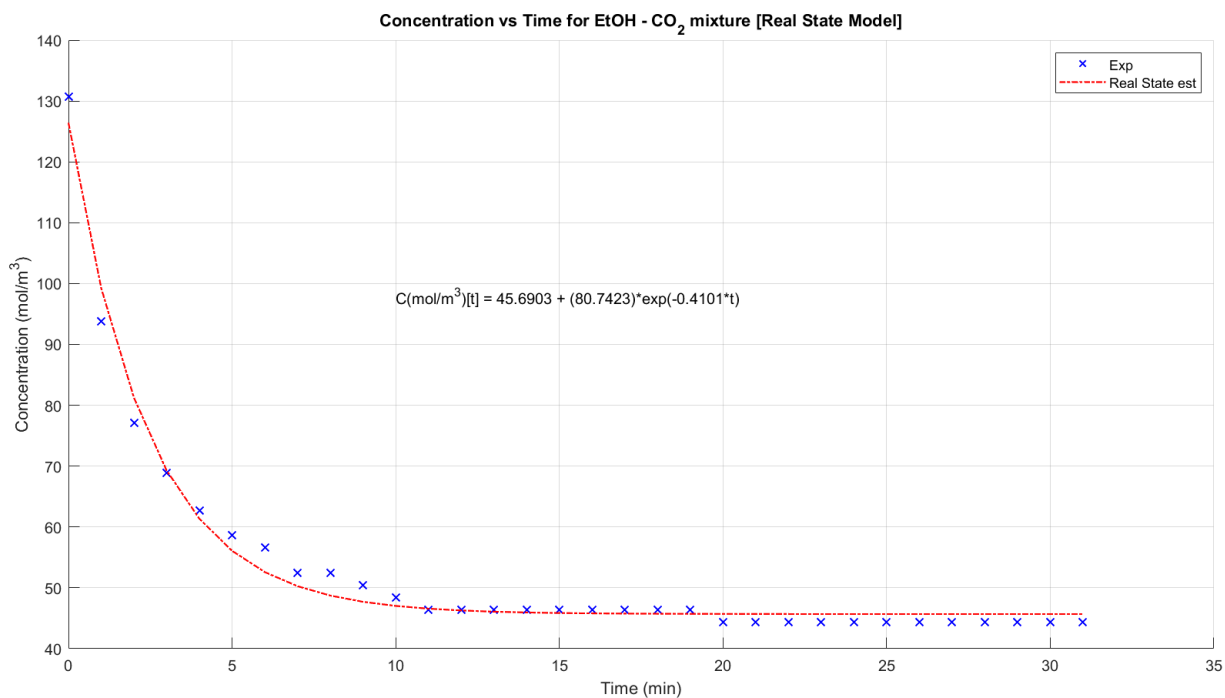


Figure 5: CO₂ absorption in Ethanol estimated using Real (PR) Equation of State

In all the results obtained, the V that is used to compute the number of moles of CO₂ being absorbed is half of the volume of the vessel used which is 67.5 mL. Now in this case, the results we obtained are:

$$\text{model: } C(t) = 45.6903 + (80.7423) \exp(-0.4101 \times t)$$

$$\text{parameters: } C^{\text{sat}} = 45.6903 \text{ mol/m}^3; (C^{\text{ini}} - C^{\text{sat}}) = 80.7423 \text{ mol/m}^3$$

$$\text{mass transfer coefficient: } k_a = 0.4101 \text{ s}^{-1}$$

$$\text{moles of CO}_2 \text{ being absorbed: } n_{\text{absorbed}} = (C^{\text{ini}} - C^{\text{sat}}) * V = 0.00545011 \text{ moles.}$$

$$\text{model accuracy: } R^2 = 0.991497$$

We have also plotted the estimated pressure values obtained from each of the above 2 models along with the experimental values of P and showed the result in the end of “Result” section in figure 8. All these plots significantly justify the experimental values obtained.

Also it is to note that the real state model got better accuracy than the idealized assumptions implying that the real equation of state (eq 2) captured the relationship between P & t better.



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Absorption of CO₂ in Water:

This sub-experiment similarly contains the following two cases. And here also the combined plot of estimated P values from both the models are shown in the end (fig. 9) along with the experimental data.

