# Report ST8 - Carbon Dioxide Absorption in a Membrane Contactor

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# Contents

# 1 Introduction

One of the biggest challenges in the world today is the climate crisis, and most of the climate scientists in the world agrees that this is due to the increasing amount of $CO_2$ and other greenhouse gasses in the atmosphere. This leads to the ocean rising and containing a lower pH, and possibly to air pollution and global warming. [1]. Gas-liquid membrane contractors can remove $CO_2$ from a gas, and is therefore very useful to solve environmental issues [2]. In this experiment, a gas-liquid membrane contactor was used to remove $CO_2$, and the absorption rate of $CO_2$ was determined as a function of the liquid velocity. Lastly, the experimental measurements of the absorption rate was compared to the theoretical absorption rate that was determined using Fick's first law.

# 2 Theory

## 2.1 Membrane Contactor

A membrane contactor is a device used to conduct mass transfer between two phases. Inside the membrane contactor there is a porous membrane, which is used to carry out mass transfer between the two phases without allowing one phase to disperse into the other. [2] The membrane does not work as a selective barrier, and does not control the transport between the phases. Its' main function is to keep the phases separated and in contact at the same time. [3]

The selectivity of the process is governed by the difference in the absorbents affinity for the target component. Columns, mixers and towers are usually used to allow mass transfer between the phases. In these units, the phases are in direct contact with each other, which leads to operational problems such as foaming and flooding. In a membrane contactor, the phases can be controlled separately, which eliminates such problems. [4]

## 2.2 Theoretical Model of the Absorption Rate

The mass transport through a membrane is a diffusive transport, assuming steady-state conditions, the molar absorption rate can be described using Fick's first law: [2]

$$J_A = -D_A \left( \frac{\partial \mu_A}{\partial x} \right) \tag{2.1}$$

Where $J_A$ is the molar flux of component A across the surface, $D_A$ is the diffusion coefficient, $\mu_A$ is the chemical potential and $x$ is the distance. $J_A$ is the same as the absorption rate of component A.

The chemical potential across the interface is a continuous function, to simplify the calculations, the diffusion is split into three parts. From the gas phase onto the membrane surface (phase $\alpha$), through the membrane, membrane-phase, and from the membrane surface into the liquid bulk (phase $\beta$). At steady state, the flux through all phases are equal. By assuming that the diffusion during the phase $\alpha$ and the membrane-phase is much faster than the diffusion during phase $\beta$, the flux will be controlled by the absorption of the target component into the liquid phase. Then the flux can be described using equation (2.2) [2]:

$$J_A = k_L \left( C_A^i - C_A^b \right) \tag{2.2}$$

Where $k_L$ is the average liquid phase mass transfer coefficient, $C_A^i$ is the interface concentration as given by Henry's law and $C_A^b$ is the liquid bulk concentration.

The mass transfer coefficient $k_L$ can be determined from the Sherwood number, using equation 2.3:

$$Sh = \frac{k_L d_i}{D_A} \tag{2.3}$$

Where $Sh$ is the Sherwood number, $d_i$ is the inner diameter of the fibers and $D_A$ is the diffusion coefficient. The Sherwood number can be used to describe the ratio between convective and diffusive mass transport. By applying the analogy of Leveque's solution for heat transfer, the Sherwood number can be estimated from Table 2.1[2].

**Table 2.1:** Values for estimating the Sherwood number from Graetz number[2]

| Graetz number (Gz) | Sherwood number (Sh) |
|---|---|
| $< 10$ | 3.67 |
| $10 < \text{Gz} < 20$ | $(3.67^3 + 1.62^3\text{Gz})^{1/3}$ |
| $20 <$ | $1.62\text{Gz}^{1/3}$ |

The Graetz number, $Gz$, is defined by equation (2.4):

$$G_z = \frac{v_L d_i^2}{D_A L} \tag{2.4}$$

Where $v_L$ is the velocity of the liquid, and $L$ is the length of the fiber.

By assuming that the liquid flow in the fibers are laminar, and that the velocity profile is fully developed, the liquid bulk concentration, at any axial distance $z$, can be calculated using equation (2.5)[2].

$$C_A^b|_z = C_A^i \left[1 - exp\left(-\frac{4k_L z}{v_L d_i}\right)\right] \tag{2.5}$$

The average liquid bulk concentration in the fiber, which will be used in equation (2.2), can be found by taking integrating $C_A^b$ over the length of the fiber:

$$\langle C_A^b \rangle = \frac{1}{L}\int_0^L C_A^b dz \tag{2.6}$$

Inserting the expression for $C_A^b$ from equation (2.5) into equation (2.6), and integrating, finally gives the expression for the liquid bulk concentration in the fibers.

$$C_A^b = \frac{C_A^i}{L}\left[L + \frac{v_L d_i}{4k_L}\exp\left(-\frac{4k_L L}{v_L d_i}\right) - \frac{v_L d_i}{4k_L}\right] \tag{2.7}$$

The interface concentration, $C_A^i$, used in equations (2.2) and (2.7), can be found using Henry's law[5]:

$$C_A^i = K_A P_A \tag{2.8}$$

$K_A$ is the Henry's law constant of component A and $P_A$ is the partial pressure.

Equation (2.2) is only valid when the gas-liquid interface conditions are constant, which is not the case in this experiment. For high partial pressures of $CO_2$, the absorption rate will be high, which will lead to a decrease in both pressure, and partial pressure. This causes a lower concentration of $CO_2$ in the gas-liquid interface. For this reason, large deviations are to be expected between the theoretical model and the experimental results, especially at high liquid flow rates[2].

### 2.3 Experimental Model of the Absorption Rate

The experimental absorption rate is calculated using equation (2.9):

$$J_A = \frac{\dot{n}_A^{\text{in}} - \dot{n}_A^{\text{out}}}{A_{\text{tot}}} \tag{2.9}$$

Where $\dot{n}_A^{\text{in}}$ and $\dot{n}_A^{\text{out}}$ is the molar flow of component A in and out the membrane contactor, and $A_{\text{tot}}$ is the total inner surface area of the membrane contactor.

### 2.4 The First Humidifier

The first humidifier adds water vapor to the gas inlet. This is to make sure that the partial water vapor is higher than, or equal to, the total vapor pressure. The reason why this step is important is because liquid phase water will not go into the pores in the membrane (this is called wetting). Wetting will increase the mass transfer coefficient. This means that a higher amount of gas is able to pass through the membrane.[6]

### 2.5 BTB

BTB (Bromothymol blue) is an indicator which indicates the pH of the solution. When the pH is under 6.8, the solution is yellow, and at pH over 6.8 the solution will be blue if BTB is in the solution.[7]

During the absorption of $CO_2$, the following reaction will occur:

$$\mathrm{CO_2 + H_2O \rightleftharpoons HCO_3{}^- + H^+} \tag{2.10}$$

When $CO_2$ is absorbed, the water will become more acidic. When this happens, the BTB will change the color from blue to yellow. Since the experiment happens at a close-to neutral pH, BTB is a good choice of indicator, and the change from blue to yellow will be clear.

