DEVELOPMENT OF A COMPUTER SOFTWARE FOR DESIGN AND OPTIMIZATION OF PACKED GAS ABSORPTION COLUMN

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DECLARATION

I declare that this work was carried out in its original form by me, Joseph Cornelius,of the Department of Chemical Engineering, Modibbo Adama University of Technology, Yola, Nigeria.

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Sign Date

APPROVAL PAGE

This thesis entitled “Development of a Computer Software for Design and Optimization of Packed Gas Absorption Column” meets the regulations governing the award of Master of Engineering in Chemical Engineering, Modibbo Adama University of Technology, Yola and is approved for its contribution to knowledge and literary presentation.

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DEDICATION

This work is dedicated to God Almighty, my late mother, Mrs. Roseline Joseph, and my entire family members who were instrumental to my success in life.

ACKNOLEDGEMENT

First, I wish to express my sincere gratitude to my supervisor, Prof.K.R.Onifade who supervised and guided this work to completion. His patience, humility and constructive criticisms were extremely useful in the successful execution of the work.

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Above all to God be the Glory because He stays in Heaven and watches the affairs of men. He gives us hope, provides for us in abundance, He gives us courage that our stay on earth will be to his glory through Christ our Lord.

ABSTRACT

A Computer Aided-Design module was developed for the design and optimization of packed gas absorption column. The program was tested using a problem statement. The design parameters calculated agreed with those obtained from manual solution, with a correlation coefficient of 1.000. Optimization of the total annual variable cost of the absorber and its operation was also done by studying the trend in the operating parameters. The optimum total annual variable cost for the absorber and its operation was found to be $22,480.07 per year for temperature of 0^0C, pressure drop of 21 mm H_2O/ m of packing, flooding velocity of 0.7, gas flow rate of 0.126 Kg/s and 0.016 m polypropylene packing material.

TABLE OF CONTENTS

Title Page

CHAPTER ONE

INTRODUCTION

CHAPTER TWO

LITERATURE REVIEW

CHAPTER THREE

METHODOLOGY

CHAPTER FOUR

RESULTS AND DISCUSSION

CHAPTER FIVE

CONCLUSION AND RECOMMENDATION

LIST OF TABLES

LIST OF FIGURES

LIST OF SYMBOLS

Symbols	Units
a , surface-to- volume ratio	m^2/m^3
a_w, wetted surface area	m^2
A_C, cross-sectional area of absorber(tower)	m^2
AF, absorption factor	m^2
A_S, surface area	m^2
C_A, annual cost of absorber per unit surface area	$\$/m^2$
C_E, unit cost of electricity	\$/KW-hr
C_L, solvent unit cost	
C_p, cost of packing materials	$\$/m^3$
D_c, diameter of column	m
D_L, diffusivity of solute in liquid	m^2/s
dp, packing size	m
D_v, diffusivity of solute in gas	m^2/s
$E_{(Fan + Pump)}$, power (energy) required by pump and fan	
F_P, packing factor	
F_v, flooding velocity	%
g acceleration due to gravity	
G, gas mass flow rate	kg/s

G_1, gas flow rate entering absorber	m^3/s
G_2, gas flow rate exiting absorber	m^3/s
G_l, superficial liquid flow rate entering absorber	kg/m^2s
$G_{mol,1}$, gas molar flow rate entering absorber	mol/s
$G_{mol,2}$, gas molar flow rate exiting absorber	mol/s
G_S, molar flow rate of solute free gas	mol/s
$G_{v,}$ superficial gas flow rate entering absorber	kg/m^2s
H_G, height of gas transfer unit	m
H_L, height of liquid transfer unit	m
H_{OG}, height of overall transfer units	m
H_{tower}, tower height	m
K_4, packing characteristics	
K_G, gas phase mass transfer coefficient	$Kmol/sm^2$
K_L, liquid phase mass transfer coefficient	m/s
L_1, liquid flow rate exiting absorber	m^3/s
L_2, liquid flow rate entering absorber	m^3/s
Lgr, liquid-gas flow rate ratio	
$L_{mol,\ 1}$,liquid molar flow rate exiting absorber	mol/s
$L_{mol,2}$, liquid molar flow rate entering absorber	mol/s
L_S, molar flow rate of solute free solvent	mol/s
m, slope of equilibrium curve	
m_A, molecular weight of the non-diffusing gas	kg/kg-mole
m_B, molecular weight of the diffusing gas (solute)	kg/kg-mole
ms, molecular weight of the solvent	kg/kg-mole