Case 3: Ideal behaviour is assumed

The resulting plot we obtained is shown below:

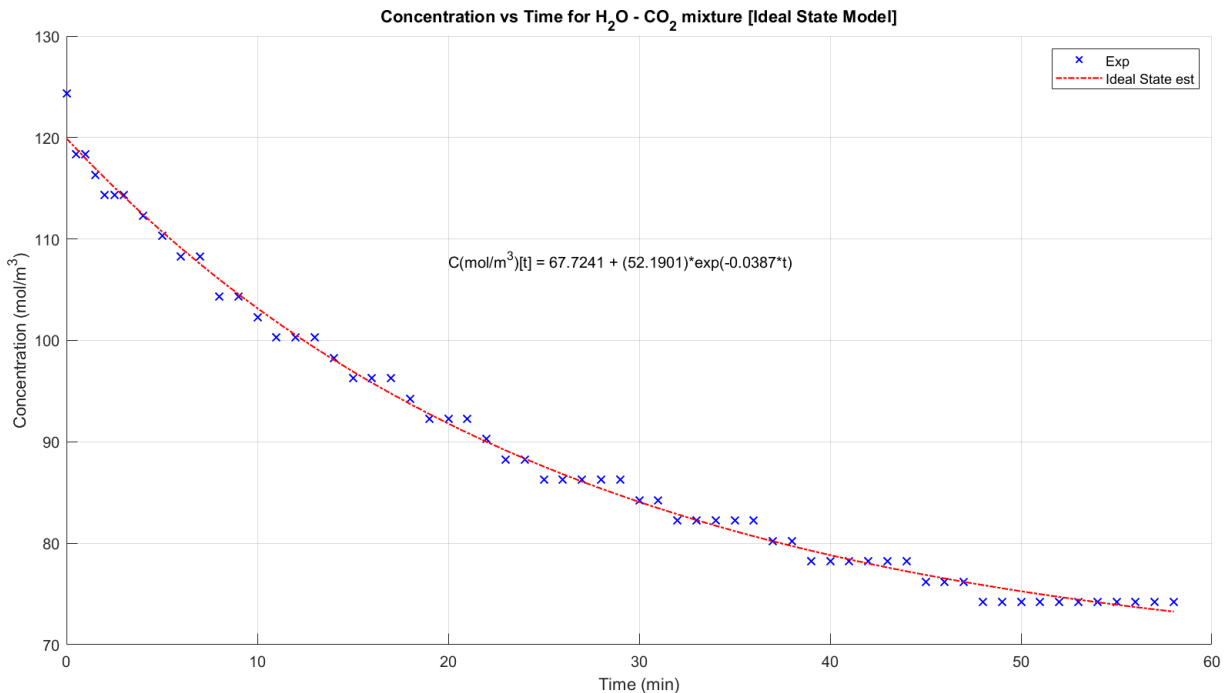


Figure 6: CO₂ absorption in H₂O estimated using Ideal Equation of State

Here also, the notations are self-explanatory. So we provide the results we obtained from this case.

$$\text{model: } C(t) = 67.7241 + (52.1901) \exp(-0.0387 \times t)$$

$$\text{parameters: } C^{\text{sat}} = 67.7241 \text{ mol/m}^3; (C^{\text{ini}} - C^{\text{sat}}) = 52.1901 \text{ mol/m}^3$$

$$\text{mass transfer coefficient: } k_a = 0.0387 \text{ s}^{-1}$$

$$\text{moles of CO}_2 \text{ being absorbed: } n_{\text{absorbed}} = (C^{\text{ini}} - C^{\text{sat}}) \times V = 0.00352283 \text{ moles.}$$

$$\text{model accuracy: } R^2 = 0.995182$$

Case 4: Real behaviour is assumed

The resulting plot we obtained is shown below (figure 7):



