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# Modeling Gas Absorption

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Project Number: WMC 4028

# Modeling Gas Absorption

A Major Qualifying Project Report

submitted to the Faculty

of the

WORCESTER POLYTECHNIC INSTITUTE

in partial fulfillment of the requirements for the

Degree of Bachelor of Science

by

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Date: April 24, 2008

Approved:

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**Professor William M. Clark, Project Advisor**

## **ABSTRACT**

This project sought to analyze the gas absorption process as an efficient way in which to remove pollutants, such as carbon dioxide from gas streams. The designed absorption lab for CM 4402 was used to collect data based on the change in composition throughout the column. The recorded and necessary calculated values were then used to create a simulation model using COMSOL Multiphysics, as a supplemental learning tool for students in CM 4402.

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## **INTRODUCTION**

Carbon dioxide emissions are abundant in numerous processes used in today's industry and pose a great threat to the surrounding environment and public health and safety. Carbon dioxide is a colorless, odorless gas, primarily produced when any form of carbon or carbon compound is burned in excess of oxygen. CO<sub>2</sub> emissions are a direct result of its natural abundance in the atmosphere as well as human activity. It is one of the most abundant gases in the atmosphere and plays an important role in vital plant processes, such as photosynthesis and respiration. CO<sub>2</sub> is also a popular commercial product, used in applications such as soft drinks, dry ice for creating stage fog, and safety measures in regards to blanketing fires. Some natural sources of carbon dioxide include: volcanic eruptions, decay of dead plant and animal matter, and breathing. However, although atmospheric carbon dioxide contributes to the growth and abundance of plant life as well as commercial utilization, the effects of increasing levels of CO<sub>2</sub> and other greenhouse gases are believed to generate more negative effects on the environment.

### **Anthropogenic Sources**

The amount of carbon dioxide released into the atmosphere has risen extensively in the last 150 years [5]. As a result of continuous combustion of fossil fuels, such as coal, oil, and natural gases, current levels have exceeded the amount sequestered in biomass, oceans, and carbon dioxide sinks, making up twenty-two percent of atmospheric concentrations [1]. According to the United States Department of Energy (DOE), the United States produced 1,161,444,000 short tons of coal and consumed 1,114,176 short tons in the year 2006 [7]. It is believed, that due to an increase in human processes which has led to an increase in greenhouse gases, the earth's climate is changing because of rising temperatures. This phenomenon, known as global warming, has become the forefront of environmental concern throughout the world. Although fossil fuel combustion provides an effective source of energy, the risks associated with the emissions resulted in the Environmental Protection Agency (EPA) proposing to set guidelines for acceptable amounts of hazardous substances in emissions; the ultimate goal and hope being to put limits on the acceptable amount of carbon dioxide that can be released in the air [2]. Another similar effort took place in November 2007, when 175 parties ratified the Kyoto Protocol, whose primary objective is to achieve "stabilization of greenhouse gas concentrations in the atmosphere at a level that would prevent dangerous anthropogenic interference with the climate system [1]."

Although environmental effects of atmospheric carbon dioxide are still being debated, there is evidence of some harmful effects to public health and safety. Being exposed to higher concentrations of CO<sub>2</sub> can affect respiratory function and cause excitation, followed by depression of the central nervous system. High concentrations of CO<sub>2</sub> can also displace oxygen in the air, resulting in lower oxygen concentrations, causing suffocation [1].

### **Finding a Solution**

Considering the previously mentioned effects of atmospheric carbon dioxide, investigations have begun on the most efficient ways in which to prevent continual increase as well as carbon dioxide removal and air purification techniques. One of the natural ways in which to remove carbon dioxide from the atmosphere is through a carbon dioxide “sink,” which is a carbon reservoir that increases in size. Primary natural sinks are oceans, plants, and other organisms that use photosynthesis to remove carbon from the atmosphere. Since the 1997 Kyoto Protocol, the use of carbon sinks has been increasingly allowed, by the parties who signed the treaty, in hopes of offsetting the increase of carbon dioxide.

Oceans, the largest active carbon sinks on Earth are driven by two processes: the solubility pump and the biological pump, both chemical processes that transport carbon from the ocean’s surface to its interior. At the present time, approximately one third of anthropogenic emissions are estimated to be entering the ocean [1]. The solubility pump is the primary mechanism driving this, with the biological pump playing a negligible role. Another natural alternative is the use forests, which are also considered to be carbon sinks when they are increasing in area. However, with constant deforestation, forest cannot be considered a major contributor to the cause until all available land has been reforested with mature forests.

In addition to natural solutions for removing carbon dioxide from the atmosphere, industrial methods have also been implemented. One of the most common being gas purification through the process of absorption. Currently, capture of carbon dioxide is performed on a large scale by absorption onto various amine-based solvents and is generally carried out in the chemical industry using packed towers, whereby a solute is transferred between a gas and a liquid phase. A liquid and a gas are contacted, and based on the solubility of the gas; components of it can be absorbed into the liquid [6].

In this lab we used pure liquid water as the desired solvent for the absorption of carbon dioxide from the packed column. Water was chosen due to its ability to effectively work for this

particular system, it's a cheaper, and it doesn't cause fast deterioration to the absorber equipment. However, in various industrial absorption processes, the use of amines, such as MEA (monoethanolamine), as solvents is very popular. In brief, flue gas streams and natural gas streams are bubbled through an amine solution and the CO<sub>2</sub> in these streams becomes bound to the amine groups in the solution. Consequently, the CO<sub>2</sub> content in the resulting gas stream is significantly reduced [9]. Although this process has been technologically proven through rigorous experimentation, some of the problems encountered in the system are degradation, corrosion, as well as expensive operational costs [10].

This report explains and illustrates the gas absorption process and tests its reliability as an efficient way in which to remove carbon dioxide from gas, specifically air, streams. The process is tested using the pilot scale absorption column in the Unit Operations Laboratory using the designed experiment for course CM4402. The acquired data is further analyzed through the model simulation program COMSOL Multiphysics that will be used as an additional learning tool for understanding the concepts of absorption.

## **BACKGROUND**

This study focused on the gas absorption process for gas purification, as an efficient way in which to remove carbon dioxide from air. Water was used as an absorbent for the recovery of CO<sub>2</sub> from a gas stream, containing CO<sub>2</sub> and air. Background research on the description of the absorption process, uses, and common absorbate/absorbent systems for carbon dioxide is presented. Additionally, a computer modeling program, COMSOL Multiphysics, was studied as an alternative to analyze and understand the fundamentals of absorption.

### **Applications and Uses of Gas Absorption**

Gas absorption is the unit operation in which one or more soluble components of a gas mixture are dissolved in a liquid. Gas absorption is the chief method for controlling industrial air pollution, and generally aims at separation of acidic impurities from mixed gas streams [3]. Impurities include carbon dioxide, hydrogen sulfide, and organic sulfur compounds, the most important being CO<sub>2</sub>. For both air pollution control and recovery of process gases, packed towers are one of the most common mass transfer devices in current use. They are used for control of soluble gases such as halide acids and to remove soluble organic compounds such as alcohols and aldehydes. When the scrubbing solution is charged with an oxidant such as sodium hypochlorite, they are used to control sulfide odors from wastewater treatment facilities and chemical plants. When gases and aerosols are both present, the packed tower is frequently used ahead of aerosol collectors such as fiber beds and wet electrostatic precipitators. Packed towers are even sometimes used as gas coolers and condensers [8].

### **Packed Tower Design**

Absorption equipment generally includes: stirred vessels, packed beds, and bubble columns. One of the most common and rapidly developing systems used to carry out the absorption process on an industrial scale is the packed tower. A packed tower is essentially a piece of pipe set on its end and filled with inert material or tower packing [3]. Generally, the packed tower operates in countercurrent flow, where the liquid enters the system through the top and wets the surfaces of the packing, and the gas stream mixed with the effluent enters the bottom. As the liquid and the gas are contacted with one another, the components of the effluent can be absorbed into the liquid.

Gas absorption in a countercurrent flow packed tower is dictated by the equilibrium conditions between the contaminant gas and the absorbing liquid. The overall controlling mechanisms are ruled by the solubility of the gas in the liquid and by any reactions that may be caused to occur in the liquid with the reacting chemical [6]. Diffusion is used to move the gas to the liquid surface and the overall gas/liquid equilibrium controls the design of the tower. Since the gas is absorbed at the liquid surface, the more liquid to gas interactions that can be caused to occur, the closer the exiting streams will approach equilibrium [3].

### **Packing Material**

The most important contributing factors in the probability of absorption is attributed to the tower packing. The packing material provides a large area of contact between the liquid and the solute-containing gas entering the bottom of the absorber. There are two primary types of packing, dumped (random) or structured packing. For this project, we will focus on random packing. Generally, random packing is made of cheap, inert materials such as clay, porcelain, or various plastics.

### **Theory**

One essential part of gas absorption is determining the rate of absorption of the material under the desired operating conditions. Reported literature allows us to predict the effect of certain operating variables on the absorption rate for a given type of apparatus. The absorption rate is generally expressed as an overall mass transfer coefficient,  $K$ , which may be based on either a gas or liquid-phase driving force [4]. In the instance, similar to this project, in a dilute system a design equation for the volume of a gas absorption tower can be expressed as:

$$W = K_y a (V_t) \Delta \bar{y}_L \quad (1)$$

where

$W$  = absorption rate of solute gas (mol/h)

$K_y a$  = overall mass transfer coefficient based on the gas-phase driving force (mol/h/m<sup>3</sup>)

$V_t$  = gross tower volume occupied by packing (m<sup>3</sup>)

$\Delta y_L$  = logarithmic mean driving force ( $y_b - y_b^*$ ) and ( $y_a - y_a^*$ )

$y_b$  = mole percent CO<sub>2</sub> in the gas phase at column bottom

$y_a$  = mole percent CO<sub>2</sub> in the gas phase at column top

$y_b^*$  = mole percent CO<sub>2</sub> in the gas phase in equilibrium with liquid at column bottom  
 $y_a^*$  = mole percent CO<sub>2</sub> in the gas phase in equilibrium with the liquid at column top

### Material Balances

In this section, the literature-based concepts of gas absorption will be presented. In order to grasp the principles of absorption, we must also understand its design and how it affects the gas- liquid interactions and the mass transfer coefficients. For instance, the diameter of a packed tower depends on the quantities of gas and liquid properties, and the height of the tower depends on the desired concentration changes and rate of mass transfer [4]. In other words, the column height alone is based on material balances, estimates of driving forces, and mass transfer coefficients. In a contact based system such as a packed absorption column, there are continuous variations in concentrations throughout the length of the equipment. So we use the overall material balance equation based on terminal streams for the system shown in Figure 2.1

$$L_a + V_b = L_b + V_a \quad (2)$$

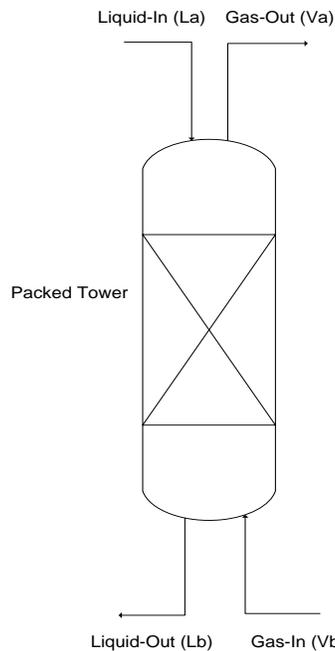


Figure 2.1 Absorber Schematic



### *Rate of absorption*

The rate of absorption can be expressed in four different ways, either using individual coefficients or overall coefficients based on the gas or liquid phases. Volumetric-based calculations are generally used in order to determine the total absorber volume. For this project, the following rate of absorption per unit volume was used

$$r = K_y a(y - y^*) \quad (3)$$

### *Calculating Height on Packed Tower*

Using the above rate equation, literature shows a distinct correlation between the mass transfer coefficient and the tower height. For dilute gases the change in molar flow rate is neglected and the differential volume is expressed as

$$-Vdy = K_y a(y - y^*) SdZ \quad (4)$$

After rearrangement and integration, the equation for the packed tower height can be written as

$$Z_T = \frac{V/S}{K_y a} \int_a^b \frac{dy}{y - y^*} \quad (5)$$

where the integral, also called the number of transfer unit ( $N_{Oy}$ ), represents the change in vapor concentration divided by the average driving force. The other half of the equation, based on length, is called the height of the transfer unit ( $H_{Oy}$ ) based on the overall gas phase driving force [4]. So the column height can be given as

$$Z_T = H_{Oy} N_{Oy} \quad (6)$$

where  $N_{Oy}$  can be determined using the logarithmic mean and the number of transfer units, expressed as

$$N_{Oy} = \frac{y_b - y_a}{\Delta \bar{y}_L} \quad (7)$$

The overall resistance to mass transfer can be considered to be made of a gas phase film resistance and a liquid phase film resistance. As a result, the height of a transfer unit can be considered to be made up of a contribution from the liquid film and a contribution by the gas film

$$H_{Oy} = H_y + m \frac{G}{L} H_x \quad (8)$$

Where  $m$  is the slope of the equilibrium line and  $G$  and  $L$  are the average molar flow rates of the gas and liquid. For the purpose of design, we can also find correlations for  $H_x$  and  $H_y$  [12], where

$$H_y = \left( \frac{0.226}{f_p} \right) \left( \frac{Sc}{0.660} \right)^{0.5} \left( \frac{G_x}{6.782} \right)^{-0.5} \left( \frac{G_y}{0.678} \right)^{0.35} \quad (9)$$

and

$$H_x = \left( \frac{0.357}{f_p} \right) \left( \frac{Sc}{372} \right)^{0.5} \left( \frac{G_x/\mu}{6.782/(0.8937 \cdot 10^{-3})} \right)^{0.3} \quad (10)$$

where

$Sc$ = Schmidt number =  $\mu/(\rho D_{AB})$

$\mu$ = viscosity

$\rho$ = density

$D_{AB}$ = diffusivity of solute A in B

$f_p$ = relative coefficient for packing material (assumed to be 1.5 for Raschig rings)