MW_G, molecular weight of the gas stream	kg/mole
MW_L, molecular weight of the liquid stream	kg/mole
N_{OG}, number of overall transfer units	
P, operating pressure	N/m^2
P_{ch}, Sugden's parachor	
P_p, pump operating pressure	
R, universal gas constant	bar m^3/Kmol K
T, operating temperature	K
V_m, liquid molar volume	
V_p, volume of packing materials	
W_F, waste (make-up) fraction	
X_1^*, maximum mole ratio of solute in the liquid phase if it were allowed to come to equilibrium with the solute entering the column in the gas phase	
x_1, mole fraction of solute exiting absorber in liquid	
X_1,mole ratio of solute exiting absorber in liquid	
x_2, mole fraction of solute entering absorber in liquid	
X_2, mole ratio of solute entering absorber in liquid	
Y, operating hours per year	hr/year
y_1^*, mole fraction of solute in gas phase in equilibrium with mole fraction of solute exiting in the liquid phase	
Y_1^*, mole ratio of solute in gas entering absorber in equilibrium with concentration in liquid phase	
y_1, mole fraction of solute entering absorber in gas	

Y_1, mole ratio of solute entering absorber in gas	
y_2^*, mole fraction of solute in gas phase in equilibrium with mole fraction of solute entering in the liquid phase	
y_2, mole fraction of solute exiting absorber in gas	
Y_2, mole ratio of solute exiting absorber in gas	
Zc, packing height	m

Greek Letter	unit
ΔP, pressure drop through the system	mmH_2O/m of packing
ε , combined fan and pump motor efficiency	
η, solute removal efficiency	%
μ_L, liquid viscosity	mN s/m^2
μ_v, gas viscosity	kg/m-s
ρ_G, density o the gas stream	kg/m^3
ρ_L, density o the liquid stream	kg/m^3
σ, surface tension	N/m
σ_c, critical surface tension	N/m
ϕ_L, liquid association factor	

Subscripts

A	refers to non-diffusing gas

B	refers to diffusing gas
C	refers to column, absorber, tower
c	refers to critical
E	refers to electricity
F	refers to fraction
G	refers to gas
L	refers to liquid (solvent)
m, mol	refers to molar
OG	overall gas
P	refers to pump
p	refers to packing materials
S	refers to solute free
s	refers to surface
tower	refers to tower
v	refers to velocity
w	refers to wetted
1,2	refers to inlet and outlet points

Abbreviations

CAD	Computer Aided Design
DIPPR	Design Institute for Physical Properties
ESDU	Engineering Science Data Unit
CAM	Computer-Aided Manufacturing

BASIC	Beginners All-purpose Symbolic Instruction Code
COBOL	Common Business Oriented Language
FORTRAN	Formula Translation

CHAPTER ONE

INTRODUCTION

1.1 General Introduction and Background of Study

The chemical industry has undergone significant changes during the past 35 years due to the increased cost of energy, increasingly stringent environmental regulations and global competition. One of the most important engineering tools for addressing these issues is optimization (Edgar and Himmablau, 2001). Modifications in plant design and operating procedures have been implemented to reduce cost and meet constraints, with an emphasis on improving efficiency and increasing profitability. Optimization can therefore be defined as the use of specific methods to determine the most cost-effective and efficient solution to a problem or design for a process (Edgar and Himmablau, 2001). It involves the study of optimality criteria for problems, the determination of algorithmic methods of solution, the study of the structure of such methods both under trial conditions and on real life problems.

