To: Professor Wilfred Chen
From: Group 4b
Date: May 5th, 2021
Subject: Mass Contactor Design

Motivation

Designing a mass contactor requires fully understanding the system being designed and optimized. The system in question is designed around removing acetone from a wastewater stream through the use of TCE (trichloroethylene), with the wastewater stream having specific purification parameters that need to be met. Specific to this design, one-stage and two-stage countercurrent mass contactors are analyzed and compared in the following pages. While presenting a system that meets this criteria is an important objective of this project, ultimately optimization is the key to real world process design, and an attempt at optimizing this process from an economic standpoint will be further explored throughout the report.

Approach

The methodology used to realize the goal of this design consisted of several steps. Firstly, the mass transfer load was calculated using the following equation:

$$m_{load} = -(q^{II}C_A^{II} - q_F^{II}C_{AF}^{II}) \qquad \textbf{(Eq. 1)}$$

where phase II refers to dispersed phase, or wastewater stream, which is enriched in species A, acetone. To facilitate extraction, trichloroethane, TCE, was chosen as it is both largely immiscible in water and has a high affinity for acetone. From there, the minimum flow rate of this solvent, or phase I, was determined from a level II analysis as follows:

$$q_{min}^{I} = q^{II}\left(\frac{C_{AF}^{II} - C_A^{II}}{MC_A^{II} - C_{AF}^{I}}\right) \qquad \textbf{(Eq. 2)}$$

This calculation only serves as an estimate since operating at a minimum flow rate requires an infinite interfacial area which is impractical. Furthermore, industrial equipment is not designed to be operated at equilibrium; therefore, a larger volumetric flow rate must be chosen. This is done by employing the concept of stage efficiency, χ, which dictates how far from equilibrium the system is operating. For this analysis, a range of efficiencies (i.e. 50%-95%) was chosen so as to gain a better understanding of system performance under different operating conditions. This directly translates to a range of TCE volumetric flow rates as shown in **Eq. 3** below:

$$q^{I} \approx \frac{q_{min}^{I}}{\chi} \qquad \textbf{(Eq. 3)}$$

Next, the outlet concentration of acetone in TCE, C_A^I, is calculated using the following equation, assuming a pure feed,

$$C_A^{I} = C_{AF}^{I} + \chi(C_{A,eq}^{I} - C_{AF}^{I}) \qquad \textbf{(Eq. 4)}$$

where the equilibrium concentration of acetone in phase I at equilibrium is obtained from a level II analysis. Using this newly acquired concentration, the average driving force can be determined and, in turn, the interfacial area as follows:

$$< \Delta C_A^{I-II} >= - (C_A^I - M C_A^{II}) \quad \textbf{(Eq. 5)}$$
$$a = \frac{m_{load}}{K_m < \Delta C_A^{I-II} >} \quad \textbf{(Eq. 6)}$$

where the values of K_m and M can be found in **Appendix A** along with other parameters. Then, the volume of phase II was determined from which the total volume of both the TCE and wastewater can be calculated:

$$V^{II} = \frac{1}{6}(ad) \quad \textbf{(Eq. 7)}$$
$$V = V^I + V^{II} \quad \textbf{(Eq. 8)}$$

where V^I can be found by assuming homogeneity and, thus, equal residence times (i.e $\tau^I = \tau^{II}$) and d can be obtained from the *Agitated Vessels* range in **Figure 7.3** from Russel, Robinson, and Wagner.[1] The latter then fixes the power input per mass of fluid for each selected diameter (see **Appendix B** and **C** for sample calculations on single-stage and two-stage mass contactors and the respective cost analysis).

Results

The outcome of the described calculations is the following graphs for single-stage and two-stage mass contactors. The total operating cost of the system is a sum of the cost due to TCE flow (directly based on q^I and efficiency), the cost due to agitation (dependent on diameter as described above) for a 24-hour period, and the capital cost from building the contactor itself. This is plotted as a function of both total volume and efficiency, with efficiency presented as contours.