$G_y$ = gas mass velocity in  $\text{kg/m}^2\text{s}$

$G_x$ = liquid mass velocity in  $\text{kg/m}^2\text{s}$

The previous correlations are only used to provide reasonable estimates and to illustrate appropriate trends in mass transfer behavior, given

$$K_y a = \frac{V}{S \cdot H_{Oy}} \quad (11)$$

## COMSOL Multiphysics

After understanding the principle concepts, the use of modeling software, COMSOL, can be implemented. COMSOL Multiphysics is a software package which can be used to model an assortment of processes. COMSOL is particularly useful for modeling processes involving transport phenomena. The models created using this software are interactive and ideal for use as visual aids in classroom instruction, study guides, and student self-tutorials. Models may be created in 1, 2, or 3 dimensions. Partial differential equation based scientific and engineering models can also be solved using COMSOL, and the software facilitates the extension of conventional single physics models to multiphysics models which are capable of simultaneously solving coupled physics phenomena, hence the name COMSOL Multiphysics.

There are six basic steps that should generally be followed to successfully create a model using COMSOL. The first is creating or importing the desired geometry of the model. Different geometries may be selected based on the number of dimensions of the model, i.e. 1, 2, or 3. After the geometry has been created or imported, it is meshed. A mesh is a partition of the model's geometry into small, simple shapes. The types of meshes which are available are free, mapped, extruded, revolved, swept, and boundary layer meshes. Smaller meshes offer more precision when it comes to solving, but there is a lower limit to the sizes of meshes. Following the meshing of the geometry, the physics must be defined on the domains and at the desired boundaries of the model. After these steps are completed, the model can be solved. After using the software to solve the model, the solution can be post-processed. In post-processing, plots can be created, as well as extrapolated and interpolated in time or beyond parametric solutions. Parametric studies may then be performed on the process.

## METHODOLOGY

### Absorption Lab Experiment

First, in order to begin the modeling portion of the project, experimentation using the gas absorption lab had to be completed. The values obtained were later input into COMSOL. For the lab experiment, four runs were completed at four different water flow rates (0.5, 1.0, 1.5, and 2.0 L/min) using a 3 in. diameter, six foot tall absorber, partially packed with ¼ in. glass Raschig rings. For the varying liquid rates, the air and CO<sub>2</sub> rates remained constant. Twenty minutes was allowed to pass between each collection of data. The initial and exiting concentrations are shown below for all runs. Refer to Appendix A for more details.

Air Flow	Air Flow (L/min)	CO2 Flow	CO2 Flow in (L/min)	Water Flow	Water Flow (L/min)	y <sub>b</sub> (comp. at bottom)	y <sub>a</sub> (comp. at top)
150	1.419	25	0.315	0.5	0.516	0.185	0.141
150	1.419	25	0.315	1	1.047	0.185	0.099
150	1.419	25	0.315	1.5	1.578	0.185	0.063
150	1.419	25	0.315	2	2.109	0.185	0.038

Table 3.1 Experimental Data from Absorption Lab Runs 1-4

### 3.2 COMSOL Model using Experimental Values

#### MODEL NAVIGATOR

- 1 Start **COMSOL Multiphysics 3.4** and click **Multiphysics**.
- 2 In the Model Navigator, select **Axial Symmetry (2D)** from the **Space dimension** list.
- 3 From the **Application Modes** list, select **Chemical Engineering>Mass Transport>Convection and Diffusion**.
- 4 In the **Dependent variables edit field**, type the name of the concentration variable: **c1** and click **Add**.
- 5 From the **Application Modes** list, select **Chemical Engineering>Mass Transport>Convection and Diffusion** again.
- 6 In the **Dependent variables** edit field, type the name of the concentration variable: **c2** and click **Add**.
- 7 Select **Lagrange-Quadratic** from the **Element list** for both modes.
- 8 Click **OK**.

By implementing the Convection and Diffusion application mode, we model the mass balance of the system under the equation:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \cdot \nabla \cdot c_i) = R_i - u \nabla \cdot c_i \quad (12)$$

where  $c_i$  denotes the concentration of a species ( $\text{mol}/\text{m}^3$ ),  $D_i$  denotes the diffusion coefficient ( $\text{m}^2/\text{s}$ ), and  $u$  denotes the velocity vector ( $\text{m}/\text{s}$ ). In this mode, the following assumptions are also made: the pressure drop is negligible, carbon dioxide is diluted in air, there is laminar flow in the liquid phase, the system is isothermal, and the contribution of diffusion to the flux is negligible in the vertical direction. Additionally, COMSOL models the simulation based on a liquid moving through one end of the column and gas coming through the other, without any contact between the two. However, the carbon dioxide in the gas stream is diffused into the liquid stream. On the other hand, in the lab, the water and gas flowed through the absorber simultaneously, and gas-liquid interaction was observed.

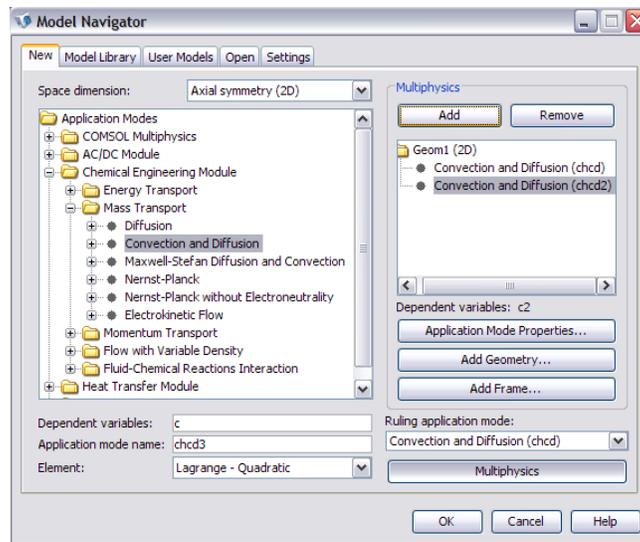


Figure 3.1 Model Navigator Window

Once you click **OK**, a blank screen will appear in the middle of the screen once all settings have been specified. This dotted line is called the axis of revolution.

#### *OPTION AND SETTINGS*

1 Define the following constants in the **Options>Constants** dialog box (the descriptions are optional); when finished, click **OK**.

Name	Expression	Value	Description
D1	1.6e-5	1.6e-5	diffusivity of CO2 in air
D2	1.6e-9	1.6e-9	diffusivity of CO2 in water
v1	$(1.419+.315)*(1/1000)*(1/60)*(1/0.00456)$	0.006338	velocity of gas
v2	$-(0.516)*(1/1000)*(1/60)*(1/0.00456)$	-0.001886	velocity of water
c10	$0.185*101325/8.314/298$	7.565925	initial concentration of CO2 in gas
c20	0	0	initial concentration of CO2 in water
Kya	770.067/3600	0.213908	calculated mass transfer coefficient
Ke	1400	1400	equilibrium constant (atm)

Note: The velocities of the gas and liquid phases are in the m/s, and concentration values represent units of mol/m<sup>3</sup>. All units in COMSOL are formatted in metric units so the appropriate conversions and calculations are available in Appendix D. As shown in the dialog box, the mass transfer coefficient is calculated using Equation 1, and is accounted for in the reaction rate term; disappearing in the gas phase via a reaction, and appearing in the liquid phase via reaction.

2 Define the following expressions in the **Options>Expressions>Global Expressions** dialog box; when finished, click **OK**. The global expressions, y and x, are specified to illustrate the carbon dioxide activity in the gas and liquid phases.

Name	Expression	Unit	Description
y	$c1*8.314*298/101325$	mol/m <sup>3</sup>	mol fraction in gas phase
x	$c2*1000/55.55/100^3$	mol/m <sup>3</sup>	mol fraction in liquid phase

### GEOMETRY MODELING

1 Click the **Specify Objects>Rectangle** from the Draw toolbar.

2 Specify the following dimensions and click **OK** when done.

Size		Rotation angle	
Width:	0.0762	α:	0 (degrees)
Height:	1.8288		
Position		Style: Solid	
Base:	Corner	Name:	R2
r:	0		
z:	0		

The following dimensions are based on the actual gas absorber size used in the Units Operations Laboratory. Although the absorber was previously reported to be 3 in. in diameter and 6 feet in length, these values are the equivalent in meters. When the dialog box is closed, click on the Zoom Extents button in the toolbar located at the top of the page. Although the actual shape of an absorber resembles a cylinder, we can use a rectangle to represent the absorber because COMSOL performs calculations about the axis of symmetry.

*PHYSICS SETTINGS*

*Subdomain Settings*

Now that the geometrical representation of the absorber was established, the gas and liquid properties representing the transport occurring in the absorption column were defined. The equation located at the top of the dialog box represents the mass balance implemented in the **Convection and Diffusion** application mode, and describes the concentration of the species, diffusion coefficients and the velocity vector.

- 1 Select **1 Convection and Diffusion (chcd)** from the **Multiphysics** toolbar.
- 2 From the Physics menu, choose **Subdomain Settings**. Select Subdomain 1.
- 3 On the c1 species page, the applicable settings for diffusion constant was entered, reaction rate, and dimensionless velocity. Keep in mind that all values were the same as reported in Run 1 of the data Appendix B, and illustrated based on the necessary conversions made (included in Appendix D).

For c1, the Subdomain settings should contain the following values:

Subdomain		1
Diffusion coefficient (D)	m <sup>2</sup> /s	D1
Reaction Rate <sup>®</sup>	mol/(m <sup>3</sup> ·s)	-Kya*(c1*8.314*298/101325-Ke*c2*1000/55.55/100^3)
z-velocity (v)	m/s	v1

As shown, the mass transfer coefficient was used as the basis for the reaction rate, whereas, in our experimental data, the mass transfer coefficient was calculated based on the rate of absorption taken place in the packed tower. The COMSOL reaction rate is basically defined as

$$y = \frac{c_1 \times R(\text{ideal gas constant}) \times T}{P}$$

Where y is the mole fraction of CO<sub>2</sub> in the gas phase, Ke is the equilibrium constant for the reaction (specified at 1400), and x is the mole fraction of CO<sub>2</sub> in the liquid phase. The conversion for mole fraction to mol/m<sup>3</sup>, which is the default unit for COMSOL, comes from the ideal gas law:

Similarly, for the liquid mole fraction we used for conversion

$$x = c_2 \left( \frac{\text{mol}}{\text{m}^3} \right) \times \frac{1}{1000} \left( \frac{\text{m}^3}{\text{L}} \right) \times \frac{1}{55.55} \left( \frac{\text{L}}{\text{mol}} \right) - K_{ya} \times (y - K_e \times x)$$

For the initial concentration of CO<sub>2</sub> in the liquid, we gave the value of zero or c20.

Subdomain initial value		<b>1</b>
Concentration, c1 (c1)	mol/m <sup>3</sup>	<b>c20</b>

For **2 Convection and Diffusion** application mode, the following should be included:

Subdomain		<b>1</b>
Diffusion coefficient (D)	m <sup>2</sup> /s	<b>D2</b>
Reaction rate (R)	mol/(m <sup>3</sup> ·s)	<b>K<sub>ya</sub>*(c1*8.314*298/101325-Ke*c2*1000/55.55/100^3)</b>
z-velocity (v)	m/s	<b>v2</b>

Subdomain initial value		<b>1</b>
Concentration, c2 (c2)	mol/m <sup>3</sup>	<b>c10</b>

Click **OK** to close the dialog box.

