

Appendix D - UNIVERSITY HONORS PROGRAM
SENIOR PROJECT - APPROVAL

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PROJECT TITLE: Mathematical Modeling and Computer
Simulation of a Gas Stripping Tower

I have reviewed this completed senior honors thesis with this student and certify that it is a project commensurate with honors level undergraduate research in this field.

Signed: Tse-Wer Wang, Faculty Mentor
Date: May 8, 2000

Comments (Optional):

Tim did a good job in the project, discovering
some insight in understanding the problem and its solution
JZW.

**Mathematical Modeling and Computer Simulation of a Gas Stripping
Tower**

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ABSTRACT

Mathematical Analysis and Computer Simulation of a Gas Stripping Tower

Separation technology is a huge field in chemical engineering. Suppose that a gas stream from a process contains an unwanted component. One way to remove that component is through a gas stripping tower. In this process, the undesirable component dissolves from the gas to a liquid solvent. The solvent might also react with the undesirable component.

The goal of this project was to carry out a mass balance of a gas stripping tower to produce partial differential equations describing the system, to solve those equations, and to use computer simulation to determine the sensitivity of the model to changes in the model parameters. Both the case involving a non-reactive solvent and a reactive solvent were studied.

A mass component balance on the system yielded partial differential equations that describe the concentration profile of this system as it moves down the tower. The method of combination was used to solve these partial differential equations. These equations depended upon the location in the tower, the diffusion coefficient, the velocity of the solvent, and the reaction rate constant (in the case of the reactive solvent).

The concentration profiles for a range of values of the model parameters was constructed using the mathematical software MATLAB®. From this information, the behavior of the system with and without reaction was plotted into graphical form and analyzed. The sensitivity of the model to various system parameters was studied, and the difference in mass flux between the non-reactive solvent and the reactive solvent was measured.

If this information were to be used in an industrial setting, the above equations could be used to optimize the tower size, the type of solvent to be used, the flow rate of the solvent, and other system parameters.

BACKGROUND

A gas stripping tower is a device for removing an undesired component from a gas stream. The gas flows down the tower, and a liquid solvent also flows down the walls of the tower. A fraction of the undesired gas component dissolves into the liquid solvent stream and leaves the tower in the liquid. Special care must be given to the choice of a solvent, as the rate of diffusion of the undesired component into the solvent determines the degree to which the undesirable component will be removed from the gas stream. If the solvent reacts with the undesirable component, then attention must also be given to the rate of reaction for the solvent being studied. The higher the rate of reaction, the faster the undesired component is reacted away and the higher the rate of diffusion of the undesired component from the gas to the solvent.

This project deals with the mathematical modeling of a gas stripping tower and sensitivity analysis of absorptivity to model parameters in such a tower. First, a mass balance on the tower will be used to generate partial differential equations. These equations will then be solved analytically to gain a concentration profile for the tower. Using this model, a computer simulation will then generate plots of the concentration profile as a function position in the tower parameterized by system variables. This will give an indication of the sensitivity of the concentration to changes in system parameters. Finally, the differential absorption of the undesirable component with and without a reaction in the solvent will be analyzed.

Mass Balance

To obtain the differential equations necessary for the analysis, a mass component balance on the concentration of the component in the solvent was first performed. Figure 1 depicts the gas stripping tower diagram close up, with the gas layer, the liquid solvent film, and the tower wall.