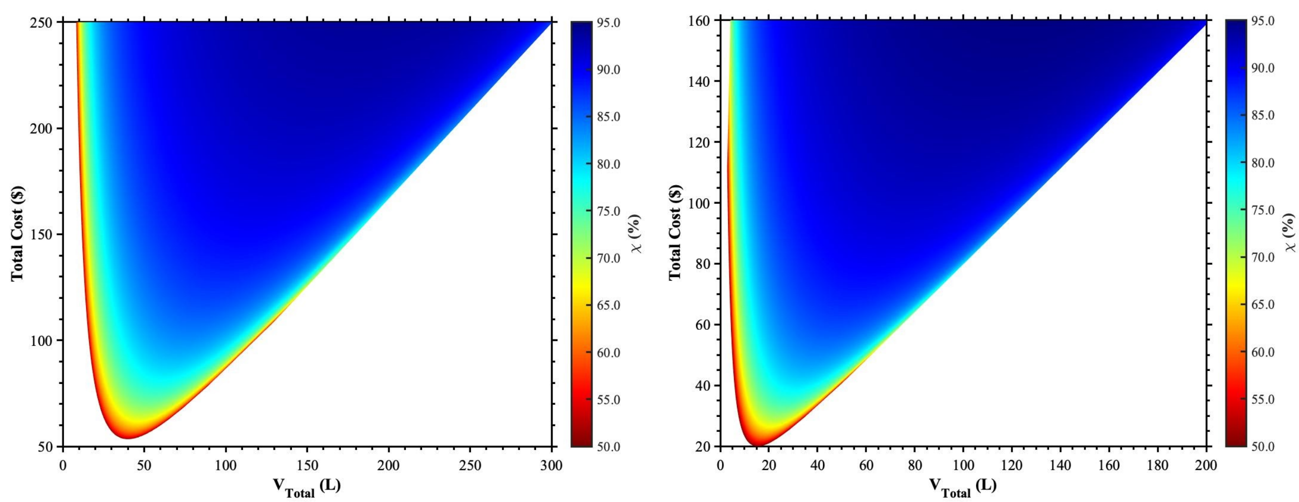

Figure 1. Total operating cost as a function of total volume for varying stage efficiency for single-stage mass contactor (left) and two-stage mass contactor (right).

Analyzing the above plots, both single and two-stage systems have the highest separation efficiencies at high system volume and high running costs. This prediction makes intuitive sense, since running cost is largely dependent on the power input into the system, where more power leads to increased interfacial area for mass transfer, and as a result higher separation efficiency. There is a balance with this though, since at lower separation efficiencies more TCE is required to achieve similar efficiencies to higher power systems, leading to an increased cost for TCE. While the cost for the TCE stream is relatively small, it is still an important factor when evaluating optimal design.

Comparing single and two-stage systems, they exhibit similar trends to one another, although two-stage systems can achieve the same efficiencies at lower system volumes as compared to single-stage systems. This makes sense as the waste stream is being treated in two different contactors, allowing more time for the stream to be purified and come into contact with TCE. Operational costs are also decreased since less TCE is required in a two-stage system. Increasing the amount of stages would then seem the ideal solution, however capital cost is an important factor to consider when designing systems like these. Two-stage systems have a higher capital cost, and there may be an initial time period where it is more cost effective to install a single-stage system. Although, after this initial time period, the two-stage or multi-stage contactor would become more cost effective in purifying the wastewater stream. A more in-depth cost analysis would be warranted if implementation of this design were to occur.

A sample calculation for a single stage contactor is included in **Appendix B** for reference. The contour plots above show the results of many different system combinations, and the appendix highlights the specifications for one system in the single-stage contactor design. If specific parameters are warranted, the same process can be completed for an array of different designs and output the specific parameters for each system being studied. While no optimal design is suggested in this report, it is left up to the reader to define what optimum design is best for each specific application. By specifying certain parameters such as separation efficiency and system volume, the resulting parameters and operational costs can be found and applied to fully design the system in question.

Conclusions & Recommendations

From the above analysis, it is evident that there are a range of design systems that can be implemented based on desired system size and operational costs. If considering two-stage systems, capital cost is also an important consideration for implementation. For further analysis, specific systems should be analyzed on whether they are viable for industrial scaling and usage. Furthermore, understanding the limitations of the above analysis is important, and further iterations of this study should include a more in-depth look at the mass transfer coefficient k_m. While treated as constant, correlative methods should be used in future analysis to more accurately depict the system being operated, as the amount of agitation in the system will influence its value. Higher amounts of agitation increases its value, while lowering agitation will lower k_m. Further analysis of this phenomena is recommended for future study of these system designs.

References

[1] T. W. F., Russel, et al. *Mass and Heat Transfer: Analysis of Mass Contactors and Heat Exchangers*. Cambridge University Press, 2008, doi:10.1017/CBO9780511810701.

[2] "Appendix D: Capital Cost Guidelines." *Rules of Thumb in Engineering Practice*, by Donald R. Woods, Wiley-VCH, 2008, pp. 376–436.

[3] "Trichloroethylene | 79–01-6." *Chemical Book*, 2017, www.chemicalbook.com/ChemicalProductProperty_EN_CB5406573.htm.