### *Boundary Conditions*

1 From the **Physics** menu, open the **Boundary Settings** dialog box. Boundary settings illustrate what is physically occurring on every side of the rectangle.

2 Select the appropriate boundary conditions for each application mode. Input the following values into appropriate edit fields. Remember that the left boundary is the axis of symmetry, so it should be specified accordingly. For the liquid phase, the lower boundary (2) is where the liquid comes out, so it is denoted as **Concentration**. The goal is to remove all carbon dioxide from the gas stream; therefore, we mark concentration as **c10**, which was previously specified. Boundary 3 is where is liquid enters the column (**Convective flux**), and at Boundary 4, select **Insulation/Symmetry** with the assumption that the column is isothermal.

#### *1 Convection and Diffusion (chcd)*

Boundary		4	1	2
Type		Insulation/Symmetry	Axial symmetry	Concentration
Concentration (c0)	mol/m <sup>3</sup>	0	0	c10

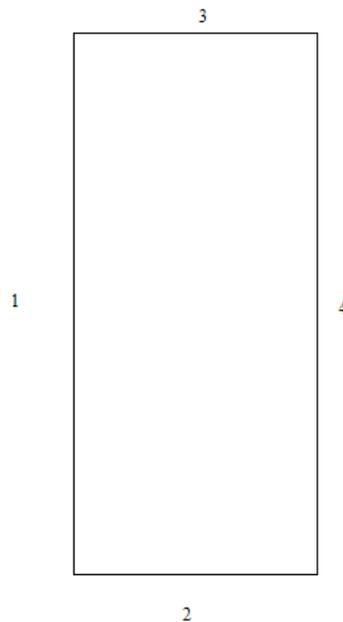
Boundary		3
Type		Convective flux
Concentration (c0)	mol/m <sup>3</sup>	0

#### *2 Convection and Diffusion (chcd2)*

For the gas phase condition, Boundaries 1 and 4 can be labeled identical to the liquid phase conditions. However, since we have a countercurrent absorber, where the gas and liquid enter on opposite ends, specify Boundaries 2 and 3 as **Convective flux** and **Concentration**, respectively.

Boundary		4	1	2
Type		Insulation/Symmetry	Axial symmetry	Convective flux
Concentration (c0)	mol/m <sup>3</sup>	0	0	0

Boundary		3
Type		Concentration
Concentration (c0)	mol/m <sup>3</sup>	c20



Boundaries are specified according to the Figure 3.1

Click **OK** when done.

### MESH GENERATION

Now that all physical components have been defined and specified, a finite mesh must be created. There are two options for meshing, allowing COMSOL to create a simple mesh, or design our own mesh parameters. For the sake of simplicity, we will allow COMSOL to provide a mesh.

- 1 From the **Mesh** menu, select **Initialize Mesh** from the drop down menu.
- 2 Select **Refine Mesh** button to generate refined solving parameters.
- 3 Click the **Solve Problem** button from the **Solve** drop-down menu to compute the model.

### POSTPROCESSING

- 1 Click **Postprocessing**> **Plot Parameters**. Click on the **Surface** tab and type “y” in the **Expression** edit field.

## RESULTS AND DISCUSSION

Figure 4.1 shows the concentration of carbon dioxide changes throughout the length of the absorber. We can see that in the gas phase,  $y$ , the air stream enters the system with a  $\text{CO}_2$  composition of 18.5 percent and leaves the absorber with a composition of 13.2 percent, with a rapid increase in absorption rate toward the top of the absorber. Recall that our experimental data showed an entering composition of 0.185 and an exiting composition of 0.141. So we can conclude that for a water velocity of  $-1.89 \times 10^{-3}$  m/s (0.5L/min), and a mass transfer coefficient of 0.214 ( $\text{mol}/\text{m}^3 \cdot \text{s}$ ), the amount of absorption reported from both the lab experiment and COMSOL are comparable.

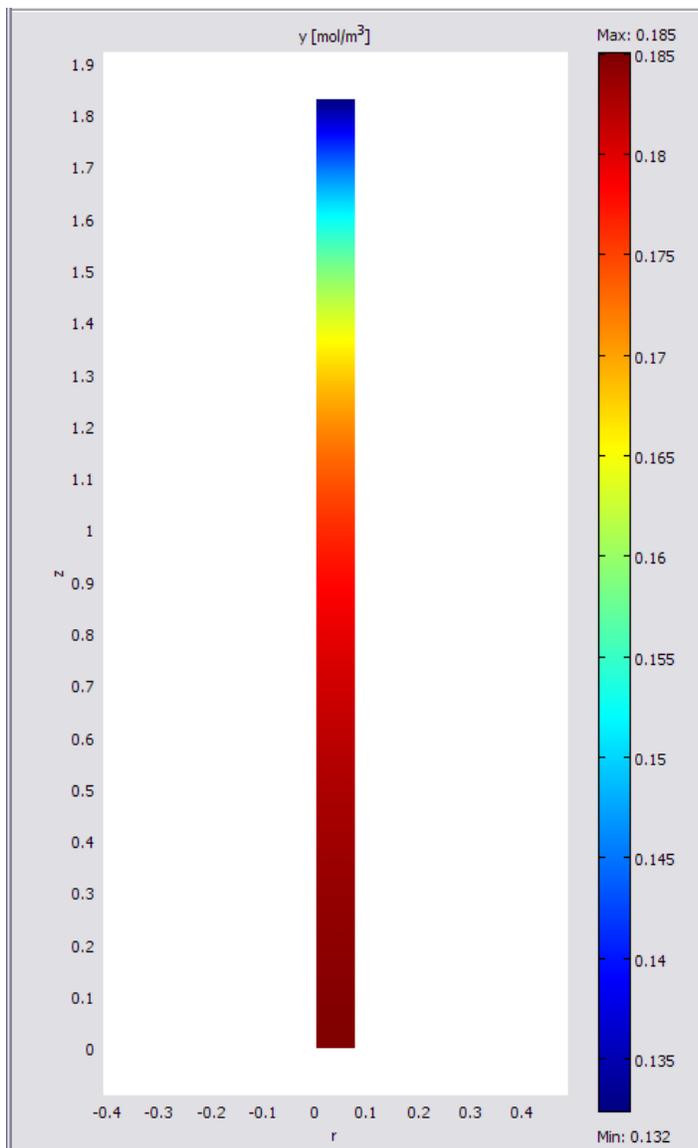


Figure 4.1 Run 1  
 $\text{H}_2\text{O}$  velocity =  $-1.89 \times 10^{-3}$  (m/s)  
 $K_{ya} = 0.214$  ( $\text{mol}/\text{m}^3 \cdot \text{s}$ )  
COMSOL  $\Delta y = 0.053$

Figure 4.2 shows similar results, however, we have a water velocity of  $-5.77 \times 10^{-3}$  (m/s) (1.5L/min) and a calculated mass transfer coefficient of 0.427 (mol/m<sup>3</sup>\*s). From our experimental data, we have an overall change in composition of 0.122, whereas COMSOL reports an overall change of 0.1284.

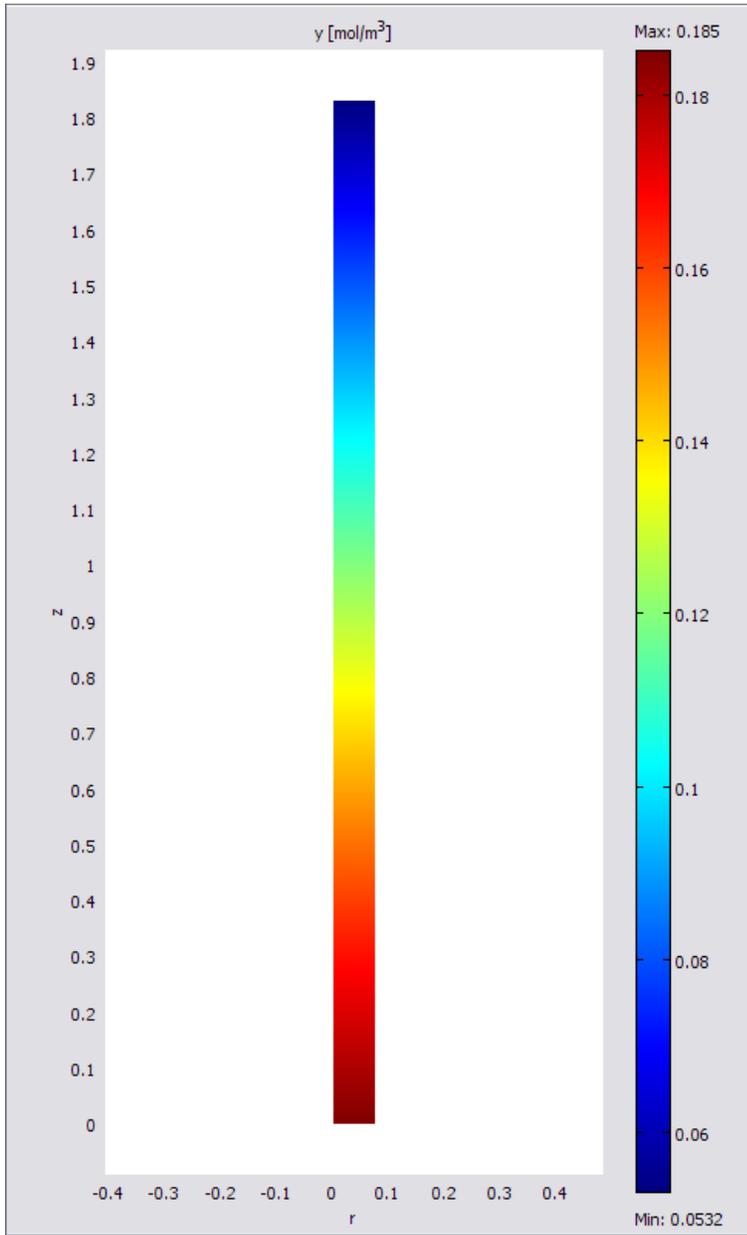


Figure 4.2-Run 3  
Water velocity =  $-5.77 \times 10^{-3}$  (m/s)  
Calculated  $K_{ya} = 0.427$  (mol/m<sup>3</sup>\*s)  
COMSOL  $\Delta y = 0.1318$

Based on Figures 4.1 and 4.2, we can see agreeable data obtained for the two water flow rates. Although the experimental and COMSOL values were in similar ranges, rate absorption trend was further evaluated.

Table 4.1 and Figure 4.3 both present experimental versus simulation values for the overall change in the mole fractions for Runs 1-4.

Water Flow (L/min)	Experimental delta y	COMSOL delta y
0.516	0.044	0.053
1.047	0.086	0.0974
1.578	0.122	0.1318
2.109	0.147	0.1539

Table 4.1: Experimental vs. COMSOL Absorption Rate

In sync with the COMSOL models, we can see that “delta y” increases as water flow rate increases. We know from literature that the packing material in the absorption column creates a larger contact area for liquid-gas interaction. As a result, when the liquid flow increases, more packing is covered and there is more uniform distribution of liquid throughout the packed tower. As flow increases, the occurrences of channeling, uneven distribution of gas or liquid flow in the column, occurs.

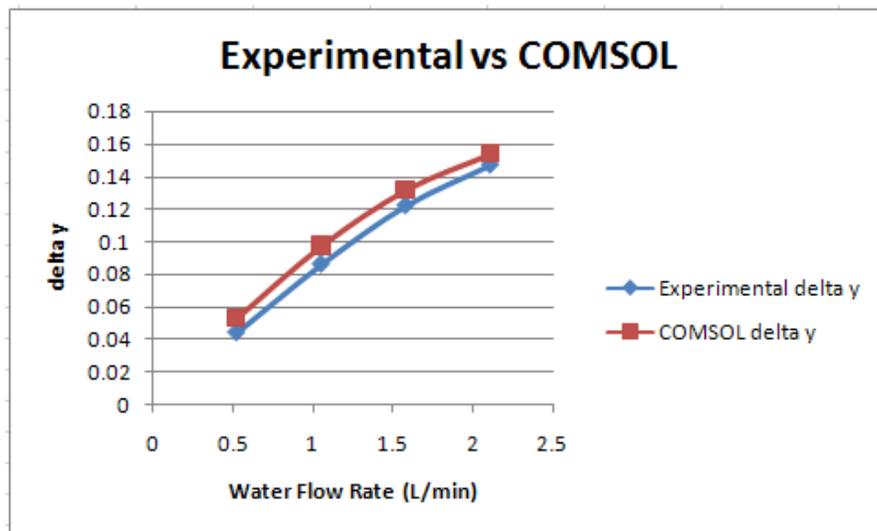


Figure 4.3 Absorption Rates for Experimental & COMSOL (Runs 1-4)

Though the COMSOL values consistently report greater changes in the overall “delta y” than the experimental, we can assume that the previously defined assumptions contribute to these variations.