## 3 Experimental Procedure

### 3.1 Apparatus

The experiment was performed in a membrane contactor rig, where a mixture of $N_2$ and $CO_2$ was be brought into indirect contact with a mixture of distilled water, 0.01 M NaOH and BTB indicator[2]. The experimental set-up is shown in Figure 3.1. Physical parameters for the set-up can be found on data sheets in the lab.

### 3.2 Execution

The experiment was performed using the following procedure[2]:

25 L of distilled water and a small amount of BTB, bromothymol blue, were added to the feeding tank. To get a pH of 7.5, approximately 0.8 mL of 0.01 M NaOH were then added to the feeding tank. The calculation of the necessary amount of NaOH solution was presented in Appendix C.1. The preselected set-points were entered into the controllers. The set-points are presented in Table 3.1. The IR-sensor was calibrated using the following procedure:

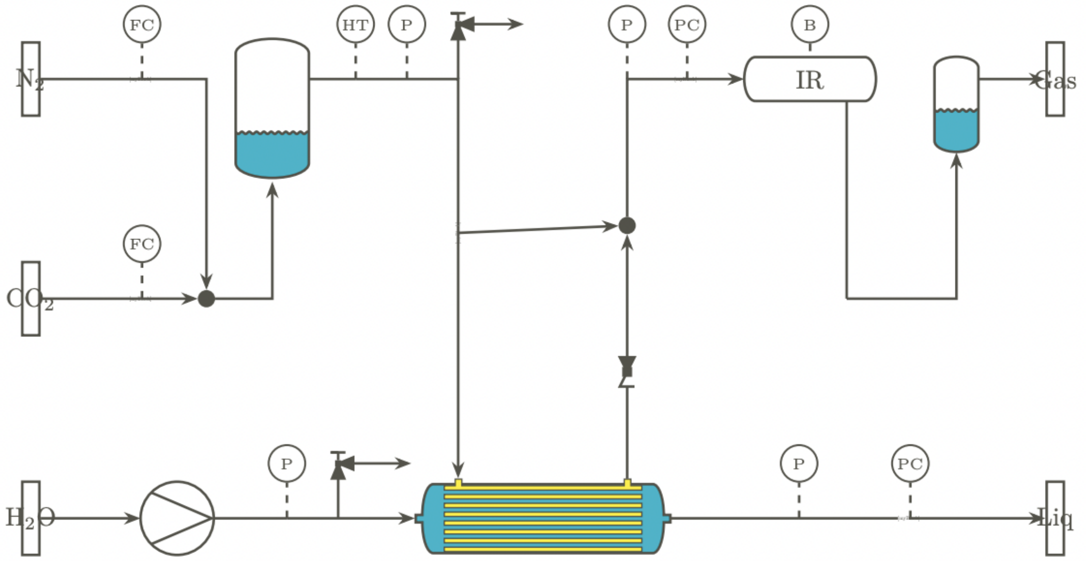

**Figure 3.1:** The experimental setup for the membrane contactor rig[2]. F stands for flow, H for humidity, P for pressure, T for temperature and C for control.

The membrane contactor unit was bypassed by using the 3-way valve and the controls was set to the set-points. When the 16-bit number stabilized, it was written down. The previous step was repeated for the different set-points presented in Table 3.2, the amount of total gas flow was constant for each set of set-points. Using the code in Appendix E.1, a linear regression was made using the 16-bit number as the x-value, and the percentage of $CO_2$ in the flow as the y-value. The result was entered into the software. The controllers was reset to the initial set-point values, and the gas flow was lead into the membrane unit using the 3-way valve. At a pump velocity of 10 rpm, the feeding water was pumped into the lumen of hollow fibers. It was ensured that there was no air in the liquid feeding hos before proceeding with the experiment. When the concentration of $CO_2$ stabilized, the necessary time it took to collect 50 mL of liquid in a 100 mL measuring cylinder was measured using a stop watch. In order to measure other necessary variables, *'Start'* was pressed in the software. The measuring was stopped after approximately two minutes by pressing *'Stop sampling'*. This was repeated for different pump velocities, increasing the pump velocities by 2 rpm for each run. In total, the experiment was run for 10 different pump flow velocities. All the controllers were reset, and the collected data was transferred to a USB-stick.

**Table 3.1:** Set-points for the membrane contactor rig. psia is absolute pressure, and psig is relative pressure.

| Controller | Description | Set-point | Units |
|---|---|---|---|
| $CO_2$ | Flow controller for pure $CO_2$ in | 0.1 | $\mathrm{L\,min^{-1}}$ (STP) |
| $N_2$ | Flow controller for pure $N_2$ in | 0.1 | $\mathrm{L\,min^{-1}}$ (STP) |
| $P_g$ | Pressure controller for the gas outlet | 18 | psia |
| $P_l$ | Pressure controller for the liquid outlet | 0.5 | psig |

**Table 3.2:** Set-points used during the calibration of the IR-sensor

| Flow rate $CO_2$ [$\mathrm{L\,min^{-1}}$] | Flow rate $N_2$ [$\mathrm{L\,min^{-1}}$] | % $CO_2$ in the gas phase |
|---|---|---|
| 0.04 | 0.16 | 20 |
| 0.06 | 0.14 | 30 |
| 0.08 | 0.12 | 40 |

# 4 Results

Due to issues with the setup, the experiment had to be stopped before all the measurements were taken. The data from the experiment is incomplete. In order to do a proper data analysis, data from the same experiment run by another group in a previous year will be used. The measured data is presented in Table A.3 and Table A.4.

The liquid velocity, the theoretical flux and the experimental flux was calculated from the measurements done during the experiment. The calculations are described in detail with example calculations in Appendix C. The results are presented in Table 4.1.

**Table 4.1:** The calculated liquid velocity, the theoretical flux and the experimental flux for the experiment.

| Run | $v_L$ [$\mathrm{cm\,s^{-1}}$] | $J_{CO_2}$ [$\mathrm{mol\,m^{-2}\,s^{-1}}$] | $J_{CO_2}^{exp}$ [$\mathrm{mol\,m^{-2}\,s^{-1}}$] |
|---|---|---|---|
| 1 | 0.767 | $7.310 \cdot 10^{-5}$ | $6.900 \cdot 10^{-5}$ |
| 2 | 0.927 | $8.830 \cdot 10^{-5}$ | $7.957 \cdot 10^{-5}$ |
| 3 | 1.071 | $10.187 \cdot 10^{-5}$ | $9.267 \cdot 10^{-5}$ |
| 4 | 1.150 | $10.931 \cdot 10^{-5}$ | $11.898 \cdot 10^{-5}$ |
| 5 | 1.350 | $12.777 \cdot 10^{-5}$ | $12.035 \cdot 10^{-5}$ |
| 6 | 1.380 | $13.053 \cdot 10^{-5}$ | $12.166 \cdot 10^{-5}$ |
| 7 | 1.350 | $12.779 \cdot 10^{-5}$ | $14.385 \cdot 10^{-5}$ |
| 8 | 1.380 | $13.066 \cdot 10^{-5}$ | $15.657 \cdot 10^{-5}$ |
| 9 | 1.445 | $13.638 \cdot 10^{-5}$ | $15.750 \cdot 10^{-5}$ |
| 10 | 1.412 | $13.341 \cdot 10^{-5}$ | $17.194 \cdot 10^{-5}$ |

The fluxes from Table 4.1 are plotted as a function of the liquid velocity in Figure 4.1. The blue colored objects are from the theoretical model, and the orange colored objects are from the experimental model.