[4] "Water - Density, Specific Weight and Thermal Expansion Coefficient." *The Engineering Toolbox*, 2003, www.engineeringtoolbox.com/water-density-specific-weight-d_595.html.

Appendix A: Nomenclature

Table A1. List of relevant parameters

Parameter	***Definition***	***Value***
C^{I}_{AF}	Acetone concentration in phase I feed	$0\ \frac{g}{L}$
C^{II}_{AF}	Acetone concentration in phase II feed	$35\ \frac{g}{L}$
$C^{II}_{A,\,goal}$	Acetone concentration in phase II exit	$3\ \frac{g}{L}$
q^{II}	Volumetric flow rate of phase II	$250\ \frac{L}{min}$
K_M	Mass transfer coefficient	$3 \times 10^{-5}\ \frac{m}{s}$
M	Distribution coefficient	2
C_{power}	Cost of power	$\frac{\$0.12}{kW \cdot h}$
C_{TCE}	Cost of TCE	$\frac{\$0.1}{kg}$
C_{volume}	Cost of mass contactor volume	$\frac{\$680}{m^3}$ [2]
ϱ^{I}	Density of phase I	$1463\ \frac{g}{L}$ [3]
ϱ^{II}	Density of phase II	$997.05\ \frac{g}{L}$ [4]

I: Continuous phase/TCE
II: Dispersed phase/Water
A: Acetone

Appendix B: Sample Calculation (Single Stage)

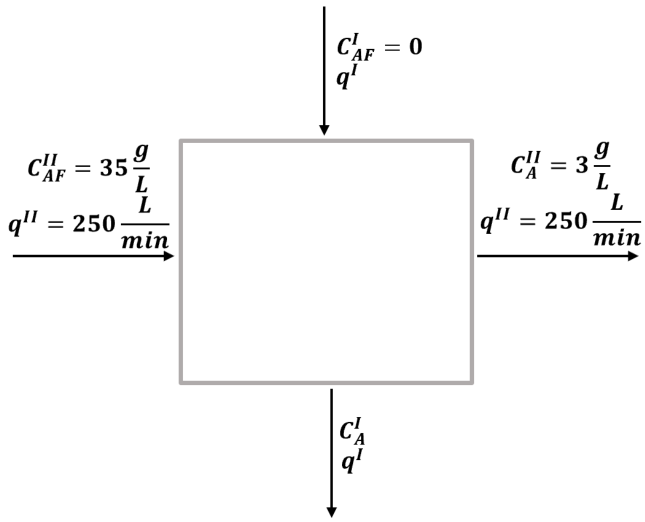

Figure B1. Single stage mass contactor schematic diagram

Using the values in Table A1

$$m_{load} =-(q^{II}C^{II}_{A,goal} - q^{II}_{F}C^{II}_{AF}) = 8000\ \frac{g}{min}$$

$$q^{I}_{min} = q^{II}\left(\frac{C^{II}_{AF}-C^{II}_{A}}{MC^{II}_{A}-C^{I}_{AF}}\right) = 1333\ \frac{L}{min}$$

Choosing $\chi = 0.90$

$$q^{I} \approx \frac{q^{I}_{min}}{0.90} = 1481\ \frac{L}{min}$$

$$\lambda = \frac{q^{II}}{q^{I}}$$

At equilibrium,

$$C^{II}_{A,eq} = \frac{C^{I}_{AF} + \lambda C^{II}_{AF}}{\lambda + M} = 2.72\frac{g}{L}$$

$$\chi = \frac{C^{I}_{A} - C^{I}_{AF}}{C^{I}_{A,eq} - C^{I}_{AF}} = \frac{C^{II}_{AF} - C^{II}_{A}}{C^{II}_{AF} - C^{II}_{A,eq}}$$

Rearranging χ,

$$C^{II}_{A} = C^{II}_{AF} - \chi(C^{II}_{AF} - C^{II}_{A,eq})$$

$$C^{I}_{A} = C^{I}_{AF} + \chi(C^{I}_{A,eq} - C^{I}_{AF})$$

$$< \Delta C^{I-II}_{A} >=-(C^{I}_{A} - MC^{II}_{A}) = 7\ \frac{g}{L}$$

This gives an interfacial area of

$$a = \frac{m_{load}}{K_m \langle \Delta C_A^{I-II} \rangle} = 634.92\ m^2$$

Next, a diameter has to be selected from **Figure 7.3**

$$d_{max} = 75\ \mu m$$

which corresponds to a power per mass of fluid of $10^3 \frac{W}{kg}$. Employing this diameter value in **Eq. 7** yields a volume value of