Another important relationship that is noticed occurs between the liquid flow rate and the mass transfer coefficient. Figure 4.4 confirms that in addition to an increase in absorption rate with flow, there is also an increase in “Kya.” This is partially due to Kya being directly proportional to the rate of absorption. One other justification is that the liquid boundary layer

resistance to mass transfer is reduced with higher flow rates, for similar reasons that absorption increases. On the other hand, at slower liquid rates, the boundary resistance is higher due to a decrease in liquid-gas stream contact and interaction.

Figure 4.4 shows a graphical representation of the overall mass transfer coefficients for both lab and COMSOL experimentation for the aforementioned water flow rates based on the absorption rates.

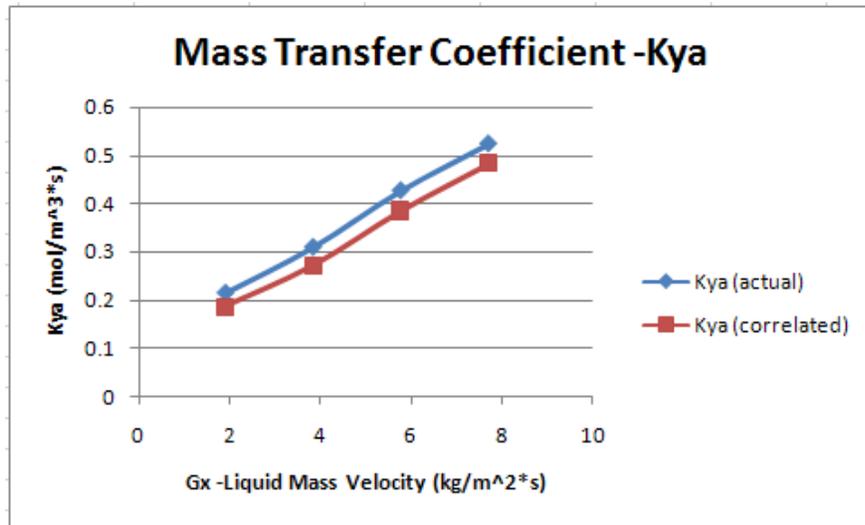


Figure 4.4 G<sub>x</sub> vs. K<sub>ya</sub>

Illustrated in Figures 4.1 and 4.2, are varying trends in the composition of CO<sub>2</sub> absorbed based on the respective flow rates. By analyzing the concentration as a function of position in the absorber, we were able to obtain the following graphs using post-processing methods in COMSOL (Input Summaries are included in Appendix E).

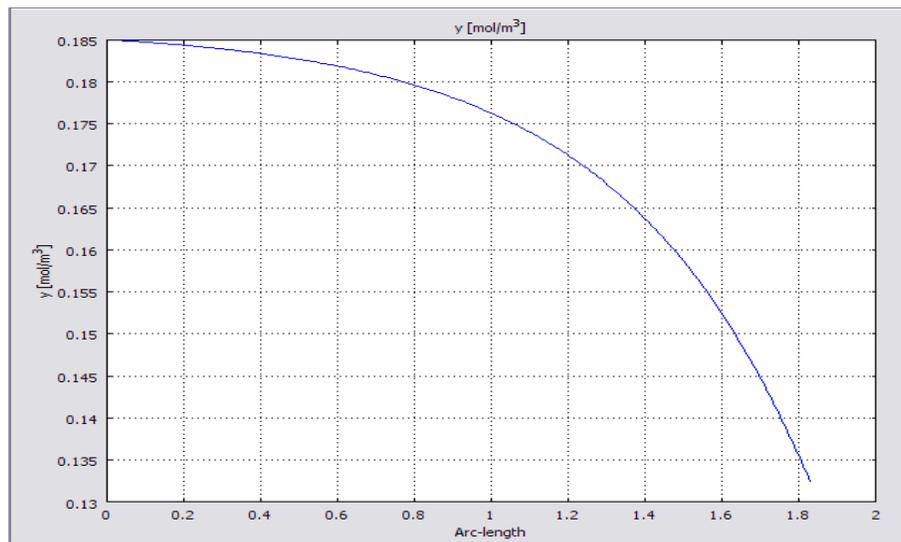


Figure 4.5 Run 1 - Concentration Profile

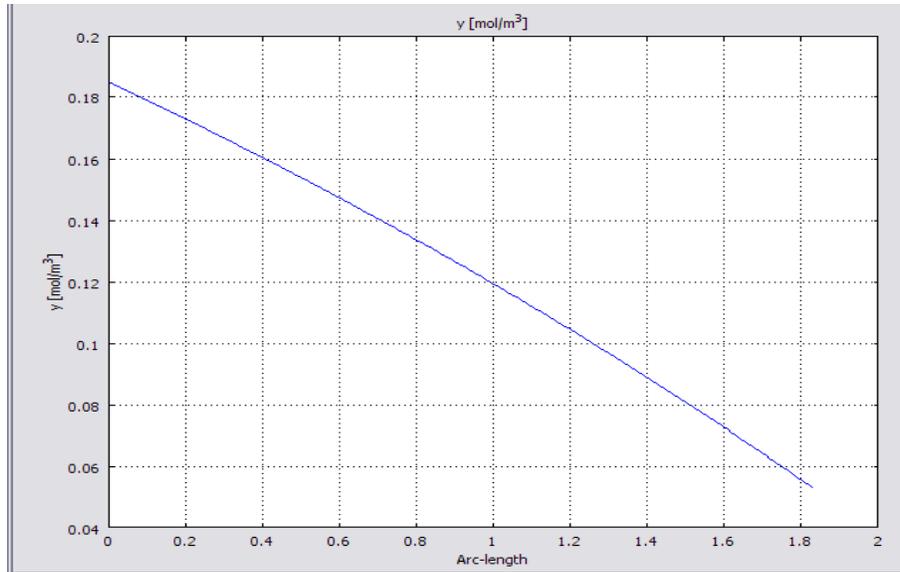


Figure 4.6 Run 3- Concentration Profile

Figure 4.5, concentration profile, for water velocity of  $-1.89 \cdot 10^{-3}$  (m/s), illustrates an exponential change in composition across the tower, whereas Figure 4.6, water velocity of  $-5.77 \cdot 10^{-3}$  (m/s), shows a more linear composition change at its respective flow rate and mass transfer coefficient. With further study and experimentation with COMSOL, these trends can be used to analyze carbon dioxide composition in the gas phase as a function of time inside the packed tower.

### Liquid Phase Analysis

We can also evaluate the accuracy of COMSOL predictions based on the previous assumptions to solve for the concentration in the liquid bottoms stream. In the post-processing used to compare CO<sub>2</sub> absorbed in the gas phase, we can perform the same analysis for the liquid phase. Figure 4.7 shows the carbon dioxide in the liquid phase, with a maximum mole fraction of 1.298e-4 compared to a value of 1.3e-4 from experimental data collection.

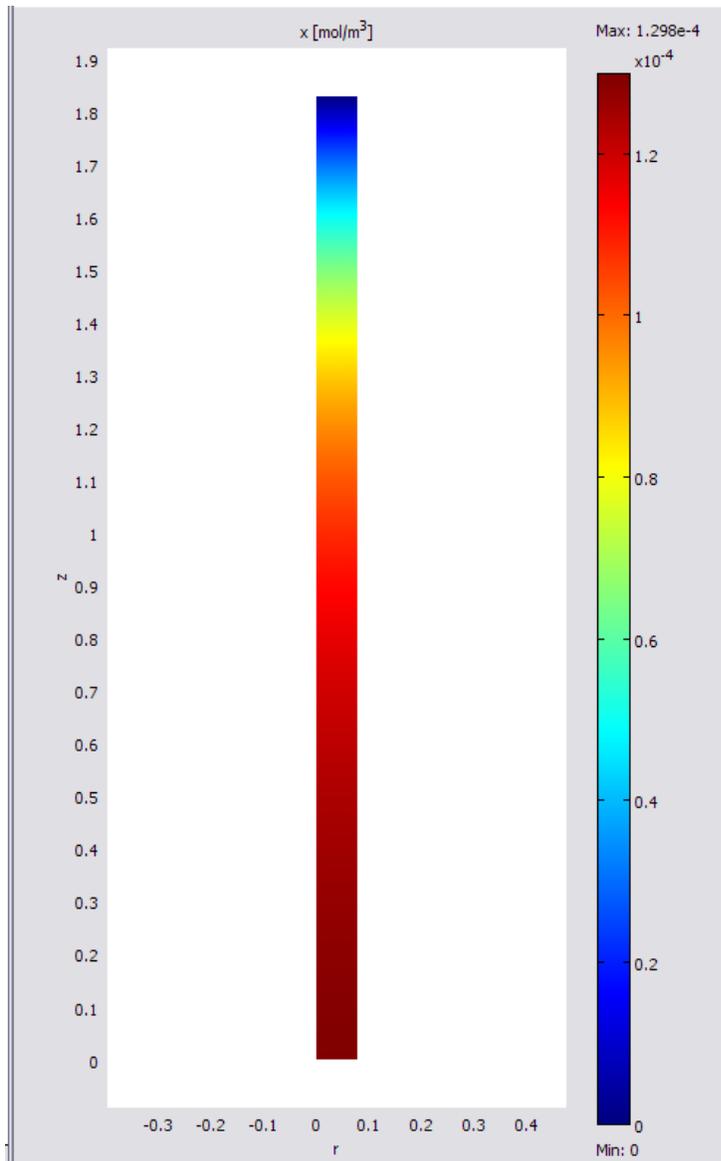


Figure 4.7 Run 1  
H<sub>2</sub>O velocity =  $-1.89 \cdot 10^{-3}$  (m/s)  
K<sub>ya</sub> = 0.214 (mol/m<sup>3</sup>\*s)  
COMSOL max. x =  $1.298 \cdot 10^{-4}$

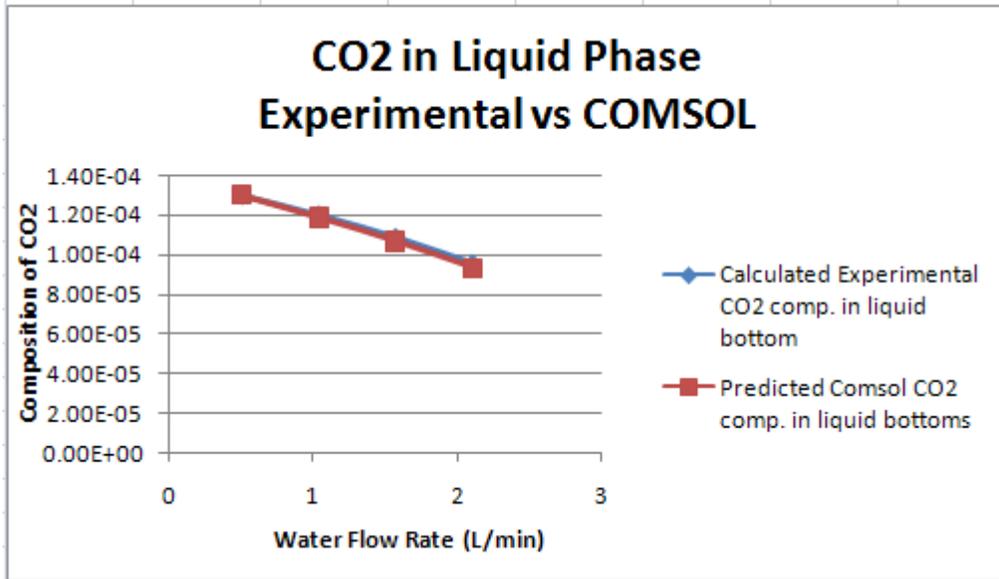


Figure 4.8 CO<sub>2</sub> Compositions in Liquid Stream Outlet

Figure 4.8 shows the experimental compositions in the liquid phase compared to values produced by COMSOL. We can see that, not lonely does COMSOL accurately model the interactions and transport in the gas phase of the absorber, but also in liquid phase.