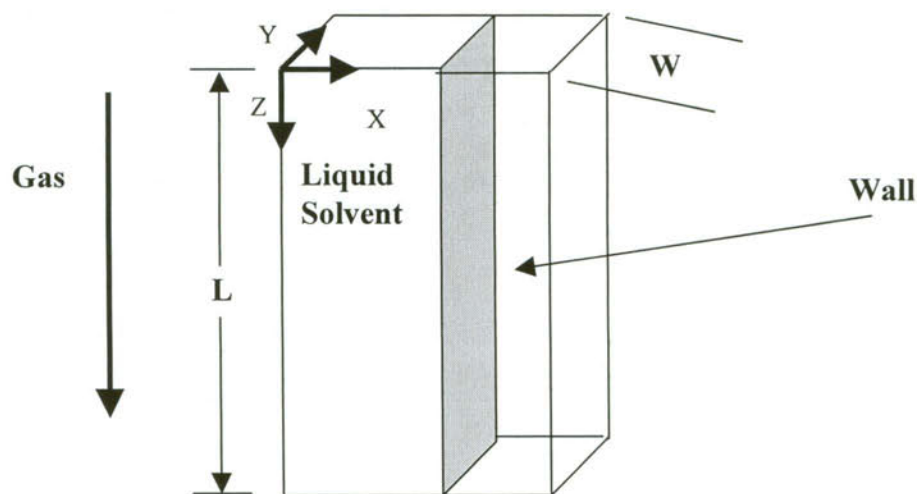


Figure 1: Gas Layer, Liquid Solvent Layer, and Tower Wall

First, an elemental volume is established over which the mass balance is made. This would be the intersection of slabs of thickness ΔX and ΔZ . The mass balance is then

$$N_{Az}|_z W\Delta x - N_{Az}|_{z+\Delta z} W\Delta x + N_{Ax}|_x W\Delta z - N_{Ax}|_{x+\Delta x} W\Delta z = 0 \quad (1)$$

where N is the molar flux of A in the specified direction, W is the width of the film, z is the vertical direction, and x is the horizontal direction (as indicated in Figure 1). If Equation 1 is divided by $W\Delta x\Delta z$ on both sides,

$$\frac{N_{Az}|_{z+\Delta z} - N_{Az}|_z}{\Delta z} + \frac{N_{Ax}|_{x+\Delta x} - N_{Ax}|_x}{\Delta x} = 0 \quad (2)$$

Now if this equation is considered in the limit where Δx and Δz go to zero, Equation 2 becomes

$$\frac{\partial N_{Az}}{\partial z} + \frac{\partial N_{Ax}}{\partial x} = 0 \quad (3)$$

The equation for mass flux indicates that

$$N_{Az} = -D_{AB} \frac{\partial c_A}{\partial z} + x_A (N_{Az} + N_{Bz}) \approx c_A v_z \quad (4)$$

where D_{AB} is the diffusion coefficient, c_A is the concentration of component A , v_z is the velocity of the solvent in the z direction, and x_A is the molar fraction of A . This approximation is good because the D_{AB} term is negligible, as the effect of fluid motion is much greater than diffusion in the z direction. Similarly, for molar flux in the x direction,

$$N_{Ax} = -D_{AB} \frac{\partial c_A}{\partial x} + x_A (N_{Az} + N_{Bz}) \approx -D_{AB} \frac{\partial c_A}{\partial x} \quad (5)$$

The above approximation can be made since the motion of A is primarily by diffusion—the fluid motion can be neglected. Substituting Equations 4 and 5 into Equation 3 gives

$$v_z \frac{\partial c_A}{\partial z} = D_{AB} \frac{\partial^2 c_A}{\partial x^2} \quad (6)$$

If the velocity of the fluid is assumed to be uniform at the value $v_{\max}$, then

$$v_{\max} \frac{\partial c_A}{\partial z} = D_{AB} \frac{\partial^2 c_A}{\partial x^2} \quad (7)$$

The assumption of uniform velocity $v_{\max}$ is justifiable because it is assumed that the component does not penetrate very far into the film (short contact time). This partial differential equation can now be solved to give the concentration profile as a function of x and z in the tower. The method of combination is used to solve this partial differential equation. That solution is not outlined here. The detailed solution of the equation is given in Appendix A. The final form of the equation describing the concentration profile is

$$\frac{c_A}{c_{A0}} = \operatorname{erfc} \left(\frac{x}{\sqrt{4zD_{AB}/v_{\max}}} \right) \quad (8)$$

where c_{A0} is the concentration of the undesirable component in the gas stream, and erfc is the complement of the error function, the values of which are given in mathematical tables. The error function is given by

$$\operatorname{erf}(n) = \frac{2}{\sqrt{\pi}} \int_0^n e^{-n^2} dn \quad (9)$$

The boundary conditions used in the solution are

1. At $z=0$, $c_A=0$ (Inlet to tower, so concentration has not changed)
2. At $x=0$, $c_A=c_{A0}$ (At gas-liquid interface, concentration is the same)
3. At $x=\infty$, $c_A=0$ (Gas does not penetrate very far into the solvent)