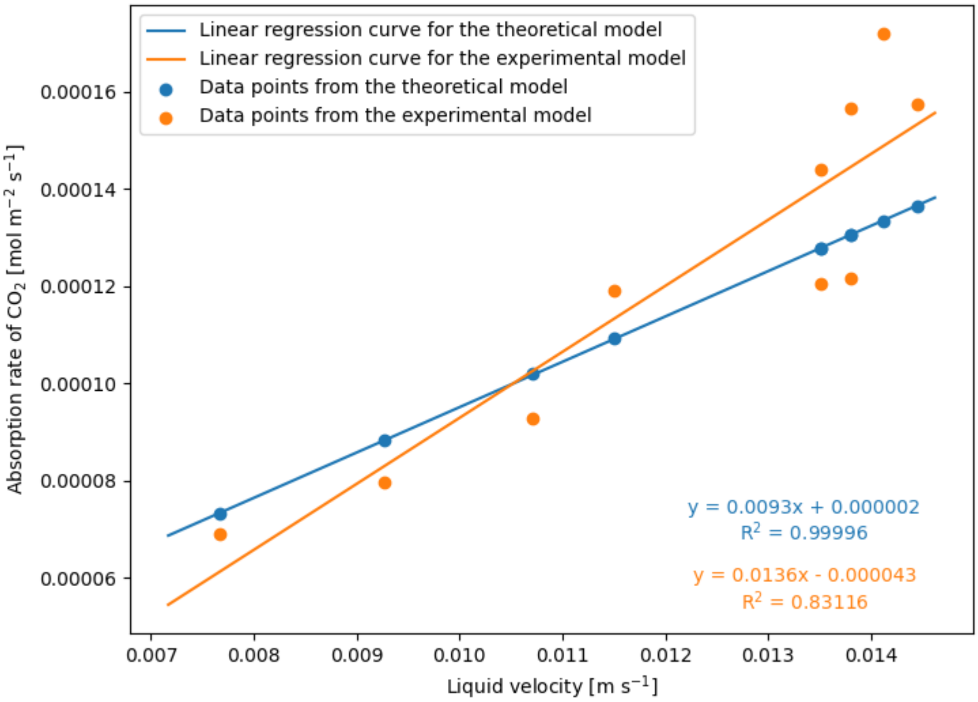

**Figure 4.1:** Plot of the results with linear regression lines for the theoretical and experimental model.

# 5 Discussion

## 5.1 Comparison of the Models

The theoretical and the experimental absorption rates are shown in Figure 4.1. The linear regression of the data points from the theoretical model is a good fit, with the R-squared value being close to 1. This is not the case for the experimental values, as the R-squared value is low. This is as expected seeing as the theoretical model is almost entirely theoretical, and does not depend on experimental world measurements. The experimental model depends on almost only experimental measurements, and is influenced more by deviations from assumptions.

The absorption rate increased with increasing liquid velocity for both models. This is as expected, as increasing the liquid velocity lowers the concentration of the absorbed $CO_2$ in the liquid. This means that the concentration gradient of $CO_2$ increases, which in turn increases the absorption rate.

For the experimental model, the increase in the absorption rate was larger than for the theoretical model. This lead to higher deviations between the two models for higher flow rates, which was expected from the theory. In the theoretical model, it was assumed that there was steady state conditions in the membrane contactor. This was not the case. Due to gas being absorbed over the length of the contactor, the pressure of the gas will decrease as the gas flows through the contactor due to the absorption of $CO_2$. This will in turn decrease the amount of $CO_2$ in the interface, which decreases the absorption rate. In the theoretical model it was assumed that the flow was laminar and fully developed, meaning that the concentration of $CO_2$ in the liquid varies with increasing distance from the membrane surface. Increasing the liquid velocity causes the liquid flow to be more turbulent, causing the liquid to mix better, which in turn makes the distribution of the absorbed $CO_2$ in the liquid more even. This lowers the concentration of $CO_2$ at the membrane surface, increasing the absorption rate. This might be part of the reason why the absorption rate increases more with increasing liquid velocity for the experimental model, than for the theoretical model. The theoretical model also assumes that the absorption of $CO_2$ into the membrane, and the diffusion through the membrane is much faster than the absorption of $CO_2$ from the membrane interface to the liquid phase. This causes the absorption from the liquid phase into the membrane, and the diffusion through the membrane, to be negligible. Although this assumption is reasonable, the mass transfer will be somewhat slower in reality. Therefore, the experimental flux is expected to be lower than the theoretical flux.

The values with the highest liquid flow rates for the experimental model does not follow the expected trend as well as the other values. This most likely stems from inaccurate measurements of the volumetric flow rate. The pump velocity, the liquid velocity should have increased for each run. This was not the case. Looking at the data in Table 4.1, the absorption rate increased for each run as expected, but for the highest pump velocities, the liquid velocities went down after increasing the pump flow rate, which does not make sense. This means that there probably were some errors done in measuring the time it took to fill the 50 mL into the measuring cylinder.

## 5.2 Composition Changes

Table A.4 shows that the gas fraction of $CO_2$ in the outlet gas flow decreases. In other words, the percentage of $CO_2$ going out of the contactor decreased for each run. The input gas flow was constant during the experiment, which means that more $CO_2$ must have been absorbed in the liquid phase for each run.

It was observed that the color of the liquid changed as it went though the membrane contactor. Table 4.1 and Figure 4.1 shows that the the absorption rate of $CO_2$ increased as the liquid velocity increased. This means that the higher the liquid velocity, the more of the $CO_2$-gas were absorbed. The more $CO_2$ that was absorbed, the lower the pH the fluid would get. This is what lead to the change in color, from blue to yellow, that the BTB caused. When the color changed, the pH must have been at approximately 6.8 were BTB change color. This is when reaction (2.10) would have shifted to the right as a result of Le Châtelier's principle.

## 5.3 Error Sources

There was no gas in the flow before the membrane, but after it had been through the membrane, there was bubbles of air in the flow for the lowest three pump velocities. This suggests that there was a leakage somewhere, allowing air or gas from the gas phase to enter the liquid flow. Parts of the outside of the membrane contactor was glued from previous leakages, and this air leakage might come from that part of the membrane. Another possibility is that $CO_2$ leaked through the fibers in the membrane. Increasing the pump velocity past 18 rpm caused a small liquid leakage, therefore, the gas bubbles probably came from an air leakage. This is probably not applicable to the data analyzed in this report, as that data was collected from an experiment performed three years ago, when the membrane contactor presumably was in a better state.
In addition, the system and the data program was very old. The computer program got froze some times. A more updated computer, program and a new membrane would probably have caused fewer faults.

When the time it took to collect 50 mL of liquid was measured, it was done in an inaccurate way. When the hose was lifted, liquid started collecting in bends in the hose, this caused "pockets of liquid" to form in the hose, presumably due to vacuum. The result was a non-continuous flow down into the measuring cylinder. Because of this, the time was not stopped when the level reached exactly 50 mL, as large amounts of liquid suddenly poured down into the measuring cylinder when the pockets of liquid deformed. The precision of the measurements could have been improved if the process of collecting the liquid was automated.