## **CONCLUSIONS**

Based on our results and collected data, we can conclude that COMSOL can be a useful tool for predicting absorption rates given specific gas and liquid velocities, mass transfer coefficients and a specified initial concentration.

For all four water flow rates used in the absorption lab, COMSOL approximated very well, almost matching the change in composition at both 1.0 and 1.5 L/min water flows. We can also use COMSOL to predict concentrations as a function of time in place inside the absorber. Given such successful results, it can be a useful learning tool for students to use COMSOL before performing experimental analysis. This can assist in providing an understanding of gas-liquid interactions within a packed tower, reinforcing important concepts, and providing students with a range of expected values for particular flow rates. If used after lab experimentation, modeling can be used as a set of guidelines to verify values collected in the lab. COMSOL not only provides a quantitative analysis for the packed tower, in regards to predicting amount of CO<sub>2</sub> removed, but also a qualitative analysis, which is essential in understanding the absorption process in its entirety.

## **RECOMMENDATIONS**

Included in this section are two sets of recommendations that can be taken into account for performing the gas absorption lab experiment and modeling gas absorption using COMSOL Multiphysics and other useful software.

### **Gas Absorption Lab Experiment**

As this was the first year using the new gas absorber in the Unit Operations (UO) laboratory, there are several methods that can both be changed and implemented in the future. First, more time should be allotted before measuring/recording data. In the UO lab, twenty minutes was allowed for the system to come to equilibrium, however, the maximum absorption for that particular liquid flow rate was not achieved. I believe that permitting an extra ten minutes would give more accurate data. With this additional information, the CO<sub>2</sub> in the liquid bottoms can be analyzed. One segment of the collection procedure that was omitted from this particular lab, was the analysis of carbon dioxide in the liquid outlet. This can be tested using the

carbon electrode built specifically for the gas absorber. Techniques for assembling and using the electrode can be found in Appendix F. Another analysis tool that was not included in this years' lab was the use of equipment software. The absorber comes with a program that can be used to collect and record data without the use of the Rosemont Analyzer. Implementing these tools can help produce more accurate and reliable data.

### Modeling Component

There are some variations in modeling absorption with COMSOL Multiphysics. The basis of the modeling was focused on mass transport and the Convection/Diffusion applications. Though we only used modeling for the simplest case, a dilute system, there are applications built for the analysis of concentrated vapors, such as the Maxwell-Stefan Diffusion and Convection application. This particular mode allows for accurate modeling of a concentrated mixture by setting up the proper multi-component mass transport equations. It also permits the use of up to four species in the absorption column.

Another important segment of gas absorption that can be modeled in the future is the mass transfer theories, specifically the two film theory. As we know. In separation processes, materials must be diffused from one phase to another, which affect the overall mass transfer coefficient. In the two film theory, equilibrium is assumed at the interface, and the resistances to mass transfer in the two phases are added to an overall resistance [3]. Figure 6.1 illustrates the assumptions made under the two film theory.

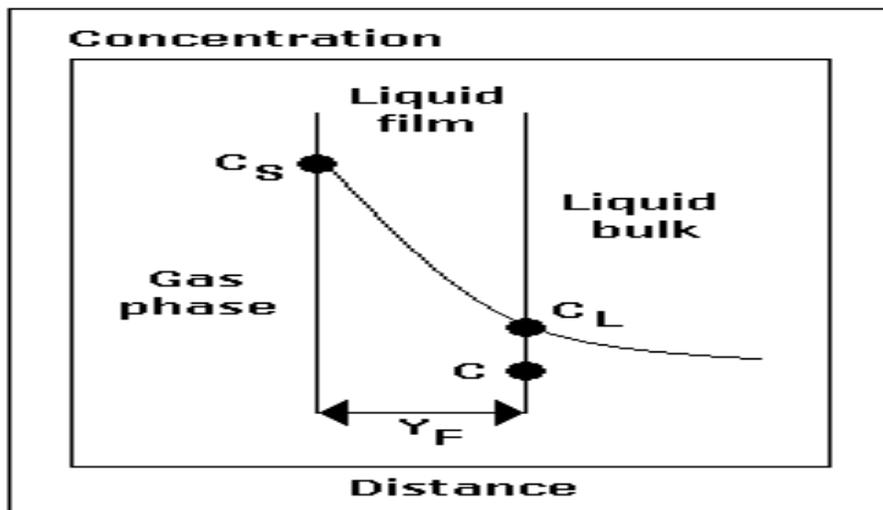


Figure 6.1 Two Film Theory (<http://web.deu.edu.tr/atiksu/ana52/aedet01.gif>)

### *Aspen Plus*

Another useful tool that can be used for understanding absorption concepts and trends is Aspen Plus. Aspen Plus can be used for various chemical engineering applications. For example, it can execute tasks as simple as describing thermodynamic properties of an ethanol and water mixture, or as complex as predicting the steady-state behavior of a full-scale petrochemical plant [11]. Aspen is also a useful tool for simulating reaction engineering scenarios, such as designing and sizing reactors, predicting reaction conversions, and understanding reaction equilibrium behavior. Though this program does not create concentration profiles, it does allow for reasonable predictions for an absorber under certain conditions. However, in order to maximize its ability, the best way to model an absorption column would be to apply Rate-Based equations in the Rad-Frac mode. A similar test was tried for this project. The input summary of the trial is included in Appendix F for future study.

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## APPENDIX A – GAS ABSORPTION IN A PACKED TOWER LAB

Worcester Polytechnic Institute  
Department of Chemical Engineering

ChE 4402

Gas Absorption in a Packed Tower

B term

### Introduction and Objectives

Carbon dioxide is considered to be the largest contributor to the global warming problem. The removal of CO<sub>2</sub> from industrial gas streams is becoming increasingly important due to the need to control greenhouse gas emissions to protect the environment. Carbon dioxide can be removed from an industrial effluent gas stream by absorption into a liquid solvent. This separation process is normally achieved in a column packed with packing materials designed to promote direct contact between the solvent flowing downward over the packing and a continuous gas phase flowing upward. In industrial processes, the solvent is usually an aqueous potassium carbonate or amine solution that provides enhanced absorption through reaction with the CO<sub>2</sub>.

In this experiment you will study the absorption of CO<sub>2</sub> from air in a packed column using water as the solvent. The main goal is to determine the effect of gas and liquid flow rates on the overall mass transfer coefficient for this absorption process. You will also be asked to use the information obtained for an absorption design calculation.

### Apparatus

#### (1) Tower

The column is a 3-inch diameter glass column partially filled with ¼ in. glass Raschig rings.

#### (2) Gas supply

CO<sub>2</sub> and air are available from tanks equipped with regulators. The regulator pressure should be set at 20 psig for each gas. Flow rates of the gases are maintained at desired levels using flow control valves and rotameters. The gases are mixed using a specially designed mixing tube located after the flow meters and prior to entering the bottom of the tower.

#### (3) Liquid supply

Water is pumped from a sump tank, through a rotameter, to the top of the column. It flows downward through the column and can be returned back to the sump tank or diverted to the drain using valves in the pipes below the column. If water is to be diverted to the drain, it is necessary to open valves to provide make-up tap water to the sump tank. A float mechanism in the sump tank will maintain a constant level in the tank as long as the appropriate valves are opened. During column operation with gas flowing upward, a liquid seal must be maintained in the pipes

below the column by appropriate adjustment of the return or drain valves. That is, the rate of water flow returned to the sump or diverted to the drain must be maintained at a rate equal to the inlet water flow rate to maintain a constant height of water in the pipe below the column. That way, water does not backup and flood the column and the gas entering the column at the bottom does not escape into the sump or out the drain.

#### (4) Measurements

Flow rates of air, CO<sub>2</sub> and water are obtained from rotameters. Calibration data is attached. Thermocouples at the column top and bottom provide temperature measurements that can be read on the column control panel. Pressure drop across each of two sections of the column can be obtained from digital readings of differential pressure gages. A water-filled manometer provides a measure of the difference between the pressure at the column top and atmospheric pressure. Inlet and outlet gas CO<sub>2</sub> compositions are measured with a Rosemount Analytical Inc. non-dispersive infrared analyzer located in Goddard 116 on the main floor of the lab, just above the column outlet. The Rosemount analyzer provides a digital readout of the volume percent CO<sub>2</sub> in the air.

### Procedure

#### (1) Preliminary inspection of equipment

It is necessary that each student understand the arrangement and operation of the equipment before any experimental work is undertaken. A complete inspection of the equipment should be made and the function of each part of the apparatus should be determined. A detailed schematic should be drawn. Each member of the lab group will be expected to answer questions about the equipment during the lab session.

#### (2) Preliminary work

The Rosemount infrared spectrometer should be calibrated prior to the experiment using nitrogen gas and two available standard CO<sub>2</sub>/air mixtures. The standard gas cylinders have regulators that should be set at about 10-15 psig. Sample valves on a panel above the analyzer can be opened one at a time to introduce the samples individually. A pressure of 1 inch of water at the manometer on the panel gives suitable flow rates for gases flowing into the analyzer. The flow control valve next to the manometer should be opened slowly to establish the flow that provides 1 inch of water. The pure nitrogen gas is used as the zero point reference. Once nitrogen is introduced at the sample port and has been flowing for at least two minutes, press **zero** then **enter** on the Rosemount front panel. After a minute or two, the instrument should read zero (or nearly so). Close the flow control valve and the N<sub>2</sub> sample valve. To calibrate the instrument over the range from zero to 20% CO<sub>2</sub>, a 20% CO<sub>2</sub> mixture is introduced in the sample port.

After this flow has been established for a minute or two by opening the flow control valve just enough to get 1 inch of water on the manometer, press **span** then **enter**. The instrument should read 20% (or nearly so). Close the flow control valve and the 20% sample valve. You can check the accuracy of the instrument by recording the reading for a standard 12 % CO<sub>2</sub> mixture. Simply establish the flow of the 12 % mixture with the flow control valve giving a 1 inch pressure difference at the manometer and record the Rosemount reading after it becomes steady. Our 12 % often reads slightly higher than 12%; about 12.7%. Don't forget to close the flow control valve and the 12 % sample valve.

### (3) Experimental conditions

Inlet gas CO<sub>2</sub> composition should be maintained at a nearly constant value somewhere between 18 and 20 % by volume. It is recommended that the air flow be no less than 750 ml/min and no more than 1400 ml/min. Therefore, the required CO<sub>2</sub> flow should be between 200 and 320 ml/min. The calibration curves were obtained at 70 °F and 20 psig at the regulator. Correction for other T and P conditions might need to be made. The water flow can be varied between 0.5 and 2.0 L/min. Inlet CO<sub>2</sub> composition in the water entering the column can be assumed to be zero as long as the outlet water is completely diverted to the drain. It is suggested that you study four different water rates at a fixed gas rate during the first experimental period and that you study the same four water rates at a different gas rate for the second experimental period. The CO<sub>2</sub> composition of the outlet gas stream can be monitored continuously (by opening the column top sample valve and opening the flow control valve on the panel above the instrument just enough to provide 1 inch of water at the manometer). It is important to wait long enough for steady state to be achieved. It normally takes about 20 minutes for the outlet concentration to settle to a constant value.

### Theory

The engineer who is required to design an absorption tower is interested in the rate of absorption of the material under the desired operating conditions. Considerable experimental work on a few systems has been reported in the literature that will enable the designer to predict the effect of certain operating variables on the rate of absorption for a given type of apparatus. The absorption rate is generally expressed as an overall mass transfer coefficient, K, which may be based on either a gas or a liquid-phase driving force. In most cases it is impossible to determine the area of contact of the gas and liquid. Therefore, the coefficients are reported on a volume basis. For dilute systems with straight operating and equilibrium lines, a design equation for the volume of a gas absorption tower may be written as:

$$W = K_y a (V_t) \Delta \bar{y}_L \quad (1)$$

where

W = absorption rate of solute gas; mol/h

K<sub>y</sub>a = overall mass transfer coefficient based on the gas-phase driving force, mol/h/m<sup>3</sup>

V<sub>t</sub> = gross tower volume occupied by packing, m<sup>3</sup>

Δ $\bar{y}_L$  = logarithmic mean driving force; logarithmic mean of (y<sub>b</sub>-y<sub>b</sub><sup>\*</sup>) and (y<sub>a</sub>-y<sub>a</sub><sup>\*</sup>)

y<sub>b</sub> = mole percent CO<sub>2</sub> in the gas phase at column bottom

$y_a$  = mole percent CO<sub>2</sub> in the gas phase at column top

$y_b^*$  = mole percent CO<sub>2</sub> in the gas phase that would be in equilibrium with the liquid at column bottom

$y_a^*$  = mole percent CO<sub>2</sub> in the gas phase that would be in equilibrium with the liquid at the column top

The equilibrium relation for CO<sub>2</sub> dissolved in water can be represented by Henry's law

$$y_{CO_2}^* P = H x_{CO_2}$$

Henry's constant may be assumed to be 1400 atm at 20 °C [1].