With Reaction

Now the special case can be considered where the solvent reacts with the undesired component to neutralize that component (i.e., the solvent “eats up” some of the undesired component). The change in the mass balance will simply be the rate of reaction between the solvent and undesired component. For a first order, irreversible reaction, this is given by

$$-r_A = kc_A \quad (10)$$

where k is the specific reaction rate constant. Inserting this into Equation 7 gives

$$v_{\max} \frac{\partial c_A}{\partial z} = D_{AB} \frac{\partial^2 c_A}{\partial x^2} - kc_A \quad (11)$$

After some manipulations, Equation 11 can also be solved. The details of that solution are not given here, but are outlined in Appendix A. The final solution of the case with reaction is

$$\frac{c_A}{c_{A0}} = \left(e^{-\left(\frac{k}{v_{\max}}\right)} \right) \operatorname{erfc} \left(\frac{x}{\sqrt{4zD_{AB}/v_{\max}}} \right) \quad (12)$$

The same boundary conditions apply as with the case without reaction. However, some modifications must be made to accommodate the changes in variables required to perform the solution. Note that the exponential term will always be between 0 and 1. This means that the concentration in the case with reaction will always be less than the case without reaction. Because the concentration is lower in the case with reaction, the driving force for diffusion from gas to liquid is greater, and thus the case with a reactive solvent will have a higher mass flux.

To find the total mass flux in both cases, it is necessary to first differentiate concentration with respect to x and then evaluate that derivative at $x=0$. For the case without reaction,

$$\left. \frac{\partial c_A}{\partial x} \right|_{x=0} = -\frac{2c_{A0}}{\sqrt{\pi}} \left(e^{-\left(\frac{x}{\sqrt{4D_{AB}z/v_{\max}}}\right)^2} \right) \left(\frac{1}{\sqrt{\frac{4D_{AB}z}{v_{\max}}}} \right) = -\frac{2c_{A0}}{\sqrt{\pi}} \left(\frac{1}{\sqrt{\frac{4D_{AB}z}{v_{\max}}}} \right) \quad (13)$$

Then Equation 13 must be summed over the entire height of the tower by integrating with respect to z from 0 to L and multiplying by the width of the plate W :

$$\text{MassFlux} = \frac{2c_{A0}WD_{AB}}{\sqrt{\pi}} \int_0^L \left(\frac{4D_{AB}z}{v_{\max}} \right)^{-1/2} dz = \frac{c_{A0}Wv_{\max}}{\sqrt{\pi}} \left(\frac{4D_{AB}L}{v_{\max}} \right)^{1/2} \quad (14)$$

For the case with reaction, the analysis is very similar, with a slightly different result:

$$\text{MassFlux} = \frac{c_{A0}Wv_{\max}}{\sqrt{\pi}} \left(e^{k/v_{\max}} \right) \left(\frac{4D_{AB}L}{v_{\max}} \right)^{1/2} \quad (15)$$

Note that in the limiting case of $k=0$ (which would be the same as no reaction), Equation 15 is the same as Equation 14.

NUMERICAL METHODS

Equations 9 and 11 describe the concentration profile of the undesired component in the liquid solvent. These equations are then simulated using the mathematical computer program MATLAB®. The MATLAB codes used in generating the plots are attached in Appendix B.

MATLAB is a very useful program for engineers. It can work with algebraic equations, perform numerical integration, and numerically solve both ordinary and partial differential equations. An area of future study for this project might be to compare the values produced by the solved equations to the values that would be generated by numerically solving the equations using the PDE toolbox.

RESULTS AND DISCUSSION

As discussed previously, MATLAB was used to perform the simulation of the concentration profile in the liquid phase as a function of several system parameters. Figure 2 shows dimensionless concentration as a function of x for several values of z for both the reactive solvent and non-reactive solvent.