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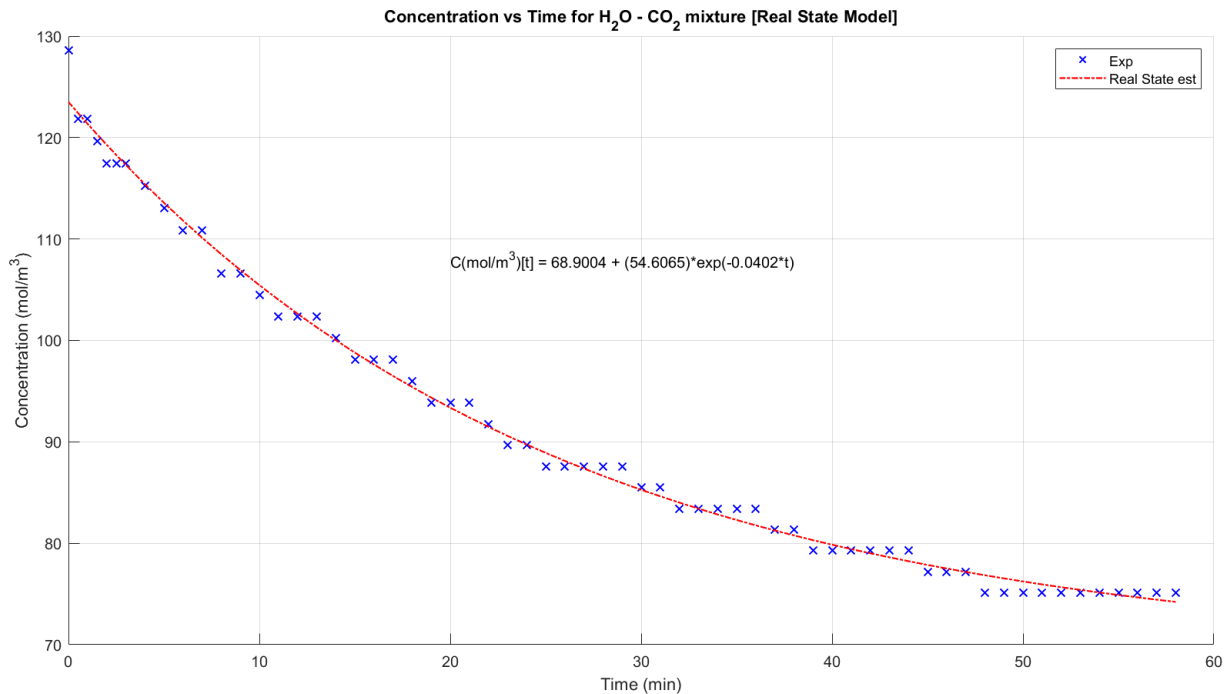


Figure 7: CO₂ absorption in H₂O estimated using Real (PR) Equation of State

model: $C(t) = 68.9004 + (54.6065) \exp(-0.0402 \times t)$

parameters: $C^{sat} = 68.9004 \text{ mol/m}^3$; $(C^{ini} - C^{sat}) = 54.6065 \text{ mol/m}^3$

mass transfer coefficient: $k_a = 0.0402 \text{ s}^{-1}$

moles of CO₂ being absorbed: $n_{absorbed} = (C^{ini} - C^{sat}) * V = 0.00368594 \text{ moles}$.

model accuracy: $R^2 = 0.995824$

Here also the results imply that the real-case assumption captured a better essence of the theory behind this experiment compared to the idealised model.

The comparative analysis between the solvents used in the absorption of CO₂ is done in the “Conclusions” section. This discussion is preceded by two more plots (figure 8 & 9) which include each of these model scenarios for a single type of solvent and contain the pattern of estimated pressure data. Though the apparent view of the two estimated models with each solvents from the following plots show almost similar trend, one might misunderstand the essence captured by each of them and that’s the reason why model adequacy checking gives us deeper understanding.