# 6 Conclusion

The $CO_2$ absorption rate was in this experiment determined as a function of the liquid velocity. This was done using a membrane contractor. The linear regression of the data from the experiment shows that the absorption rate of $CO_2$ increased as the liquid velocity increased for both the experimental and the theoretical model. For the experimental model, the absorption rate increases more than for the theoretical model. The theoretical model is only applicable for low liquid velocities, as the difference between the two models increased with increasing liquid velocity.

There were many sources that might have been a cause to error. Firstly, the system and data program were old and outdated. Secondly, there might have been a gas leakage from the membrane contractor, and thirdly, the measurement of the time it took to reach 50 mL of liquid was done in an inaccurate way.

Trondheim, January 9, 2022

Karianne Høie, Erlend Sørlie

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# A Data Tables

## A.1 Membrane Contactor Data

Table A.1 shows the physical parameters of the membrane contactor used in the experiment.

**Table A.1:** Relevant data on the membrane contactor used in the experiment. The data was found on a data sheet in the laboratory.

| Symbol | Description | Value | Unit |
|---|---|---|---|
| $L$ | Fiber length | 12.3 | cm |
| $d_i$ | Inner diameter of the fibers | 220 | µm |
| $d_o$ | Outer diameter of the fibers | 300 | µm |
| $A_{\text{tot}}$ | Total inner surface area | 0.18 | $\text{m}^2$ |

## A.2 Relevant Physical Constants

Relevant physical constants for the experiment. The temperature over the 10 runs were approximately 295 K = 22 °C. The diffusion and Henry's law constants were collected for 22 °C.

**Table A.2:** Relevant physical constants for the experiment.

| Symbol | Description | Value | Unit |
|---|---|---|---|
| $D_{\text{CO}_2}$ [8] | Diffusion coefficient for $CO_2$ in water at 22 °C | $1.784 \cdot 10^{-9}$ | $\text{m}^2\,\text{s}^{-1}$ |
| $K_{\text{CO}_2}$ [8] | Henry's law constant for $CO_2$ 22 °C | $3.615 \cdot 10^{-4}$ | $\text{mol}\,\text{m}^{-3}\,\text{Pa}^{-1}$ |
| $R$ | Molar gas constant | 8.314 | $\text{m}^3\,\text{Pa}\,\text{K}^{-1}\,\text{mol}^{-1}$ |

## A.3 Data from the Experiment

All data presented in this section were collected from a different group in a previous year. Table A.3 presents the pump velocity, the time required to fill 50 mL in a measuring cylinder and the liquid flow rate calculated from equation (C.7). Table A.4 shows the averages of the different parameters measured by the software during the experiment.

**Table A.3:** Pump velocities, time required to fill 50 mL in a measuring cylinder and calculated flowrate, $Q_L$, for the different runs during the experiment.

| Run | Pump velocity [rpm] | $t$ [s] | $Q_L$ $[\text{cm}^3\,\text{s}^{-1}]$ |
|---|---|---|---|
| 1 | 10 | 81 | 0.617 |
| 2 | 12 | 67 | 0.746 |
| 3 | 14 | 58 | 0.862 |
| 4 | 16 | 54 | 0.926 |
| 5 | 18 | 46 | 1.087 |
| 6 | 20 | 45 | 1.111 |
| 7 | 22 | 46 | 1.087 |
| 8 | 24 | 45 | 1.111 |
| 9 | 26 | 43 | 1.163 |
| 10 | 28 | 44 | 1.136 |

**Table A.4:** The average values of the measurements done by the software during the experiment for different runs. $T_{gas}$ is the temperature of the gas, $P_{\text{gas}}^{\text{in}}$ and $P_{\text{gas}}^{\text{out}}$ are the pressures of the gas at the inlet and outlet respectively, $P_{\text{liquid}}^{\text{in}}$ and $P_{\text{liquid}}^{\text{out}}$ are the pressures of the liquid at the inlet and outlet respectively, $\dot{V}_{\text{CO}_2}$ and $\dot{V}_{\text{N}_2}$ are the volumetric flow rates of $CO_2$ and $N_2$, and $y_{\text{CO}_2}^{\text{out}}$ is the molar fraction of $CO_2$ in the gas outlet.

| Run | $T_{\text{gas}}$ [K] | $P_{\text{gas}}^{\text{in}}$ [kPa] | $P_{\text{gas}}^{\text{out}}$ [kPa] | $P_{\text{liquid}}^{\text{in}}$ [kPa] | $P_{\text{liquid}}^{\text{out}}$ [kPa] | $\dot{V}_{\text{CO}_2}$ [$\text{cm}^3\,\text{s}^{-1}$] | $\dot{V}_{\text{N}_2}$ [$\text{cm}^3\,\text{s}^{-1}$] | $y_{\text{CO}_2}^{\text{out}}$ [%] |
|---|---|---|---|---|---|---|---|---|
| 1 | 295.21 | 117.94 | 117.84 | 151.63 | 144.56 | 1.24 | 1.25 | 43.92 |
| 2 | 295.26 | 117.92 | 117.82 | 151.82 | 144.45 | 1.24 | 1.25 | 42.93 |
| 3 | 295.29 | 117.91 | 117.81 | 154.18 | 144.60 | 1.24 | 1.25 | 41.66 |
| 4 | 295.34 | 117.93 | 117.83 | 156.95 | 144.74 | 1.24 | 1.25 | 38.85 |
| 5 | 295.36 | 117.91 | 117.81 | 157.49 | 144.73 | 1.24 | 1.25 | 38.76 |
| 6 | 295.41 | 117.94 | 117.84 | 158.29 | 144.77 | 1.24 | 1.25 | 38.64 |
| 7 | 295.42 | 117.93 | 117.83 | 160.89 | 144.81 | 1.24 | 1.25 | 36.04 |
| 8 | 295.43 | 118.06 | 117.96 | 162.90 | 145.30 | 1.24 | 1.25 | 34.45 |
| 9 | 295.45 | 117.98 | 117.87 | 161.46 | 145.26 | 1.24 | 1.25 | 34.14 |
| 10 | 295.47 | 117.97 | 117.86 | 166.85 | 145.27 | 1.24 | 1.25 | 32.27 |

# B IR-Calibration

Table B.1 presents the 16-bit numbers collected for different concentrations during the calibration of the IR-sensor. Due to the experiment being cut short, these values are irrelevant for the data analysis, as the analyzed data were collected from a previous year.

**Table B.1:** Data collected during the calibration of the IR-sensor.

| Flow rate $CO_2$ [$\mathrm{L\,min^{-1}}$] | Flow rate $N_2$ [$\mathrm{L\,min^{-1}}$] | % $CO_2$ in the gas phase | 16-bit number |
|---|---|---|---|
| 0.04 | 0.16 | 20 | 35258 |
| 0.06 | 0.14 | 30 | 35706 |
| 0.08 | 0.12 | 40 | 36343 |
| 0.10 | 0.10 | 50 | 37077 |

Table B.2 presents the 16-bit numbers collected for different concentrations during the calibration of the IR-sensor during the experiment of the previous group that produced the data that is analyzed in this report.