Under certain assumptions, a design equation for the column height is given by [2]:

$$Z = \frac{V/S}{K_y a} \int_a^b \frac{dy}{y - y^*} \quad (2)$$

where

$S$  = cross sectional area, m<sup>2</sup>

$V$  = molar flow rate of the gas phase, mol/h

The integral in this equation represents the change in vapor composition divided by the average driving force and is called the number of transfer units based on the overall gas phase driving force,  $N_{Oy}$ . The other part of Equation 2 has units of length and is called the height of a transfer unit based on the overall gas phase driving force,  $H_{Oy}$ . Thus the height of the column is given by:

$$Z = H_{Oy} N_{Oy} \quad (3)$$

For dilute systems or those with otherwise straight operating and equilibrium lines, the integral in Equation 2 is easily determined using the logarithmic mean and the number of transfer units is given by:

$$N_{Oy} = \frac{y_b - y_a}{\Delta \bar{y}_L} \quad (4)$$

The overall resistance to mass transfer can be considered to be made of a gas phase film resistance and a liquid phase film resistance and the height of a transfer unit can be considered to be made up of a contribution from the liquid film and a contribution from the gas film as given by [3]:

$$H_{Oy} = H_y + m \frac{V}{L} H_x \quad (5)$$

where  $m$  is the slope of the equilibrium line and  $V$  and  $L$  are the average molar flow rates of the gas and liquid. This formulation is useful for design purposes because correlations are available for  $H_x$  and  $H_y$ . For example, Geankoplis [4] gives

$$H_y = \left( \frac{0.226}{f_p} \right) \left( \frac{Sc}{0.660} \right)^{0.5} \left( \frac{G_x}{6.782} \right)^{-0.5} \left( \frac{G_y}{0.678} \right)^{0.35} \quad (6)$$

and

$$H_x = \left( \frac{0.357}{f_p} \right) \left( \frac{Sc}{372} \right)^{0.5} \left( \frac{G_x / \mu}{6.782 / (0.8937 \cdot 10^{-3})} \right)^{0.3} \quad (7)$$

where  $H_x$  and  $H_y$  have units of meters,

$Sc = \text{Schmidt number} = \mu / (\rho D_{AB})$

$\mu = \text{viscosity}$

$\rho = \text{density}$

$D_{AB} = \text{diffusivity of solute A in B (gas phase for } H_y \text{ and liquid phase for } H_x)$

$f_p = \text{a relative mass transfer coefficient for a given packing material compared to a reference packing material. } f_p \text{ can be assumed to be 1.5 for } 1/4 \text{ Raschig rings.}$

$G_y = \text{gas mass velocity in kg/m}^2\text{s}$

$G_x = \text{liquid mass velocity in kg/m}^2\text{s}$

These correlations are not generally expected to give accurate quantitative predictions, but they should provide reasonable rough estimates and show appropriate trends in mass transfer behavior.

Note that 
$$K_y a = \frac{V}{S H_{Oy}} \quad (8)$$

For design purposes, the height of column required to provide a specified separation can be obtained from Equation 3, if correlations like Equations 6 and 7 are used together with equilibrium information to estimate  $H_{Oy}$  in Equation 5. Alternatively, if the column height is given, and an estimate is obtained for  $H_{Oy}$ , the outlet compositions that will result for given inlet flows and compositions can be determined from Equation 3 together with a mass balance. Equations 3 and 8 could also be used to evaluate  $H_{Oy}$  from experimental data obtained on a given column.

Also note that mass transfer coefficients and transfer units can alternatively be based on the liquid phase driving force and that although  $H_{Oy} \neq H_{Ox}$  and  $N_{Oy} \neq N_{Ox}$  design results in terms of column heights or product stream compositions based on the two methods should be similar.

### Calculations

The following calculations should be performed:

- (a) a value of  $K_y a$  should be calculated for each run. The value of  $W$  to be used in this calculation should be obtained from a material balance on  $\text{CO}_2$  in the gas phase.
- (b) estimates of error should be attached to any value of  $K_y a$  and error bars should be provided on all plots.
- (c) Plots of  $K_y a$  versus liquid mass velocity,  $G_x$ , should be made and a correlation of  $K_y a$  as a function of liquid mass velocity should be attempted.  $G_x$  should be based on the total cross sectional area of the tower, and has units of  $\text{kg/m}^2\text{-h}$ .
- (d) Estimates of  $H_{Oy}$  and  $K_y a$  obtained should be obtained from correlations and compared with the experimental results, including a comparison of the expected and experimental dependence of  $K_y a$  on  $G_x$  and  $G_y$ .

### Design Requirements

Determine the outlet compositions (vapor and liquid) for an absorption process at  $20^\circ\text{C}$  using our column with  $2.5 \text{ L/min}$  water flow rate to treat a  $20\% \text{ CO}_2/\text{air}$  stream flowing at  $2 \text{ L/min}$ .

Determine how this water flow rate compares to the minimum water rate required to accomplish the same removal of CO<sub>2</sub> from the vapor phase.

Hint: an equation for the operating line can be determined to be [5]:

$$L' \left( \frac{x_2}{1-x_2} \right) + V' \left( \frac{y_1}{1-y_1} \right) = L' \left( \frac{x_1}{1-x_1} \right) + V' \left( \frac{y_2}{1-y_2} \right)$$

where L' and V' are the CO<sub>2</sub> free water and air molar flow rates, respectively.

For the case where x<sub>2</sub> = 0 (pure water entering at column top), the operating line can be plotted as [6]:

$$y(x) = \frac{\frac{L'}{V'} \left( \frac{x}{1-x} \right) + \left( \frac{y_2}{1-y_2} \right)}{1 + \frac{L'}{V'} \left( \frac{x}{1-x} \right) + \left( \frac{y_2}{1-y_2} \right)}$$

where y<sub>2</sub> is the mole fraction of CO<sub>2</sub> in the gas exiting the top of the column.

## Results and Discussion

A discussion of the errors in the results due to experimental uncertainty and their effect on the results through propagation of error should be included. How meaningful are your results when errors are considered. It is not sufficient to simply state your results in numerical form. They should be interpreted in terms of physical phenomena occurring within the process. Do the trends in the data make sense? Do your results agree with published information or correlations? What is happening physically inside the column when the water rate is changed that can account for the observed dependence of the mass transfer coefficient on the water rate?

## Report Requirements

The pre-lab report should contain an introduction stating the objective of the experiments, including the rationale for expecting K<sub>y</sub>a to depend on the liquid flow rate, some background on gas absorption, a detailed derivation of the design equation from first principles, including the assumptions and simplifications made, a description of the equipment and purpose of each item, including a detailed schematic drawing, and a stepwise procedure, that would allow someone who is unfamiliar with the equipment to perform the experiment. Following the first week of experiments, calculations of K<sub>y</sub>a for all liquid flow rates should be made and correlated against G<sub>x</sub>.

These results are to be presented informally to the instructor before the second week's experiments. Error analysis is not required at this stage. The final report should contain the usual sections as specified in the course descriptions. In addition, an error analysis is required for all calculated values of K<sub>y</sub>a, and error bars are to be included on all plots.

## Calibration Curves

A calibration curve for the digital water flow meter is provided in Figure 1. Note that the measured water flow was 2.1 L/min when the meter read 2.0 L/min. Figures 2 and 3 show calibration curves for air and CO<sub>2</sub> rotameters, respectively. Note that the float travel is measured at the center of the float. Equations for best fit lines provided on these curves should not be extrapolated beyond the ranges shown.

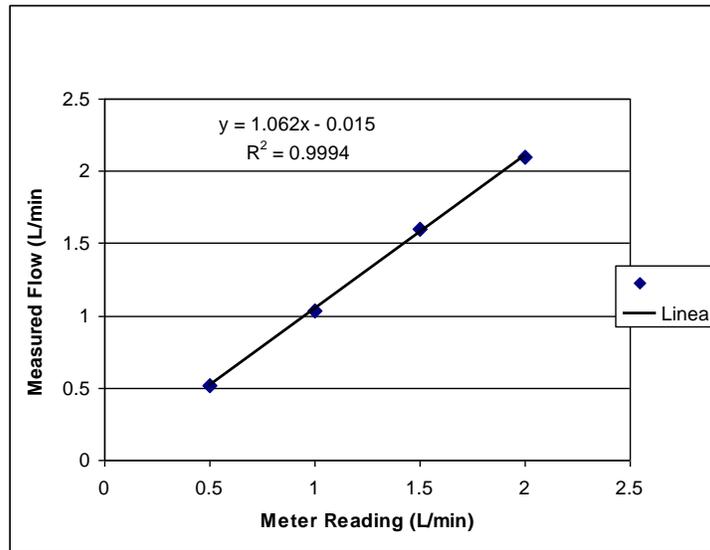


Figure 1. Calibration curve for absorption column water flow meter.

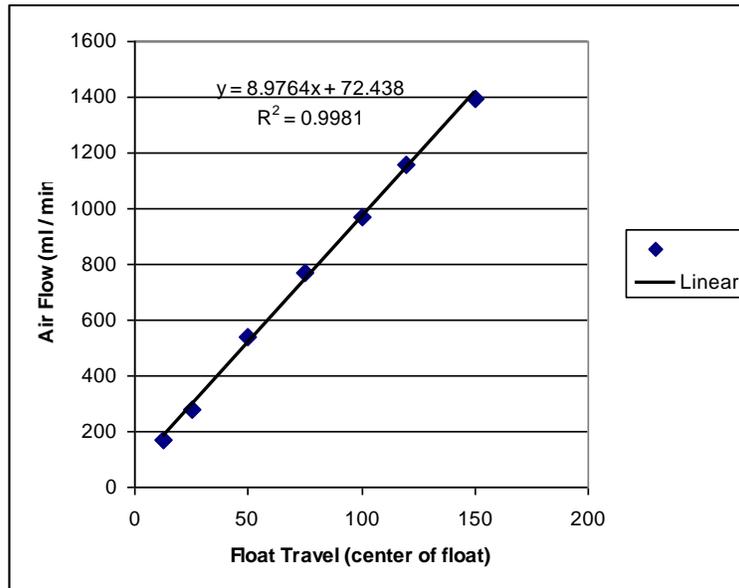


Figure 2. Calibration curve for absorption column air rotameter.

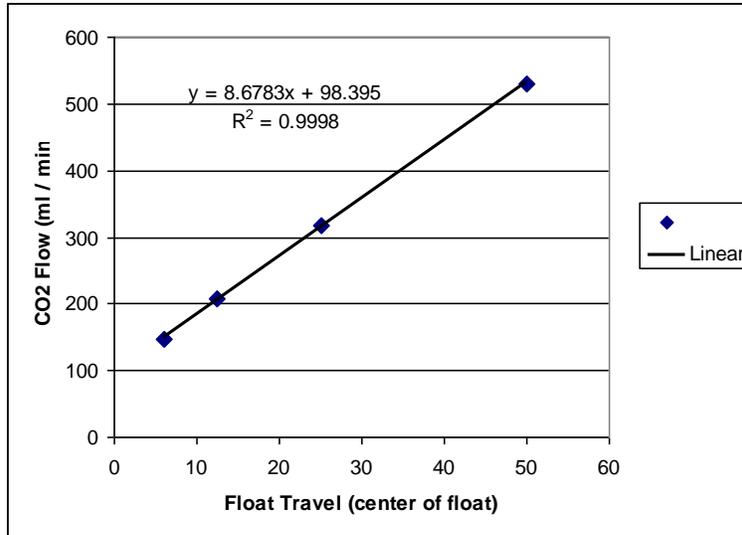


Figure 3. Calibration curve for absorption column CO<sub>2</sub> rotameter.

### References

1. McCabe, W. L., Smith, J. C., and Harriott, P., Unit Operations of Chemical Engineering, 7<sup>th</sup> Ed., McGraw-Hill, New York, (2005), p. 580.
2. Ibid, p. 581.
3. Ibid, p. 584.
4. Geankoplis, C. J., Transport Processes and Separation Process Principles, 4<sup>th</sup> Ed., Prentice Hall, Upper Saddle River, NJ, (2003), p. 686.
5. Ibid, p. 665.
6. Cussler, E. L., Diffusion: Mass Transfer in Fluid Systems, 2<sup>nd</sup> Ed., Cambridge University Press, NY, (1997), p. 260.