$$V^{II} = \frac{1}{6}(ad) = 7.94\ L$$

Since $\tau^I = \tau^{II}$,

$$V^I = \frac{V^{II}}{\lambda} = 47.03\ L$$

Therefore, the total volume of the tank is

$$V = V^I + V^{II} = 54.97\ L$$

Cost Analysis

From **Figure 7.3**, it was found that in order to attain particles with a diameter of $75\ \mu m$, the power input per mass of fluid must be $10^3 \frac{W}{kg}$. The total mass of fluid can be calculated as follows:

$$m_f = \varrho^I V^I + \varrho^{II} V^{II} = 76.72\ kg$$
$$P = 76.72\ kW$$

To calculate the total power cost, assume the system is operating for a full day, or 24 hours:

$$Total\ Power\ Cost = P \times C_{power} \times 24 = \$2210$$

Next, the cost of total TCE was accounted for using the following equation:

$$Total\ TCE\ Cost = \varrho^I V^I C_{TCE} = \$6.88$$

Then, the capital cost of setting up the reactor tank is as following:

$$Total\ Volume\ Cost = V \times C_{volume} = \$37.38$$

Therefore, the total cost of operating the unit comes out to

$$Total\ Cost = Total\ Power\ Cost + Total\ TCE\ Cost + Total\ Volume\ Cost = \$2254$$

Appendix C: Sample Calculation (Multi-stage - Two Stage)

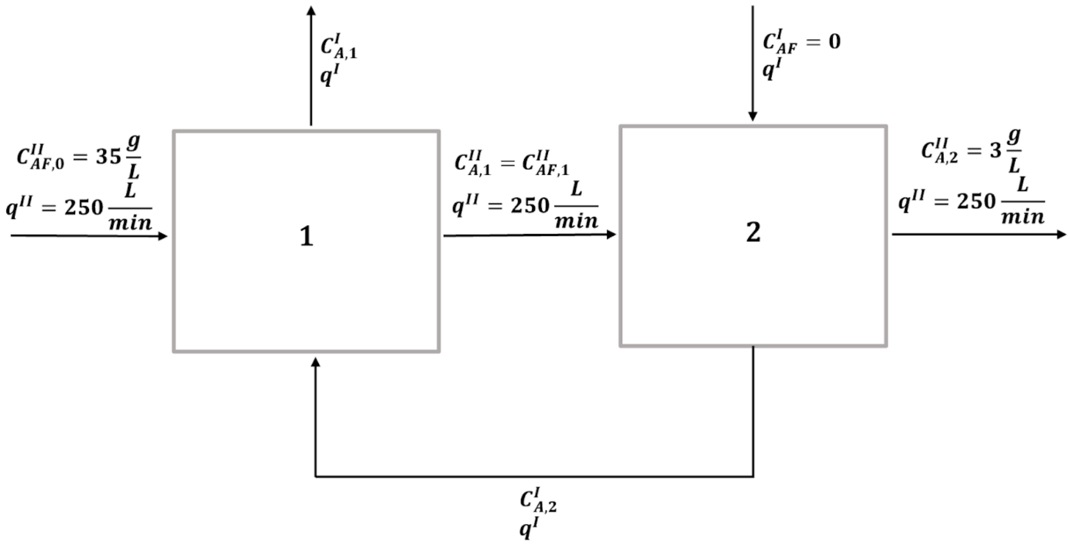

Figure C1. Two stage mass contactor schematic diagram

Using the values in Table A1

$$m_{load,1} = -(q^{II}C^{II}_{A,1\ eq} - q^{II}_{F}C^{II}_{AF,0}) = 5897\ \frac{g}{min}$$
$$m_{load,2} = -(q^{II}C^{II}_{A,goal} - q^{II}_{F}C^{II}_{A1,eq}) = 2103\ \frac{g}{min}$$
$$q^{I}_{min} = q^{II}\left(\frac{C^{II}_{AF}-C^{II}_{A}}{MC^{II}_{A}-C^{I}_{AF}}\right) = 350.50\ \frac{L}{min}$$

Choosing $\chi = 0.90$

$$q^{I} \approx \frac{q^{I}_{min}}{0.90} = 389.45\ \frac{L}{min}$$
$$\lambda = \frac{q^{II}}{q^{I}}$$