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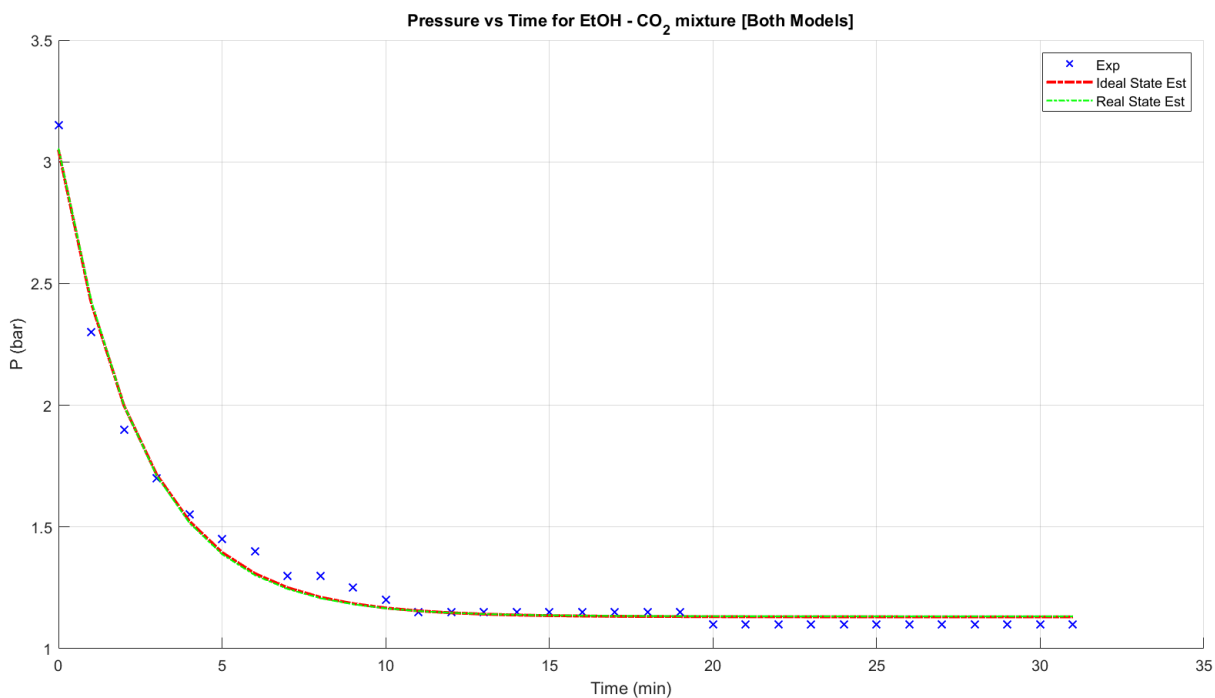