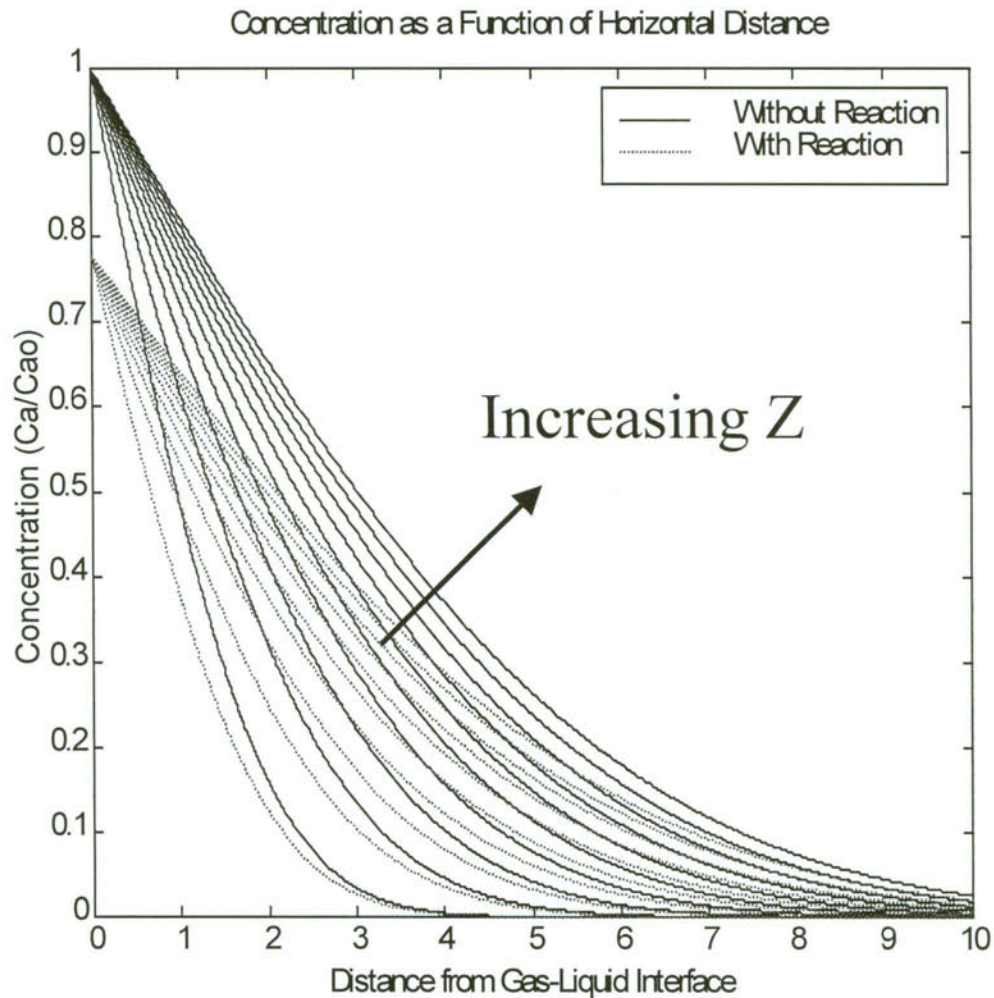


Figure 2: Concentration as a Function of x for Several z

Note that the concentration decreases most steeply nearest the gas-liquid interface. Also notice that the difference between the non-reactive solvent and the reactive solvent is greatest near the interface. This is because the concentration is higher at the interface, resulting in a higher rate of reaction and thus more undesirable component eaten away by reaction. As z increases, the concentration gradient is less steep because the material from the top of the tower has collected and flowed to the bottom of the tower, resulting in further penetration of the undesirable component into the solvent. Also, as z increases,

the effect of increasing z becomes less noticeable. Thus, the change of concentration with respect to x decreases with increasing z .

Figure 3 shows concentration as a function of z for several x .