## APPENDIX B – LAB CALCULATIONS

### Calculating Volumetric and Molar Flows

Note: Calculations for conversions into molar flow rate are only given for one species.

Conversions for the other species were calculated using the identical formats.

CO<sub>2</sub> (L/min) entering column (Correlation given in Absorption Lab Appendix 1):

$$(8.6783 * 25) + 98.395 / 1000 = 0.3153525$$

CO<sub>2</sub> (mol/hr) entering column:

$$(0.3153525 * 10^{-3}) * \rho_{CO_2} * \left(\frac{1}{44.01}\right) * 1000 * 60 = 0.8512583$$

where

$$\rho_{CO_2} = 1.98 \text{ (kg / m}^3\text{)}$$

Amount of CO<sub>2</sub> coming out of the system:

$$(y_a * \text{Airflow (L / min)}) / (1 - y_a)$$

$$y_a = \frac{CO_2\_out}{CO_2\_out + Air\_out} = \frac{x}{(x + 1.419198 \text{ (L / min)})}$$

$$0.141(x + 1.419198 \text{ (L / min)}) = x \Rightarrow \frac{0.200107}{(1 - .141)} = .232953$$

Amount of CO<sub>2</sub> absorbed:

$$CO_2\_in \text{ (mol / hr)} - CO_2\_out \text{ (mol / hr)}$$

$$0.8512583 - 0.628831 = 0.222427$$

Amount of CO<sub>2</sub> in liquid:

$$x_b = \frac{[(\text{AirFlow (mol / hr)} + CO_2\_in \text{ (mol / hr)}) * y_b] - [(\text{AirFlow (mol / hr)} + CO_2\_out) * y_a]}{\text{WaterFlow (mol / hr)}}$$

$$[(3.523526069 + 0.8512583 * 0.186)] - [(3.523526069 + 0.232953 * 0.141)] / 171809101 = 0.000132838$$

Concentration of CO<sub>2</sub> in entering gas phase:

$$yb' = 1400 * xb = 0.185973$$

Logarithmic mean driving force:

$$\Delta yL = \frac{[(yb - yb') - (ya - ya')]}{\ln\left[\frac{yb - yb'}{ya - ya'}\right]} = 0.0164674$$

Number of Transfer Units:

$$N_{oy} = \frac{\Delta y}{\Delta yL} = 2.73266$$

Liquid mass velocity:

$$Gx = \text{Waterflow} * MW_{H_2O} * (1/1000) * (1/3600) * (1/S)$$

$$171809101 * 18.02 * (1/1000) * (1/3600) * (1/0.004560367) = 1.885813$$

Gas Mass Velocity:

$$Gy = \frac{\text{Gasflow}(kg/hr) * (1/3600)}{0.004560367} = 0.008506077$$

Gas phase film resistance:

$$Hy = \left(\frac{0.226}{f_p}\right) \left(\frac{Scy}{0.660}\right)^{0.5} \left(\frac{Gx}{6.782}\right)^{-0.5} \left(\frac{Gy}{0.678}\right)^{0.35} = 0.074412$$

Liquid phase film resistance:

$$Hx = \left(\frac{0.357}{f_p}\right) \left(\frac{Scx}{372}\right)^{0.5} \left(\frac{Gx/\mu}{6.782/(0.8937 \cdot 10^{-3})}\right)^{0.3} = 0.198482983$$

Schmidt number (Sc):

$$Sc = \frac{\mu}{\rho D_{AB}}$$

$$Scx = \frac{8.9 * 10^{-4}}{1000 * (1.6 * 10^{-9})} = 556.25$$

$$Sc_y = \frac{1.842 * 10^{-5}}{1.2 * (1.6 * 10^{-5})} = 0.959375$$

Height of a Transfer Unit:

$$H_{oy} = \frac{Z}{N_{oy}} = \frac{1.8288}{2.73266} = 0.669238$$

Mass Transfer Coefficient:

$$K_y a = \frac{V}{S * H_{oy}} = \frac{4.3747844}{(0.004560367)(0.669238)} = 1433.429134$$

Rate of Absorption:

$$W = K_y a \cdot (V_t) \cdot \Delta y L = 1433.43 \cdot (0.00834) \cdot 0.01647 = 0.19687$$

## APPENDIX C – MODEL CONVERSIONS/CALCULATIONS

Note: COMSOL reports velocity in m/s, so values calculated from the lab portion of this project were further converted to fit into the model properly.

Velocity of gas:

$$\left[ (1.419 + 0.315) \frac{L}{min} \right] * \left[ \left( \frac{1}{1000} \right) \frac{m^3}{L} \right] * \left[ \left( \frac{1}{60} \right) \frac{min}{sec} \right] * \left[ \left( \frac{1}{0.00456(S)} \right) \left( \frac{1}{m^2} \right) \right] = 0.006338$$

Velocity of liquid:

$$\left[ -(0.516) \frac{L}{min} \right] * \left[ \left( \frac{1}{1000} \right) \frac{m^3}{L} \right] * \left[ \left( \frac{1}{60} \right) \frac{min}{sec} \right] * \left[ \left( \frac{1}{0.00456(S)} \right) \left( \frac{1}{m^2} \right) \right] = -0.001886$$

Initial concentration of CO<sub>2</sub>:

Note: COMSOL accepts concentration in units of (mol/m<sup>3</sup>), unlike our reported concentrations from the absorption lab which were without units. As a result, the following conversions must be done.

$$c_{10} \left( \frac{mol}{m^3} \right) = \frac{y_{ao} P}{RT} = \frac{(0.185)(101325)}{(8.314)(298)} = 7.56$$

CO<sub>2</sub> in gas and liquid phases:

$$y_{ao} \left( \frac{mol}{m^3} \right) = \frac{c_1 * 8.314 * 298}{101325}$$

$$x_{ao} \left( \frac{mol}{m^3} \right) = \left[ \frac{c_1 * 1000}{55.55 * 101325} \right]$$

Reaction Rate:

$$-K_{ya} * (y_{ao} - Ke * x_{ao}) = -0.185 \left( \left( \frac{c_1 * 8.314 * 298}{101325} \right) - 1400 * \left( \frac{c_1 * 1000}{55.55 * 101325} \right) \right)$$



## APPENDIX E – COMSOL MODEL SUMMARY

### Table of Contents

- Title - COMSOL Model Report
- Table of Contents
- Model Properties
- Constants
- Global Expressions
- Geometry
- Geom1
- Solver Settings
- Postprocessing
- Variables

### Model Properties

Property	Value
Model name	
Author	
Company	
Department	
Reference	
URL	
Saved date	Apr 23, 2008 5:42:22 PM
Creation date	Apr 22, 2008 9:09:40 PM
COMSOL version	COMSOL 3.4.0.248

File name: R:\MQP\absorber1actualfinal.mph

Application modes and modules used in this model:

- Geom1 (Axial symmetry (2D))
  - Convection and Diffusion (Chemical Engineering Module)
  - Convection and Diffusion (Chemical Engineering Module)

### Constants

Name	Expression	Value	Description
D1	1.6e-5		diffusivity of CO2 in air
D2	1.6e-9		diffusivity of CO2 in water
v1	$(1.419+.315)*(1/1000)*(1/60)*(1/0.00456)$		velocity of gas

v2	$-(0.516) \cdot (1/1000) \cdot (1/60) \cdot (1/0.00456)$		velocity of water
c10	$0.185 \cdot 101325 / 8.314 / 298$		initial concentration of CO2 in gas
c20	0		initial concentration of CO2 in water
Kya	$770.067 / 3600$		calculated mass transfer coefficient
Ke	1400		equilibrium constant (atm)

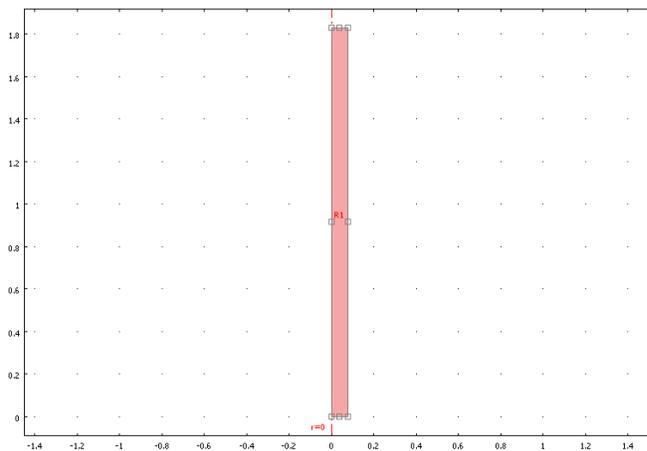
## Global Expressions

Name	Expression	Unit	Description
y	$c1 \cdot 8.314 \cdot 298 / 101325$	mol/m <sup>3</sup>	mol fraction in gas phase
x	$c2 \cdot 1000 / 55.55 / 100^3$	mol/m <sup>3</sup>	mol fraction in liquid phase

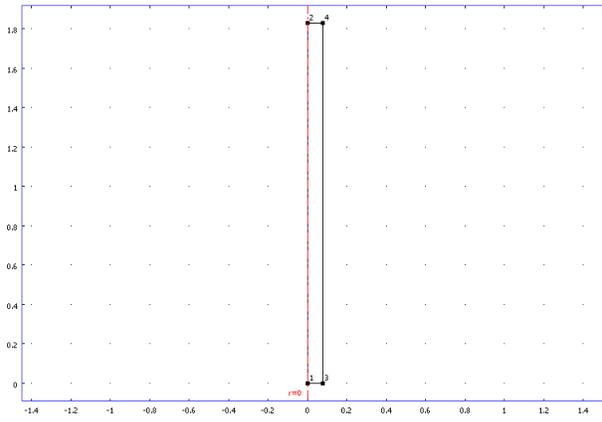
## Geometry

Number of geometries: 1

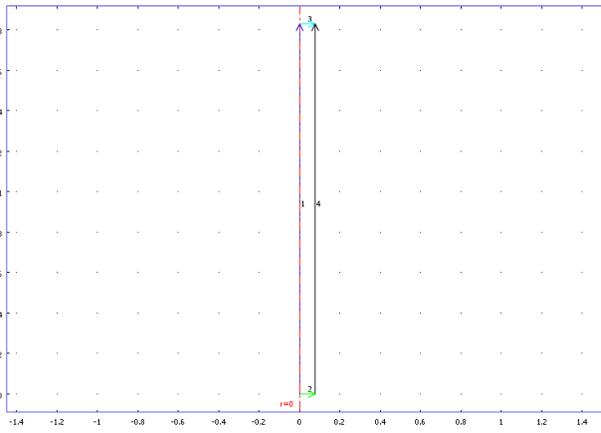
### Geom1



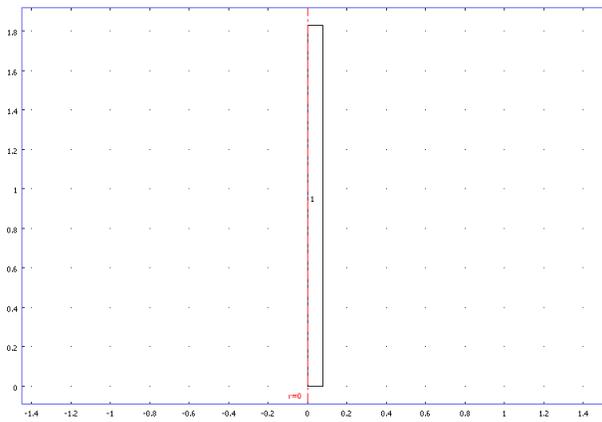
### Point mode



## Boundary mode



## Subdomain mode



## Geom1

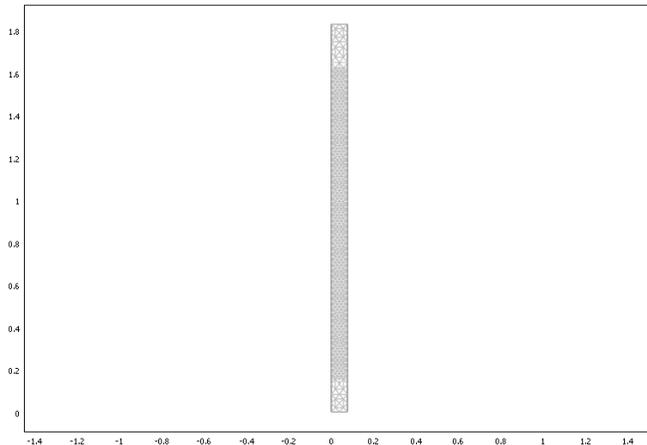
Space dimensions: Axial symmetry (2D)