**Table B.2:** Data collected by a previous group during the calibration of the IR-sensor.

| Flow rate $CO_2$ [$\mathrm{L\,min^{-1}}$] | Flow rate $N_2$ [$\mathrm{L\,min^{-1}}$] | % $CO_2$ in the gas phase | 16-bit number |
|---|---|---|---|
| 0.00 | 0.20 | 0 | 34457 |
| 0.02 | 0.18 | 10 | 34844 |
| 0.04 | 0.16 | 20 | 35338 |
| 0.05 | 0.15 | 25 | 35650 |
| 0.06 | 0.14 | 30 | 36009 |
| 0.08 | 0.12 | 40 | 36553 |
| 0.10 | 0.10 | 50 | 37222 |
| 0.12 | 0.08 | 60 | 38159 |
| 0.14 | 0.06 | 70 | 38821 |
| 0.16 | 0.04 | 80 | 39745 |

Figure B.1 shows the linear regression of the data in Table B.2. The curve is a good fit for the data points, as the $R^2$ value is quite high. The parameters of the fitted curve were used to calibrate the IR-sensor so that during the main experiment, it presented the molar fraction of $CO_2$ in percentage instead of 16-bit numbers.

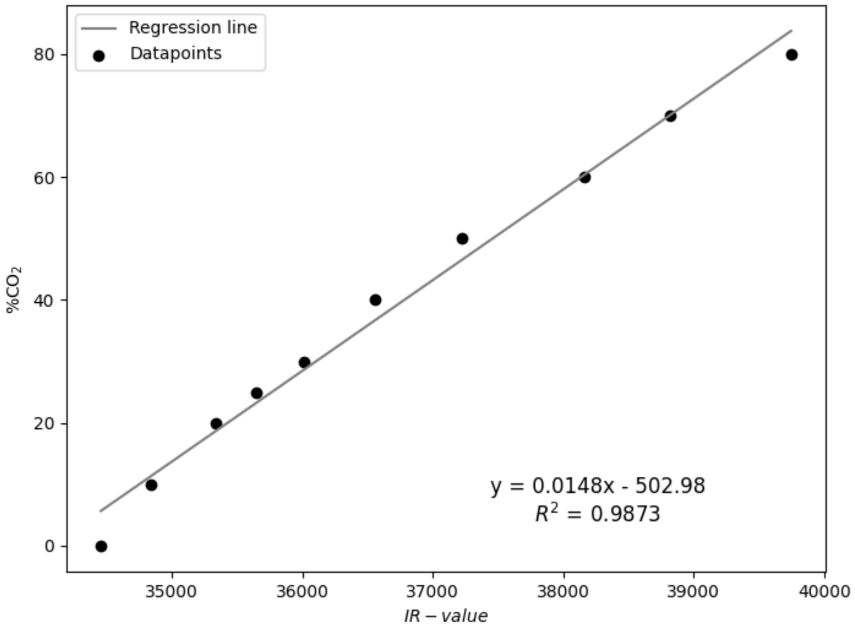

**Figure B.1:** Plot of the linear regression made from the 16-bit values and the concentrations of $CO_2$ in Table B.2.

# C Calculations

## C.1 Preparing the Feed Tank Solution

The feeding tank is to be filled with 25 L of a solution with a pH of 7.5. This is to be achieved by adding an amount of 0.01 M NaOH. In water, NaOH dissolves by the following reaction:

$$\mathrm{NaOH(aq)} \longrightarrow \mathrm{Na^{+}(aq)} + \mathrm{OH{-}(aq)} \tag{C.1}$$

NaOH is a strong base, and is assumed to dissolve completely. As pH is dependent on the concentration of $H^+$, it is more convenient to use pOH. The relation between pH and pOH is given by,

$$\mathrm{pH} + \mathrm{pOH} = 14 \tag{C.2}$$

Which gives pOH = 6.5. pOH can be defined by this expression[9]:

$$\mathrm{pOH} = -\log\,[\mathrm{OH^-}] \tag{C.3}$$

Rearranging equation (C.3), the necessary concentration of $OH^-$ in the solution can be found:

$$c_{\mathrm{OH^-}} = 10^{-\mathrm{pOH}} = 3.163 \cdot 10^{-7} [\mathrm{mol\,L^{-1}}] \tag{C.4}$$

From reaction (C.1), the number of moles of NaOH needed in the mixture is equal to the number of moles of $\mathrm{OH}^-$. This can be calculated using,

$$n_{\mathrm{NaOH}} = n_{\mathrm{OH}^-} = c_{\mathrm{OH}^-} \cdot V = 3.163 \cdot 10^{-7} \mathrm{mol\,L^{-1}} \cdot 25\,\mathrm{L} = 7.905 \cdot 10^{-6}\,\mathrm{mol} \tag{C.5}$$

The necessary amount of 0.01 M NaOH can then be found,

$$V_{\mathrm{NaOH}} = \frac{n_{\mathrm{NaOH}}}{c_{\mathrm{NaOH}}} = \frac{7.905 \cdot 10^{-6}\,\mathrm{mol}}{0.01\,\mathrm{mol\,L^{-1}}} = 0.79\,\mathrm{mL} \tag{C.6}$$

To make a 25 L solution with a pH of 7.5, 0.79 mL of 0.01 M NaOH solution needs to be added to the feeding tank.

## C.2 Liquid Velocity

The volumetric flow rate of the liquid, $Q_L$, can be calculated using equation (C.7), where $V$ is the volume passing through a cross section of the pipe during the time $t$. In the experiment, $V$ was 50 mL for all runs, and $t$ was measured.

$$Q_L = \frac{V}{t} = \frac{50\,\mathrm{mL}}{t} \tag{C.7}$$

In order to calculate the liquid velocity through the membrane contactor, the total inner cross sectional area of the contactor, $A_{\mathrm{CS,\ tot}}$, needs to be found.

The number of fibers in the membrane contactor can be calculated as the ratio between the total surface area of the contactor, $A_{\mathrm{tot}}$, and the surface area of a single fiber, $A_{\mathrm{fiber}}$:

$$N_{\mathrm{fiber}} = \frac{A_{\mathrm{tot}}}{A_{\mathrm{fiber}}} = \frac{A_{\mathrm{tot}}}{\pi d_i L} = \frac{0.18\,\mathrm{m}^2}{\pi \cdot 220\,\mu\mathrm{m} \cdot 12.3\,\mathrm{cm}} \approx 2117 \tag{C.8}$$

Where the values for the parameters of the membrane contactor can be found in Table A.1. The inner cross sectional area of one fiber is found using,

$$A_{\mathrm{CS,fiber}} = \pi \cdot \left(\frac{d_i}{2}\right)^2 \tag{C.9}$$

Where $d_i$ is the inner diameter of the fibers in the contactor. $A_{\mathrm{CS,\ tot}}$ can be calculated using the following equation:

$$A_{\mathrm{CS,tot}} = N_{\mathrm{fiber}} \cdot A_{\mathrm{CS,fiber}} = 2117 \cdot \pi \cdot \left(\frac{d_i}{2}\right)^2 = 0.805\,\mathrm{cm}^2 \tag{C.10}$$

Finally, the liquid velocity, $v_L$ can be calculated using equation ():

$$v_L = \frac{Q_L}{A_{\mathrm{CS,tot}}} = \frac{Q_L}{0.805\,\mathrm{cm}^2} \tag{C.11}$$

### C.2.1 Example Calculation

Inserting the required time to fill a measuring cylinder with 50 mL of liquid, for Run 1 from Table A.3, into equations (C.7) and (C.11), gives:

$$Q_L = \frac{50\,\mathrm{mL}}{81\,\mathrm{s}} = 0.617\,\mathrm{mL\,s^{-1}} = 0.617\,\mathrm{cm^3\,s^{-1}}$$

$$v_L = \frac{0.617\,\mathrm{cm^3\,s^{-1}}}{0.805\,\mathrm{cm^2}} = 0.767\,\mathrm{cm\,s^{-1}}$$

Which are the values presented for run 1 in Table 4.1 and Table A.3.