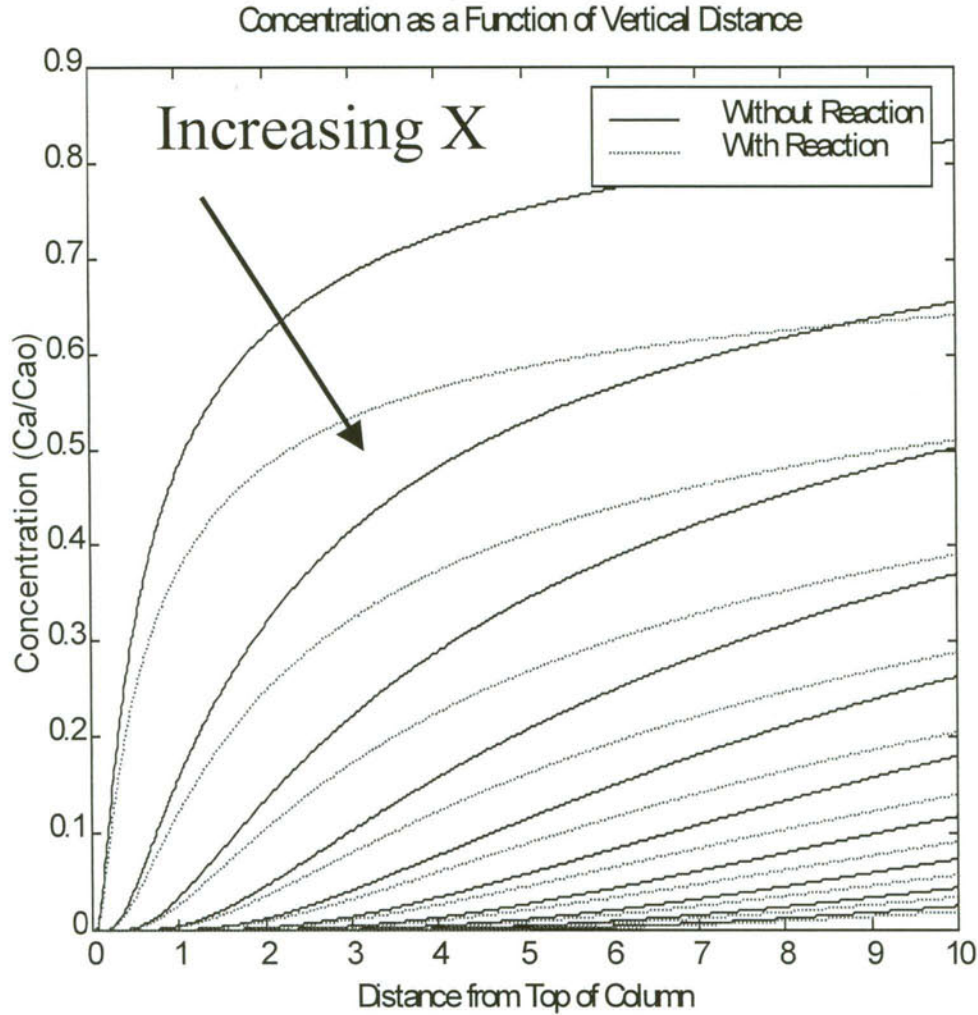


Figure 3: Concentration as a Function of z for Several x

Note that the concentration profile as a function of z resembles half of a Gaussian distribution curve. This can be attributed to the resemblance in form of the error function to the Gaussian distribution. As z increases (as one moves further down the tower), the concentration increases, but the rate of that increase decreases with increasing z . Also, the difference between the non-reactive solvent and reactive solvent increases as z increases. This is because the concentration increases down the tower, making the reactive solvent more effective. As x increases, the reactive solvent behaves closer to the non-reactive solvent because the concentration is very low at deeper penetration. Thus,

the concentration is diffusion-limited. Also, as x increases, the sensitivity of the concentration profile to z decreases.

Figure 4 shows a three-dimensional plot depicting concentration as a function of x and z . Note that the axes are configured to mimic the physical setup of the tower.