At equilibrium,

$$C^{II}_{A2,eq} = \frac{\frac{C^{I}_{AF}}{\lambda+M} + \frac{\lambda^{2}C^{II}_{AF,0}}{(\lambda+M)^{2}}}{1-\frac{\lambda\cdot M}{(\lambda+M)^{2}}} = 2.532\ \frac{g}{L}$$
$$C^{I}_{A2,eq} = MC^{II}_{A2,eq} = 5.064\ \frac{g}{L}$$
$$C^{II}_{A1,eq} = \frac{C^{I}_{A2,eq} + \lambda C^{II}_{AF,0}}{\lambda + M} = 10.42\ \frac{g}{L}$$
$$C^{I}_{A1,eq} = MC^{II}_{A1,eq} = 20.84\ \frac{g}{L}$$

$$\chi_{1} = \frac{C^{I}_{A1} - C^{I}_{A2}}{C^{I}_{A1,eq} - C^{I}_{A2}} = \frac{C^{II}_{AF,0} - C^{II}_{A1}}{C^{II}_{A0} - C^{II}_{A1,eq}}$$

$$\chi_2 = \frac{C^I_{A2} - C^I_{AF}}{C^I_{A2,eq} - C^I_{AF}} = \frac{C^{II}_{A1} - C^{II}_{A2}}{C^{II}_{A1} - C^{II}_{A2,eq}}$$

Rearranging χ_1 and χ_2,

$$C^I_{A1} = C^I_{A2} + \chi_1(C^I_{A1,eq} - C^I_{A2})$$
$$C^{II}_{A1} = C^{II}_{AF,0} - \chi_1(C^{II}_{AF,0} - C^{II}_{A1,eq})$$
$$C^I_{A2} = C^I_{AF} + \chi_2(C^I_{A2,eq} - C^I_{AF})$$
$$C^{II}_{A2} = C^{II}_{A1} - \chi_2(C^{II}_{A1} - C^{II}_{A2,eq})$$

$$< \Delta C^{I-II}_A >_1 = -(C^I_{A1} - MC^{II}_{A1}) = 6.54\ \tfrac{g}{L}$$
$$< \Delta C^{I-II}_A >_2 = -(C^I_{A2} - MC^{II}_{A2}) = 2.58\ \tfrac{g}{L}$$

This gives an interfacial area of

$$a_1 = \frac{m_{load,1}}{K_m < \Delta C^{I-II}_A >_1} = 500.61\ m^2$$
$$a_2 = \frac{m_{load,2}}{K_m < \Delta C^{I-II}_A >_2} = 453.59\ m^2$$

Next, a diameter has to be selected from **Figure 7.3**

$$d_{max} = 75\ \mu m$$

which corresponds to a power per mass of fluid of $10^3\ \frac{W}{kg}$. Employing this diameter value in **Eq. 7** yields a volume value of

$$V^{II}_1 = \tfrac{1}{6}(a_1 d) = 6.258\ L$$
$$V^{II}_2 = \tfrac{1}{6}(a_2 d) = 5.670\ L$$

Since $\tau^I = \tau^{II}$,

$$V^I_1 = \frac{V^{II}_1}{\lambda} = 9.749\ L$$
$$V^I_2 = \frac{V^{II}_2}{\lambda} = 8.833\ L$$

Therefore, the total volume of the tank is

$$V = V^I_1 + V^{II}_1 + V^I_2 + V^{II}_2 = 30.51\ L$$

Cost Analysis

From **Figure 7.3**, it was found that in order to attain particles with a diameter of 75 μm, the power input per mass of fluid must be $10^3 \frac{W}{kg}$. The total mass of fluid can be calculated as follows:

$$m_{f1} = \varrho^I V_1^I + \varrho^{II} V_1^{II} = 20.50\ kg$$
$$m_{f2} = \varrho^I V_2^I + \varrho^{II} V_2^{II} = 18.58\ kg$$
$$P_1 = 20.50\ kW$$
$$P_2 = 18.58\ kW$$

To calculate the total power cost, assume the system is operating for a full day, or 24 hours:

$$Total\ Power\ Cost\ = (P_1 + P_2) \times C_{power} \times 24 = \$112.54$$

Next, the cost of total TCE was accounted for using the following equation:

$$Total\ TCE\ Cost = (V_1^I + V_2^I) \times \varrho^I C_{TCE} = \$2.72$$

Then, the capital cost of setting up the reactor tank is as following:

$$Total\ Volume\ Cost\ = V \times C_{volume} = \$20.75$$

Therefore, the total cost of operating the unit comes out to

$$Total\ Cost\ = Total\ Power\ Cost\ + Total\ TCE\ Cost\ + Total\ Volume\ Cost = \$136$$

Appendix D: MATLAB Codes

The Matlab code used to generate the plots and carry out the calculations can be found here.