## C.3 Theoretical Model

Almost all necessary equations are shown in Section 2.2. Equation (C.12) was used to calculate the partial pressure of $CO_2$ from the pressure at the gas inlet.

$$P^{\mathrm{in}}_{\mathrm{CO_2}} = y^{\mathrm{in}}_{\mathrm{CO_2}} P^{\mathrm{in}}_{\mathrm{gas}} \tag{C.12}$$

### C.3.1 Example Calculation

In this section, an example calculation of the flux for run 1 will be presented.

The Graetz number were calculated using equation (2.4):

$$G_z = \frac{0.767\,\mathrm{cm\,s^{-1}} \cdot (0.022\,\mathrm{cm})^2}{1.784 \cdot 10^{-5}\mathrm{cm^2\,s^{-1}} \cdot 12.3\,\mathrm{cm}} = 1.69$$

All the Graetz numbers were calculated to be less than 10. From table 2.1, the Sherwood number were found to be 3.67 for all 10 runs. By rearranging equation (2.3), the mass transfer coefficient $k_L$ were found:

$$k_L = \frac{Sh \cdot D_{\mathrm{CO_2}}}{d_i} = \frac{3.67 \cdot 1.784 \cdot 10^{-5}\mathrm{cm^2\,s^{-1}}}{0.022\,\mathrm{cm}} = 2.976 \cdot 10^{-3}\,\mathrm{cm\,s^{-1}}$$

To calculate interface concentration, equations (2.8) and (C.12) were combined. It was assumed that the amount of $CO_2$ and $N_2$ in the inlet gas flow were equal,

$$C^i_{\mathrm{CO_2}} = K_{\mathrm{CO_2}} P^{\mathrm{in}}_{\mathrm{gas}} y^{\mathrm{in}}_{\mathrm{CO_2}} = 3.615 \cdot 10^{-4}\mathrm{mol\,m^{-3}\,Pa^{-1}} \cdot 117\,940\,\mathrm{Pa} \cdot 0.5 = 21.32\,\mathrm{mol\,m^{-3}}$$

The liquid bulk concentration were calculated from equation (2.7):

$$C^b_{\mathrm{CO_2}} = \frac{21.32\,\mathrm{mol\,m^{-3}}}{12.3\,\mathrm{cm}} \cdot \left[12.3\,\mathrm{cm} + \frac{0.767\,\mathrm{cm\,s^{-1}} \cdot 0.022\,\mathrm{cm}}{4 \cdot 2.98 \cdot 10^{-3}\,\mathrm{cm\,s^{-1}}} \exp\left(-\frac{4 \cdot 2.98 \cdot 10^{-3}\,\mathrm{cm\,s^{-1}} \cdot 12.3\,\mathrm{cm}}{0.767\,\mathrm{cm\,s^{-1}} \cdot 0.022\,\mathrm{cm}}\right) - \frac{0.767\,\mathrm{cm\,s^{-1}} \cdot 0.022\,\mathrm{cm}}{4 \cdot 2.98 \cdot 10^{-3}\,\mathrm{cm\,s^{-1}}}\right] = 18.87\,\mathrm{mol\,m^{-3}}$$

Finally, the theoretical absorption rate is calculated using equation (2.2):

$$J_{\mathrm{CO_2}} = 2.98 \cdot 10^{-5}\,\mathrm{m\,s^{-1}} \cdot \left(21.32\,\mathrm{mol\,m^{-3}} - 18.87\,\mathrm{mol\,m^{-3}}\right) = 7.310 \cdot 10^{-5}\,\mathrm{mol\,m^{-2}\,s^{-1}}$$

## C.4 Experimental Model

In order to calculate the experimental absorption rate, the molar flows of $CO_2$ before and after the membrane contactor need to be found. The molar flow of $CO_2$ going in to the contactor can be calculated from the ideal gas law:

$$\dot{n}_{\mathrm{CO_2}}^{\mathrm{in}} = \frac{P_{gas}^{\mathrm{in}} \cdot \dot{V}_{\mathrm{CO_2}}}{R \cdot T} \tag{C.13}$$

Similarly, for $N_2$:

$$\dot{n}_{\mathrm{N_2}}^{\mathrm{in}} = \frac{P_{gas}^{\mathrm{in}} \cdot \dot{V}_{\mathrm{N_2}}}{R \cdot T} \tag{C.14}$$

Assuming that no $N_2$ is absorbed in the contactor, the gas flow of $N_2$ is constant:

$$\dot{n}_{\mathrm{N_2}}^{\mathrm{out}} = \dot{n}_{\mathrm{N_2}}^{\mathrm{in}} = \dot{n}_{\mathrm{N_2}}$$

The molar fraction of $CO_2$ in the gas flow out of the system, can be expressed as:

$$y_{\mathrm{CO_2}}^{\mathrm{out}} = \frac{\dot{n}_{\mathrm{CO_2}}^{\mathrm{out}}}{\dot{n}_{\mathrm{tot}}^{\mathrm{out}}} \tag{C.15}$$

Rearranging equation (C.15), an expression for the molar flow of $CO_2$ out of the system can be found:

$$\dot{n}_{\mathrm{CO_2}}^{\mathrm{out}} = y_{\mathrm{CO_2}}^{\mathrm{out}} \cdot \dot{n}_{\mathrm{tot}}^{\mathrm{out}} = y_{\mathrm{CO_2}}^{\mathrm{out}} \left( \dot{n}_{\mathrm{CO_2}}^{\mathrm{out}} + \dot{n}_{\mathrm{N_2}} \right) = y_{\mathrm{CO_2}}^{\mathrm{out}} \cdot \dot{n}_{\mathrm{CO_2}}^{\mathrm{out}} + y_{\mathrm{CO_2}}^{\mathrm{out}} \cdot \dot{n}_{\mathrm{N_2}}$$

Solving for $\dot{n}_{\mathrm{CO_2}}^{\mathrm{out}}$, gives the final expression:

$$\dot{n}_{\mathrm{CO_2}}^{\mathrm{out}} = \frac{y_{\mathrm{CO_2}}^{\mathrm{out}} \cdot \dot{n}_{\mathrm{N_2}}}{1 - y_{\mathrm{CO_2}}^{\mathrm{out}}} \tag{C.16}$$

The experimental absorption rate can then be calculated using equation (2.9).