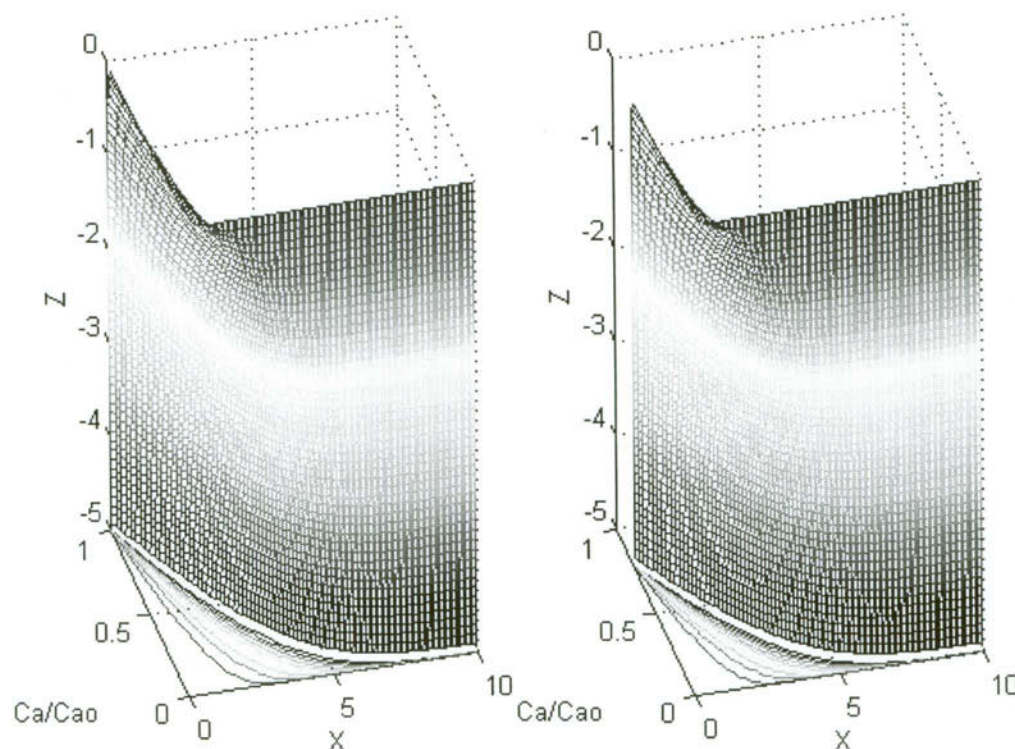


Figure 4: Three-Dimensional Representation of Concentration Profile as a Function of x and z (Reactive Solvent on Right)

Of course, these plots follow the trends shown in Figures 2 and 3. This three-dimensional view is just a way to visualize the concentration profile in the proper orientation, mimicking the orientation of the physical layout.

Finally, the mass flux was calculated to compare the performance of the non-reactive solvent against that of the reactive solvent. The mass flux was calculated over a range of values of the reaction rate constant for the reactive solvent. Figure 5 shows the difference between the use of a non-reactive and reactive solvent.

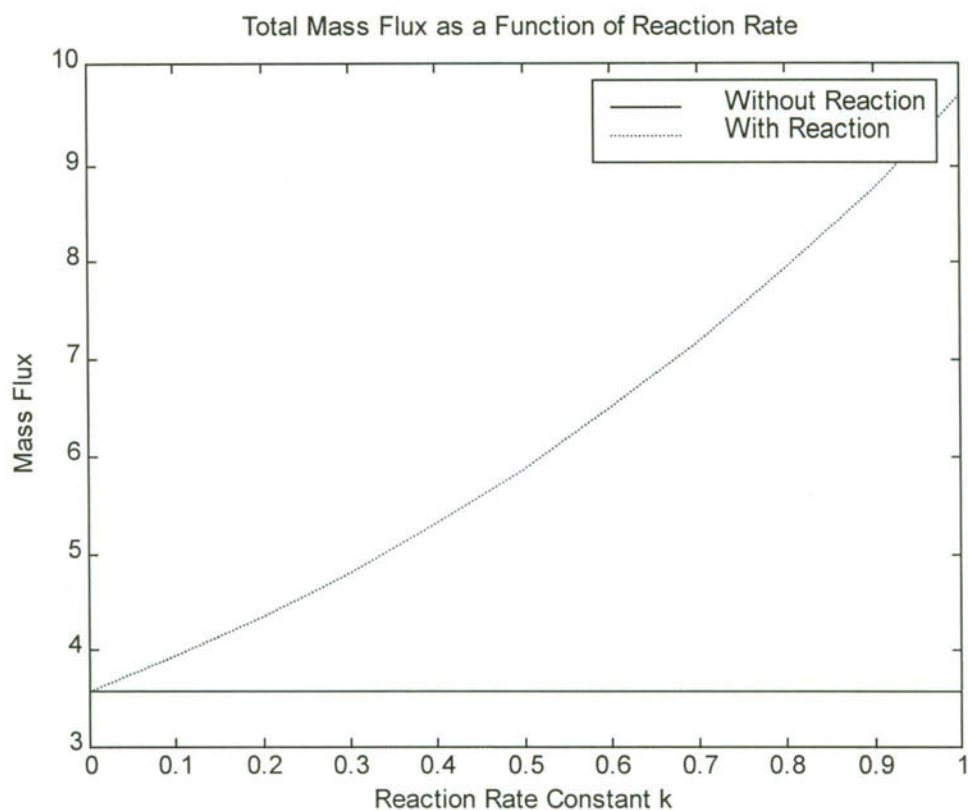


Figure 5: Comparison of Mass Fluxes with and without Reaction

As seen in the plot, the reactive solvent becomes more effective with higher reaction rates. This is because as more of the undesirable component is reacted away, the diffusion driving force between the gas and solvent becomes higher, thus allowing a higher rate of diffusion.