Figure 8: CO₂ absorption in Ethanol

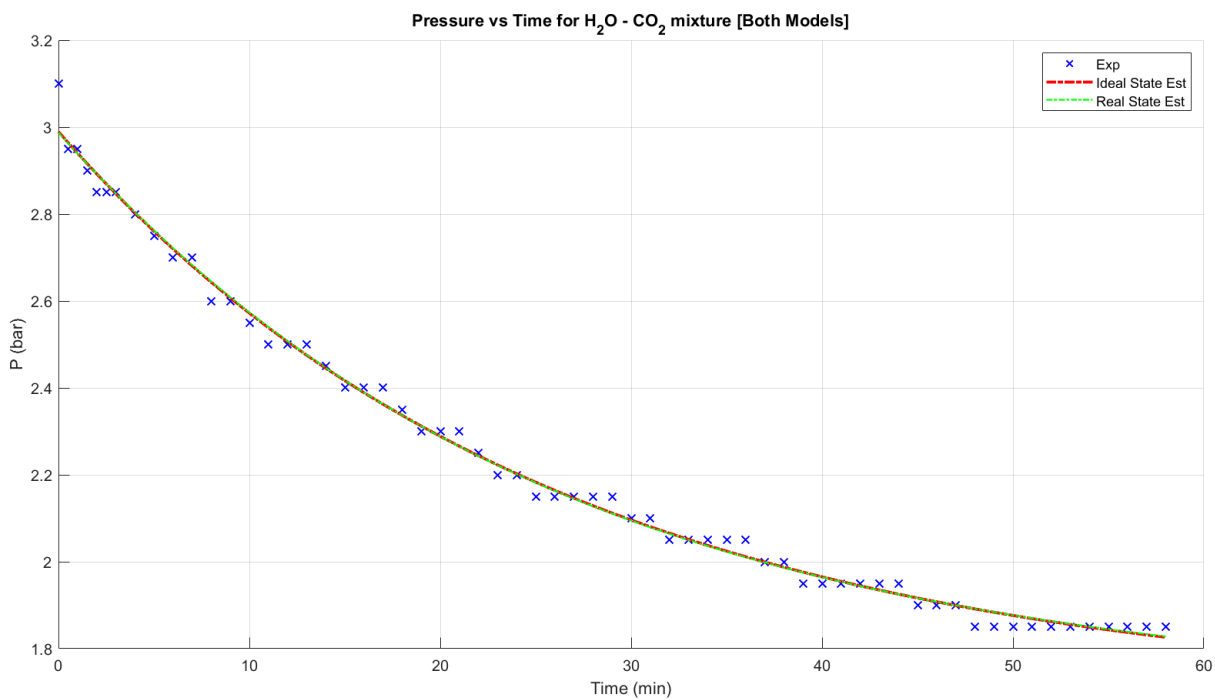


Figure 9: CO₂ absorption in H₂O



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10. Conclusions

- The absorption for carbon dioxide is thus studied with two different solvents. And from the values of mass transfer coefficient it's vivid that CO₂ gets absorbed in ethanol with a greater rate than that of in water.
- The number of moles of CO₂ that got absorbed is also higher in ethanol.
- The above findings also follow the literature.
- With each of the solvents, the real-state models capture better essence than the idealised models since the R^2 is closer to 1 in the real-state models than the other counterparts.
- These studies help researchers make better decisions in the context of choice of solvents which further helps in design aspects in industrial level where processes like CO₂ capture are taken care of.

11. References

- I. CH 3030 Applications of Mass Transfer Course Notes.
- II. Treybal, Robert E. Mass-transfer Operations. New York: McGraw-Hill, 1980.
- III. [Source of literature data used](#) for equations of state & to find values of the constants.
- IV. [Carbon Capture Science & Technology](#), to study application of CO₂ absorption.
- V. The [GitHub repository](#) contains all the related data and coded scripts used for calculations.



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Data Sheet

Experiment: Batch Absorption

Date: 22/01/2025

Batch: R

Group No 5

Roll No	Name
CH22B019	N. Pranavi
CH22B020	Deeponjhen Des
CH22B021	Siddhartha R
CH22B022	P. Ganesh

TA Signature: D.V.K. Bhagawan
22/1/25

T (min)	P (bar)	For EtOH + CO ₂ mixture	T (min)	P (bar)
0	3.15	RPM = 300-330 temp. = 27°C	16	1.15
1	2.30		17	1.15
2	1.90		18	1.15
3	1.70		19	1.15
4	1.55		20	1.10
5	1.45		21	1.10
6	1.40		22	1.10
7	1.30		23	1.10
8	1.30		24	1.10
9	1.25		25	1.10
10	1.25		26	1.10
11	1.15		27	1.10
12	1.15		28	1.10
13	1.15		29	1.10
14	1.15		30	1.10
15	1.15		31	1.10



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T(min)	P(bar)	For H_2O-CO_2 mixture	T(min)	P(bar)
0	3.10	RPM = 310-330 temp = $26.7^\circ C$ - $26.8^\circ C$	31	2.10
0.5			32	2.05
1	2.95		33	2.05
1.5	2.95		34	2.05
2	2.90		35	2.05
2.5	2.805		36	2.05
3	2.85		37	2.0
	2.85		38	2.0
4	2.80		39	1.95
5	2.75		40	1.95
6	2.70		41	1.95
7	2.70		42	1.95
8	2.60		43	1.95
9	2.60		44	1.95
10	2.55		45	1.90
11	2.50		46	1.90
12	2.50		47	1.90
13	2.50		48	1.85
14	2.45		49	1.85
15	2.40		50	1.85
16	2.40		51	1.85
17	2.40		52	1.85
18	2.35		53	1.85
19	2.30		54	1.85
20	2.30		55	1.85
21	2.30		56	1.85
22	2.25		57	1.85
23	2.20		58	1.85
24	2.20			
25	2.15			
26	2.15			
27	2.15			
28	2.15			
29	2.15			
30	2.10			