### C.4.1 Example Calculation

Performing the calculation for run 1.

The molar flow of $CO_2$ into the contactor is calculated from equation(C.13):

$$\dot{n}_{\mathrm{CO_2}}^{\mathrm{in}} = \frac{117\,940\,\mathrm{Pa} \cdot 1.24 \cdot 10^{-6}\mathrm{m^3\,s^{-1}}}{8.314\,\mathrm{m^3\,Pa\,K^{-1}\,mol^{-1}} \cdot 295.21\,\mathrm{K}} = 5.946 \cdot 10^{-5}\,\mathrm{mol\,s^{-1}}$$

The molar flow of $N_2$ into the contactor is calculated from equation(C.14):

$$\dot{n}_{\mathrm{N_2}}^{\mathrm{in}} = \frac{117\,940\,\mathrm{Pa} \cdot 1.25 \cdot 10^{-6}\mathrm{m^3\,s^{-1}}}{8.314\,\mathrm{m^3\,Pa\,K^{-1}\,mol^{-1}} \cdot 295.21\,\mathrm{K}} = 6.007 \cdot 10^{-5}\,\mathrm{mol\,s^{-1}}$$

The molar flow of $CO_2$ out the contactor is calculated from equation(C.16):

$$\dot{n}_{\mathrm{CO_2}}^{\mathrm{out}} = \frac{0.4392 \cdot 6.007 \cdot 10^{-5}\,\mathrm{mol\,s^{-1}}}{1 - 0.4392} = 4.704 \cdot 10^{-5}\,\mathrm{mol\,s^{-1}}$$

Finally, the experimental absorption rate were calculated using equation (2.9):

$$J_{\mathrm{CO_2}}^{\mathrm{out}} = \frac{5.946 \cdot 10^{-5}\,\mathrm{mol\,s^{-1}} - 4.704 \cdot 10^{-5}\,\mathrm{mol\,s^{-1}}}{0.18\,\mathrm{m^2}} = 6.900 \cdot 10^{-5}\,\mathrm{mol\,m^{-2}\,s^{-1}}$$

# D Health, Safety and Environment

This was a relatively safe experiment, but there were some possible risks. Exposure to BTB over time can cause eye irritation or lung damage. If it was spilled on the skin or eyes, it should be rinsed off with large quantities of water. This did not happen. NaOH could have been spilled, $CO_2$ could leak and the equipment could break (and lead to cuts etc.). NaOH can cause blindness if it is in contact with eyes and it can cause burning damage on the skin. Due to this, spill of NaOH was the biggest risk in this experiment. It was a low concentration, but to prevent a dangerous situation, protective gloves were used to lower the risk. Lab coat and glasses was always used.

The COVID-19 restrictions has been repealed, so it was not necessary to do much considering infection control. As a precaution, the lab space and equipment used during the experiment was wiped before leaving the lab, and the QR code was scanned.

# E Python Code

## E.1 Calibrating the IR-sensor - Linear Regression

Below is the code that were used to get the parameters for the calibration of the IR-sensor.

```
import numpy as np
import matplotlib.pyplot as plt


def Rsquared(x, y, f_regression):
    y_avg = np.average(y)
    SStot = np.sum((y-y_avg)**2)
    SSres = np.sum((y-f_regression(x))**2)
    return 1 - (SSres/SStot)

ir_values, percentageCO2 = np.loadtxt("IR/IR-data.txt", usecols=(0, 1),
                                      skiprows=1, unpack=True)
params, cov = np.polyfit(ir_values, percentageCO2, 1, cov=True)
f = np.poly1d(params)
x_values = np.linspace(ir_values[0],ir_values[-1], 100)

R2 = Rsquared(ir_values, percentageCO2, f)

fig = plt.figure(figsize=[8, 6])
ax = fig.add_subplot()
plt.plot(x_values, f(x_values), label="Regression line", color="grey")
plt.scatter(ir_values, percentageCO2, label="Datapoints", color="black")
plt.xlabel(r"$IR-value$")
plt.ylabel(r"%CO$_2$")
ax.text(0.7, 0.15, f"y = {params[0]:.4f}x - {-params[1]:.2f}", horizontalalignment='center',
        verticalalignment='center', transform=ax.transAxes, fontsize=12)
ax.text(0.7, 0.10, r"$R^2$"+f" = {R2:.4f}", horizontalalignment='center',
        verticalalignment='center', transform=ax.transAxes, fontsize=12)
plt.legend()
plt.savefig("Ir_cal")
plt.show()

print(f"a = {params[0]:.4f}")
print(f"b = {params[1]:.2f}")
print(f"R^2 = {R2:.4f}")
```

## E.2 Extracting the Relevant Data

The code below was used to extract the relevant values from the .CSV-files generated by the software and add them into a .txt-file. For each run, the values were found by taking an average of all the measurements done during the sampling.

```
import numpy as np
import pandas as pd

#Function to delete empty NA values from the dataframes
def delete_nan(list):
    if np.isnan(np.sum(list)) == True:
        nan_array = np.isnan(list)
        not_nan_array = ~ nan_array
        new_list = list[not_nan_array]
        return new_list
    else:
        return list

# Importing the data from the diffent runs as dataframes
df1 = pd.read_csv('Contactor/Run1.csv')
df2 = pd.read_csv('Contactor/Run2.csv')
df3 = pd.read_csv('Contactor/Run3.csv')
df4 = pd.read_csv('Contactor/Run4.csv')
df5 = pd.read_csv('Contactor/Run5.csv')
df6 = pd.read_csv('Contactor/Run6.csv')
df7 = pd.read_csv('Contactor/Run7.csv')
df8 = pd.read_csv('Contactor/Run8.csv')
df9 = pd.read_csv('Contactor/Run9.csv')
df10 = pd.read_csv('Contactor/Run10.csv')
DF = [df1, df2, df3, df4, df5, df6, df7, df8, df9, df10]

# Extracting the relevant data, calculating the average of the
# measurements over the time interval and saving the results to a file
f = open("Contactor/ContactorData.txt", 'w')
f.write('Run\tT_gas\tP_in(gas)\tP_out(gas)\tP_in(liquid)'
        '\tP_out(liquid)\tV(CO2)\tV(N2)\ty_CO2\n')
f.write('[#]\t[K]\t      [kPa]\t     [kPa]    '
        '   \t[kPa]        \t[kPa]    \t[cm3/s]\t[cm3/s]\t[-]\n')
for i in range(len(DF)):
    df = DF[i]
    Tgas_list = delete_nan(np.array(df[' Humidity sensor temperature [Celcius]']))
    Tgas = np.average(Tgas_list)+273 #Converting to Kelvin
    PgasIn_list = delete_nan(np.array(df[' Pressure transmitter: gas feed [psi]']))
    PgasIn = np.average(PgasIn_list)*6894.75728/1000  #Converting to kPa
    PgasOut_list = delete_nan(np.array(df[' Pressure transmitter: gas product [psi]']))
    PgasOut = np.average(PgasOut_list) * 6894.75728 / 1000  # Converting to kPa
    PliquidIn_list = delete_nan(np.array(df[' Pressure transmitter: water feed [psi]']))
    PliquidIn = np.average(PliquidIn_list) * 6894.75728 / 1000  # Converting to kPa
    PliquidOut_list = delete_nan(np.array(df[' Pressure transmitter: water product [psi]']))
    PliquidOut = np.average(PliquidOut_list) * 6894.75728 / 1000  # Converting to kPa
    VflowCO2_list = delete_nan(np.array(df[' Flow Controller: CO_2 [l/min]']))
    VflowCO2 = np.average(VflowCO2_list)*1000/60  # Converting to cm3/s
    VflowN2_list = delete_nan(np.array(df[' Flow Controller: N2 [l/min]']))
    VflowN2 = np.average(VflowN2_list)*1000/60  # Converting to cm3/s
    y_CO2_list = delete_nan(np.array(df[' CO_2 sensor [-]']))
    y_CO2 = np.average(y_CO2_list)
    f.write(f"{i+1}\t{Tgas}\t{PgasIn}\t{PgasOut}\t{PliquidIn}"
            f"\t{PliquidOut}\t{VflowCO2}\t{VflowN2}\t{y_CO2}\n")
f.close()
```