CONCLUSIONS

The kinetics of diffusion of an undesired component from a gas stream into a solvent in a gas stripping tower was the focus of this project. Two general cases were considered—the case with a non-reactive solvent, and the case with a solvent that reacts with the undesired gas component (first order, irreversible reaction).

The reaction certainly has an effect on the concentration profile and thus the rate of removal of the component from the gas stream. However, without specific numbers, the extent of this difference is not known (i.e., it would be specific to each case).

In general, the concentration decreases as one progresses further into the liquid phase. This is because the diffusion does not penetrate far into the film. In other words, the concentration becomes zero at some depth of penetration into the liquid. Also, the concentration increases as one progresses further down the tower. This is because the concentration deeper down the tower reflects the cumulative absorption of the component starting from the time when the liquid element first started out at the top of the tower.

With a reactive solvent, it is more effective when the concentration is higher. This is because the reaction rate increases with increasing concentration. Also, the mass flux increases with increasing reaction rate because the reactive solvent consumes some of the component, thus increasing the concentration difference at the interface (driving force). This enhances the absorption of more of the component into the liquid.

Results show several potential applications in industry. The equations developed here can be used as design equations in the design of a gas stripping tower. The equations could aid in the selection of solvent, tower size, and other tower parameters. The equations could also be used to optimize current conditions, knowing the specific values of the system parameters. Also, an economic comparison could be made for a real system to determine the incentive for investing in a reactive solvent. For some systems, a reactive solvent might be worth the extra cost, while in other systems that expenditure might not be warranted.

The process involved in carrying out this project was also very useful. This project was an illustration of the use of a few assumptions to simplify the solution of an otherwise very complex problem. It was also a good exercise in applying mathematical and differential equation solving skills.

Works Consulted

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Jaeger, J. and Carslaw. *Operational Methods*. Melbourne, 1941.

Pratap, Rudra. *Getting Started with MATLAB: A Quick Introduction for Scientists and Engineers*. New York: Saunders College Publishing, 1996.

Appendix A: Partial Diff. Solution

Without Reaction

From mass balance,

$$v_{\max} \frac{\partial C_A}{\partial z} = D_{AB} \frac{\partial^2 C_A}{\partial x^2}$$

Boundary conditions,

at $z=0$, $C_A=0$ (inlet to tower)

at $x=0$, $C_A=C_{A0}$ (at liquid-gas interface, concentration is same as gas)

at $x=\infty$, $C_A=0$ (short penetration into film)

Combination of variables - assume solution

$$\frac{C_A}{C_{A0}} = \phi(n)$$

and assume that

$$n = \frac{x}{\sqrt{4D_{AB}z/v_{\max}}}$$

$$\frac{\partial \phi}{\partial z} = \phi' \cdot \frac{-x}{2} \left(\frac{4D_{AB}z}{v_{\max}} \right)^{-3/2} \left(\frac{4D}{v_{\max}} \right)$$

$$= \phi' \cdot \frac{-x}{2} \left(\frac{1}{\sqrt{\frac{4Dz}{v_{\max}}}} \right)^3 \left(\frac{4D}{v_{\max}} \right)$$

$$= -\frac{\phi'}{2} n \left(\frac{4D}{v_{\max}} \right) \left(\frac{1}{\frac{4Dz}{v_{\max}}} \right)$$

$$= -\frac{\phi'}{2} n \left(\frac{1}{z} \right)$$

$$\frac{\partial^2(\phi)}{\partial x^2} = \phi''$$

Now substituting,

$$\phi'' + 2n\phi' = 0$$

Boundary conditions

$$\text{at } n=0, \phi=1$$

$$\text{at } n=\infty, \phi=0$$

Now replace

$$\psi = \phi' = C_1 e^{-n^2}$$

Integrating

$$\phi = C_1 \int_0^n e^{-n^2} dn + C_2$$

Application of boundary conditions,

$$\phi = 1 - \frac{\int_0^n e^{-n^2} dn}{\int_0^\infty e^{-n^2} dn} = 1 - \text{erf}(n)$$

$$\phi = \frac{C_A}{C_{A0}} = 1 - \text{erf}\left(\frac{x}{\sqrt{4Dz/v_{\text{max}}}}\right)$$

$$\boxed{\frac{C_A}{C_{A0}} = \text{erfc}\left(\frac{x}{\sqrt{4Dz/v_{\text{max}}}}\right)}$$