Independent variables: r, phi, z

## Mesh

### Mesh Statistics

Number of degrees of freedom	4126
Number of mesh points	550
Number of elements	964
Triangular	964
Quadrilateral	0
Number of boundary elements	134
Number of vertex elements	4
Minimum element quality	0.714
Element area ratio	0.234



## Application Mode: Convection and Diffusion (chcd)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd

### Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Non-conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

## Variables

Dependent variables: c1

Shape functions: shlag(2,'c1')

Interior boundaries not active

## Boundary Settings

Boundary		4	1	2
Type		Insulation/Symmetry	Axial symmetry	Concentration
Concentration (c0)	mol/m <sup>3</sup>	0	<b>c10</b>	<b>c10</b>
Boundary		3		
Type		Convective flux		
Concentration (c0)	mol/m <sup>3</sup>	0		

## Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m <sup>2</sup> /s	<b>D1</b>
Reaction rate (R)	mol/(m <sup>3</sup> ·s)	<b>-Kya*(c1*8.314*298/101325-Ke*c2*1000/55.55/100^3)</b>
z-velocity (v)	m/s	<b>v1</b>
Subdomain initial value		1
Concentration, c1 (c1)	mol/m <sup>3</sup>	c20

## Application Mode: Convection and Diffusion (chcd2)

Application mode type: Convection and Diffusion (Chemical Engineering Module)

Application mode name: chcd2

## Application Mode Properties

Property	Value
Default element type	Lagrange - Quadratic
Analysis type	Stationary
Equation form	Non-conservative
Equilibrium assumption	Off
Frame	Frame (ref)
Weak constraints	Off
Constraint type	Ideal

## Variables

Dependent variables: c2

Shape functions: shlag(2,'c2')

Interior boundaries not active

## Boundary Settings

Boundary		4	1	2
Type		Insulation/Symmetry	Axial symmetry	Convective flux
Concentration (c0)	mol/m <sup>3</sup>	0	0	0
Boundary		3		
Type		Concentration		
Concentration (c0)	mol/m <sup>3</sup>	<b>c20</b>		

## Subdomain Settings

Subdomain		1
Diffusion coefficient (D)	m <sup>2</sup> /s	<b>D2</b>
Reaction rate (R)	mol/(m <sup>3</sup> ·s)	<b>Kya*(c1*8.314*298/101325-Ke*c2*1000/55.55/100^3)</b>
z-velocity (v)	m/s	<b>v2</b>
Subdomain initial value		1
Concentration, c2 (c2)	mol/m <sup>3</sup>	c10

## Solver Settings

Solve using a script: off

Analysis type	Stationary
Auto select solver	On
Solver	Stationary
Solution form	Automatic
Symmetric	auto
Adaption	Off

## Direct (UMFPACK)

Solver type: Linear system solver

Parameter	Value
Pivot threshold	0.1
Memory allocation factor	0.7

## Stationary

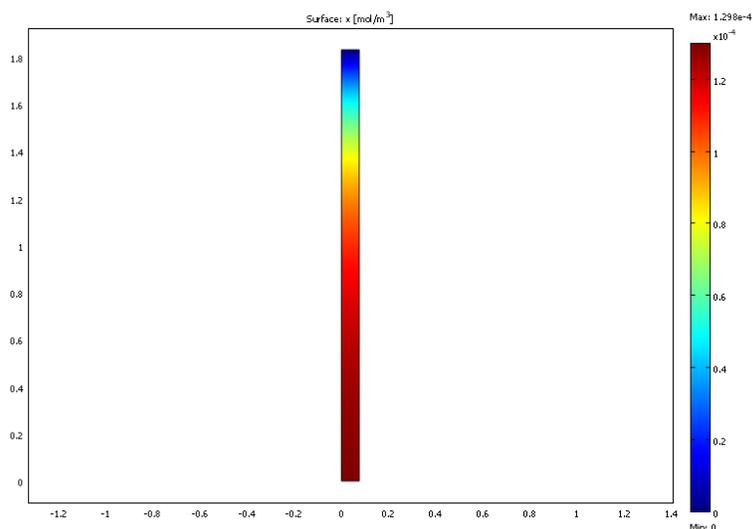
Parameter	Value
Linearity	Automatic
Relative tolerance	1.0E-6
Maximum number of iterations	25
Manual tuning of damping parameters	Off
Highly nonlinear problem	Off
Initial damping factor	1.0
Minimum damping factor	1.0E-4
Restriction for step size update	10.0

## Advanced

Parameter	Value
Constraint handling method	Elimination
Null-space function	Automatic
Assembly block size	5000
Use Hermitian transpose of constraint matrix and in symmetry detection	Off
Use complex functions with real input	Off
Stop if error due to undefined operation	On
Store solution on file	Off
Type of scaling	Automatic
Manual scaling	
Row equilibration	On

Manual control of reassembly	Off
Load constant	On
Constraint constant	On
Mass constant	On
Damping (mass) constant	On
Jacobian constant	On
Constraint Jacobian constant	On

## Postprocessing



## APPENDIX F – ASPEN PLUS INPUT SUMMARY

### RATE FRAC- MODELING ABSORPTION

;Input Summary created by Aspen Plus Rel. 20.0 at 12:46:26 Thu Apr 24, 2008

;Directory R:\Aspen Files\MQP Filename C:\DOCUME~1\yjackson\LOCALS~1\Temp\e\~ap3.tmp

TITLE 'Gas Absorption 1'

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &

HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &

VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &

MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &

MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &

PDROP=bar

DEF-STREAMS CONVEN ALL

SIM-OPTIONS ATM-PRES=1.01325

DESCRIPTION "

General Simulation with Metric Units :

C, bar, kg/hr, kmol/hr, Gcal/hr, cum/hr.

Property Method: None

Flow basis for input: Mole

Stream report composition: Mole flow

"

DATABANKS PURE20 / AQUEOUS / SOLIDS / INORGANIC / &

NOASPENPCD

PROP-SOURCES PURE20 / AQUEOUS / SOLIDS / INORGANIC

COMPONENTS

CARBO-01 CO2 /

WATER H2O /

AIR AIR

FLOWSHEET

BLOCK ABSORBER IN=LIQ-IN GAS-IN OUT=GAS-OUT LIQ-OUT

PROPERTIES NRTL

STREAM GAS-IN

SUBSTREAM MIXED TEMP=300. <K> PRES=20. <psig> &

MOLE-FLOW=4.37 <mol/hr>

MOLE-FLOW CARBO-01 0.85 <mol/hr> / WATER 0. <mol/hr> / &

AIR 3.52 <mol/hr>

STREAM LIQ-IN

SUBSTREAM MIXED TEMP=300. <K> PRES=1. <atm> &

MOLE-FLOW=1718.09 <mol/hr>

MOLE-FLOW CARBO-01 0. <mol/hr> / WATER 1718.09 <mol/hr> / &

AIR 0. <mol/hr>

BLOCK ABSORBER RATEFRAC

PARAM NCOL=1 TOT-SEGMENT=6

COL-CONFIG 1 6 CONDENSER=NO REBOILER=NO

PACK-SPECS 1 1 6 HTPACK=4.5 <ft> PACK-ARRANGE=RANDOM &

PACK-TYPE=RASCHIG PACK-MAT=GLASS PACK-DIM="8-MM" &

PACK-SIZE=8.00100E-3 SPAREA=6.290000 PACK-TENSION=73.00000 &

COL-DIAM=3. <in> VOID-FRACTIO=0.704

FEEDS LIQ-IN 1 1 / GAS-IN 1 7 ABOVE-SEGMENT

**PRODUCTS GAS-OUT 1 1 V / LIQ-OUT 1 6 L**

**P-SPEC 1 1 1. <atm>**

**COL-SPECS 1 MOLE-RDV=1.0 Q1=0.0 QN=0.0**

**RAD-FRAC –MODELING ABSORPTION**

**INPUT SUMMARY CREATED BY ASPEN PLUS REL. 20.0 AT 12:53:09 THU APR 24, 2008**

**;DIRECTORY R:\ASPEN FILES\MQP FILENAME**

**C:\DOCUME~1\YJACKSON\LOCALS~1\TEMP\E\~AP6.TMP**

**;TITLE 'GAS ABSORPTION 2'**

**IN-UNITS MET VOLUME-FLOW='CUM/HR' ENTHALPY-FLO='GCAL/HR' &**

**HEAT-TRANS-C='KCAL/HR-SQM-K' PRESSURE=BAR TEMPERATURE=C &**

**VOLUME=CUM DELTA-T=C HEAD=METER MOLE-DENSITY='KMOL/CUM' &**

**MASS-DENSITY='KG/CUM' MOLE-ENTHALP='KCAL/MOL' &**

**MASS-ENTHALP='KCAL/KG' HEAT=GCAL MOLE-CONC='MOL/L' &**

**PDROP=BAR**

**DEF-STREAMS CONVEN ALL**

**DESCRIPTION "**

**GENERAL SIMULATION WITH METRIC UNITS :**

**C, BAR, KG/HR, KMOL/HR, GCAL/HR, CUM/HR.**

**PROPERTY METHOD: NONE**

**FLOW BASIS FOR INPUT: MOLE**

**STREAM REPORT COMPOSITION: MOLE FLOW**

**"**

**DATABANKS PURE20 / AQUEOUS / SOLIDS / INORGANIC / &**

NOASPENPCD

PROP-SOURCES PURE20 / AQUEOUS / SOLIDS / INORGANIC

COMPONENTS

CARBO-01 CO2 /

WATER H2O /

AIR AIR

HENRY-COMPS HC-1 CARBO-01 AIR

FLOWSHEET

BLOCK ABSORBER IN=LIQ-IN GAS-IN OUT=GAS-OUT LIQ-OUT

PROPERTIES RK-ASPEN

PROPERTIES NRTL

PROP-DATA HENRY-1

IN-UNITS MET VOLUME-FLOW='CUM/HR' ENTHALPY-FLO='GCAL/HR' &

HEAT-TRANS-C='KCAL/HR-SQM-K' PRESSURE=BAR TEMPERATURE=C &

VOLUME=CUM DELTA-T=C HEAD=METER MOLE-DENSITY='KMOL/CUM' &

MASS-DENSITY='KG/CUM' MOLE-ENTHALP='KCAL/MOL' &

MASS-ENTHALP='KCAL/KG' HEAT=GCAL MOLE-CONC='MOL/L' &

PDROP=BAR

PROP-LIST HENRY

BPVAL CARBO-01 WATER 159.8650745 -8741.550000 -21.66900000 &

1.10259000E-3 -.150000000 79.85000000 0.0

STREAM GAS-IN

SUBSTREAM MIXED TEMP=25. PRES=1. MOLE-FLOW=4.37 <MOL/HR>

MOLE-FLOW CARBO-01 0.85 <MOL/HR> / WATER 0. <MOL/HR> / &

AIR 3.52 <MOL/HR>

**STREAM LIQ-IN**

SUBSTREAM MIXED TEMP=25. PRES=1. <ATM> &

MOLE-FLOW=3000. <MOL/HR>

MOLE-FLOW CARBO-01 0. <MOL/HR> / WATER 3000. <MOL/HR> / &

AIR 0. <MOL/HR>

**BLOCK ABSORBER RADFRAC**

PARAM NSTAGE=2

COL-CONFIG CONDENSER=NONE REBOILER=NONE

RATESEP-ENAB CALC-MODE=RIG-RATE

FEEDS LIQ-IN 1 ABOVE-STAGE / GAS-IN 2 ON-STAGE

PRODUCTS GAS-OUT 1 V / LIQ-OUT 2 L

P-SPEC 1 1.

COL-SPECS

PACK-RATE 1 1 1 RASCHIG VENDOR=GENERIC PACK-MAT=CERAMIC &

PACK-SIZE="0.25-IN" PACK-FAC=5250.000 SPAREA=7.100000 &

VOIDFR=0.62 STICH1=48. STICH2=8. STICH3=2. HETP=2. <FT> &

DIAM=3. <IN> P-UPDATE=NO

PACK-RATE2 1 RATE-BASED=YES LIQ-FILM=FILMRXN VAP-FILM=FILMRXN &

MTRFC-CORR=ONDA-68 INTFA-CORR=ONDA-68 &

PACKING-SIZE=6.35000E-3

PACK-RATE 2 2 2 RASCHIG VENDOR=GENERIC PACK-MAT=CERAMIC &

PACK-SIZE="0.25-IN" PACK-FAC=5250.000 SPAREA=7.100000 &

VOIDFR=0.62 STICH1=48. STICH2=8. STICH3=2. HETP=31. <IN> &

**DIAM=3. <IN> P-UPDATE=NO**