## E.3 Theoretical and Experimental Flux

Below is the code used to calculate the theoretical and experimental flux, and plot them as a function of the liquid velocity.

```
import matplotlib.pyplot as plt
import numpy as np

# Membrane contactor data (converted to cm-scale)
L = 12.3     # [cm]
d_i = 0.0220    # [cm]
d_o = 0.0300     # [cm]
A_tot = 1800     # [cm2]

# Calculations on the membrane dimensions
# (C.8), (C.9), (C.10)
N = A_tot / (np.pi * d_i * L)
A_CS_fiber = np.pi * (d_i/2)**2 # [cm2]
A_CS_tot = N*A_CS_fiber   # [cm2]

# Mole fraction of CO2 in gas inlet
yin_CO2 = 0.5

# Physical data
D_CO2 = 1.784*10**(-5) # [cm2/s] (converted to cm-scale)
K_CO2 = 3.615*10**(-4) # [mol/m3*Pa#]
R = 8.314*10**(6) #[cm3*Pa/K*mol]

# Collecting the values for the experiment
time_to_fill = np.array([81, 67, 58, 54, 46, 45, 46, 45, 43, 44])   # [s]
Tgas, Pgas_in, Pgas_out, Plq_in, Plq_out, VCO2, VN2, y_CO2 = \
    np.loadtxt("Contactor/ContactorData.txt", usecols=(1, 2, 3, 4, 5, 6, 7, 8)
               , skiprows=2, unpack=True)
# [K], [kPa], [kPa], [kPa], [kPa], [cm3/s], [cm3/s], [-]

# Functions used in the calculations
# Rsquared value
def Rsquared(x, y, f_regression):
    y_avg = np.average(y)
    SStot = np.sum((y-y_avg)**2)
    SSres = np.sum((y-f_regression(x))**2)
    return 1 - (SSres/SStot)

# Sherwood number, Table 2.1
def Sherwood(Gz):
    if Gz<=10:
        return 3.67
    elif Gz>10 and Gz<=20:
        return (3.67**3 + (1.62**3)*Gz)**(1/3)
    elif Gz>20:
        return 1.62*Gz**(1/3)

# Calculating the liquid velocities
# eq (C.7), (C.11)
Q_L = 50 / time_to_fill   # [cm3/s]
v_L = Q_L / A_CS_tot   # [cm/s]

# Calculating the theoretical flux
# Gratz number, eq (2.4)
Gz = (v_L*d_i**2) / (D_CO2*L)
```

```
# Sherwood number
Sh = np.array([Sherwood(Gz_number) for Gz_number in Gz])
# Mass transfer coefficient, eq (2.3)
k_L = Sh*D_CO2/d_i
# Interface concentration, eq (2.8), converting kPa to Pa
Ci_CO2 = K_CO2*(Pgas_in*1000)*yin_CO2
# Liquid bulk concentration, eq (2.7)
Cb_CO2 = Ci_CO2/L * (L + (v_L*d_i)/(4*k_L)*np.exp(-(4*k_L*L)/(v_L*d_i))
                     - (v_L*d_i)/(4*k_L))
# The flux, eq (2.2)
J_CO2 = k_L*10**(-2)*(Ci_CO2-Cb_CO2)

# Calculate the experimental flux
# Molar flow of CO2 into the membrane, eq (C.13)
n_in_CO2 = (Pgas_in*1000*VCO2)/(R*Tgas)
# Molar flow of CO2 out of the membrane, eq (C.14)
n_N2 = (Pgas_in*1000*VN2)/(R*Tgas)
y_CO2 = y_CO2/100 # From % to fraction
n_out_CO2 = (y_CO2*n_N2) / (1-y_CO2)
# The experimental flux, eq (2.9)
Jexp_CO2 = (n_in_CO2-n_out_CO2)/(A_tot*10**(-4))

v_L = v_L/100 #Converting from [cm/s] to [m/s]
# Make the linear regressions
params1 = np.polyfit(v_L, J_CO2, 1)
f = np.poly1d(params1)
params2 = np.polyfit(v_L, Jexp_CO2, 1)
g = np.poly1d(params2)
R2_Theory = Rsquared(v_L, J_CO2, f)
R2_Exp = Rsquared(v_L, Jexp_CO2, g)

# Plotting the results
fig = plt.figure(figsize=[8, 6])
ax = fig.add_subplot()
x_values = np.linspace(v_L[0]-0.0005, v_L[-1]+0.0005, 105)
plt.scatter(v_L, J_CO2, label='Data points from the theoretical model')
plt.scatter(v_L, Jexp_CO2, label='Data points from the experimental model')
plt.plot(x_values, f(x_values), label='Linear regression curve for the theoretical model')
plt.plot(x_values, g(x_values), label='Linear regression curve for the experimental model')
ax.text(0.8, 0.20, f"y = {params1[0]:.4f}x + {params1[1]:.6f}", horizontalalignment='center',
        verticalalignment='center', transform=ax.transAxes, fontsize=10, color='#1f77b4')
ax.text(0.8, 0.16, r"R$^2$"+f" = {R2_Theory:.5f}", horizontalalignment='center',
        verticalalignment='center', transform=ax.transAxes, fontsize=10, color='#1f77b4')
ax.text(0.8, 0.09, f"y = {params2[0]:.4f}x - {-params2[1]:.6f}", horizontalalignment='center',
        verticalalignment='center', transform=ax.transAxes, fontsize=10, color='#ff7f0e')
ax.text(0.8, 0.05, r"R$^2$"+f" = {R2_Exp:.5f}", horizontalalignment='center',
        verticalalignment='center', transform=ax.transAxes, fontsize=10, color='#ff7f0e')
plt.xlabel(r"Liquid velocity [m s$^{-1}$]")
plt.ylabel(r"Absorption rate of CO$_2$ [mol m$^{-2}$ s$^{-1}$]")
plt.legend()
plt.savefig('FluxVsVelocity')
plt.show()
```