With Reaction

From mass balance,

$$v_{\text{max}} \frac{\partial C_A}{\partial z} = D \frac{\partial^2 C_A}{\partial x^2} - K C_A$$

$$\frac{\partial C_A}{\partial z} = A \frac{\partial^2 C_A}{\partial x^2} - B C_A$$

$$A = \frac{D}{v_{\text{max}}}$$

$$B = \frac{K}{v_{\text{max}}}$$

K = specific reaction rate constant

Now define

$$C_A^* = C_A e^{-\gamma z}$$

Assume solution

$$C_A^* = C_1 e^{-Bz} \operatorname{erf}(n) + C_2 e^{-Bz}$$

Boundary conditions:

$$\text{at } z=0, C_A=0, C_A^*=0$$

$$\text{at } x=0, C_A=C_{A0}, C_A^*=C_{A0} e^{Bz}$$

$$\text{at } x=\infty, C_A=0, C_A^*=0$$

$$C_A^* = -C_{A0} e^{-Bz} \operatorname{erf}(n) + C_{A0} e^{-Bz}$$

$$= C_{A0} e^{-Bz} (1 - \operatorname{erf}(n))$$

$$\frac{C_A^*}{C_{A0}} = e^{-Bz} (1 - \operatorname{erf}(n))$$

$$\boxed{\frac{C_A^*}{C_{A0}} = \left(e^{-K/V_{max}} \right) \left(\operatorname{erfc} \left(\frac{x}{\sqrt{4Dz/V_{max}}} \right) \right)}$$

```

D=1;
vmax=1;
k=.25;
x=[.01:.01:10];
z=[1:1:10];

for i=1:10;
    c=1-erf(x./((4*D*z(i)/vmax)^(.5)));
    cr=c*exp(-k/vmax);
plot(x,c,x,cr,':')
hold on
xlabel('Distance from Gas-Liquid Interface')
ylabel('Concentration (Ca/Cao)')
title('Concentration as a Function of Horizontal Distance')
end
legend('Without Reaction','With Reaction')

```

```

D=1;
vmax=1;
k=.25;
x=[1:1:10];
z=[.01:.01:10];

for i=1:10;
    c=1-erf(x(i)./(4.*D.*z./vmax).^(.5));
    cr=c*exp(-k/vmax);
    plot(z,c,z,cr,':')
    hold on
    xlabel('Distance from Top of Column')
    ylabel('Concentration (Ca/Cao)')
    title('Concentration as a Function of Vertical Distance')
end
legend('Without Reaction','With Reaction')

```

```

D=1;
vmax=1;
k=.25;
x=[.01:.1:10];
z=[.01:.1:5];
[X,Z]=meshgrid(x,z);

c=1-erf(X./((4.*D.*Z./vmax).^5));
cr=c.*exp(-k/vmax);
subplot(1,2,1),meshc(X,c,-Z)
axis([0 10 0 1 -5 0])
view(-15,20)
xlabel('X')
ylabel('Z')
ylabel('Ca/Cao')

subplot(1,2,2),meshc(X,cr,-Z)
axis([0 10 0 1 -5 0])
view(-15,20)
xlabel('X')
ylabel('Z')
ylabel('Ca/Cao')

```



```

cao=1;
w=1;
vmax=1;
D=1;
L=10;
k=[0:.1:1];
for i=1:11
    flux(i)=cao*w*vmax*(pi^-.5)*(4*D*L/vmax)^.5;
end
rflux=(exp(k./vmax)).*cao.*w.*vmax.*(pi^-.5).*(4.*D.*L./vmax).^.5;
plot(k,flux,k,rflux,':')
title('Total Mass Flux as a Function of Reaction Rate')
xlabel('Reaction Rate Constant k')
ylabel('Mass Flux')
legend('Without Reaction','With Reaction')

```