Optimization is used to improve the initial design of equipment and to enhance the operation of that equipment once it is installed so as to realize the largest production, the greatest profit, the minimum cost, the least energy usage, and so on. In plant operations, benefits arise from improved plant performance, such as improved yields of valuable products, or reduced yields of contaminants, reduced energy consumption, higher processing rates and longer times between shutdowns. Optimization can also lead to reduced maintenance costs, less equipment wear and better staff utilization (Edgar and Himmablau, 2001).

> The task of formally optimizing the design of a complex processing plant involving several hundred variables, with complex iterations, is formidable, if not impossible (Richardson and Coulson, 1991). The task can be reduced by dividing the process into more manageable units, identifying the key variables and concentrating work where the effort involved will give the greatest benefit.

Generally, when setting out to optimize any system, the first step is to indentify clearly the objective and the criterion to be used to judge the system performance. In engineering design, the objective will invariably be an economic one. For a chemical process, the overall objective for the operating company will be to maximize profits. This will give rise to sub-objectives with which the designer will work to achieve the main objective. The main sub-objective will usually be to minimize operating costs. Other sub-objectives may be to reduce investments, maximize yield, reduce labour requirements, reduce maintenance and operate safely.

When choosing his sub- objectives, the designer must keep in mind the overall objective. Minimizing cost per unit of production will not necessarily maximize profit per unit time; market factors, such as quality and delivery may determine the best overall strategy.

The second step is to determine the objective function, the system of equations and other relationships, which relate the objective with the variables to be manipulated to optimize the function. If the objective is economic, it will be necessary to express the objective function in economic terms (costs).

The third step is to find the values of the variables that give the optimum value of the objective function. The best techniques to be used for this step wil depend on the complexity of the system and on the particular mathematical model used to represent the system.

A mathematical model represents the design as a set of equations (relationships) and it will only be possible to optimize the design if the number of variables exceeds the number of relationships, that is, there is some degree of freedom in the system.

A gas absorption column is a vertical cylinder in which liquid and gas are contacted. The packed columns are commonly used and the feed to the columns can be binary or multicomponent. The columns are characteristically operated with counter-flow of the gas and liquid. Gas absorbers are used extensively in industry for separation and purification of gas streams, as product recovery devices, and as pollution control devices. Gas absorbers are most widely used to remove water soluble inorganic contaminants from gas streams (Mclnnes et al., 1990)

Absorption is a process where one or more soluble components of a gas mixture are dissolved in a liquid (i.e. a solvent). The absorption process can be categorized as physical or chemical. Physical absorption occurs when the absorbed compound dissolves in the solvent; chemical absorption occurs when the absorbed compound and the solvent react. Liquids commonly used as solvents include water, mineral oils, nonvolatile hydrocarbon oils and aqueous solutions.

1.2 Problem Statements

There are two problems to be addressed in this work. One is to develop and test a CAD module for calculating the pertinent parameters of a packed absorption column, while the second is to extend the developed CAD module for the optimization of the design parameters as a function of the annual variable cost of the absorption column.

1.3 Aim and Objectives

The aim of this research work is to develop a Computer Aided-Design module for calculating and optimizing the design parameters of a packed gas absorption column in term of the overall annual variable cost

The overall aim will be achieved through the following:

1. Develop an objective function for the absorption column in terms of variables which relate the total annual variable cost of the column to the design parameters of the column. This constitutes the design algorithm
2. Solve the mathematical program obtained from (1) using a program developed in Visual Basic. The solution constitutes the CAD module
3. Test the program using a problem statement
4. Use the CAD module to optimize the design problem

1.4 Justification

Engineers work to improve the initial design of equipment and strive to enhance its operation once it is installed so as to realize the largest production, greatest profit, the minimum cost, the least energy usage, reduced maintenance cost and so on. Typical problems in chemical engineering process design or plant operation have many (possibly an infinite number) solutions. Optimization is concerned with selecting the best among the entire set of possible solutions by efficient quantitative methods. This involves tedious calculations, many (possibly an infinite number) iterations, reading of graphs and tables. Computers and associated software make the necessary computations feasible and cost-effective. The software (CAD module) is practically relevant as it will be developed to contain procedures for design and optimization of packed absorption column.

1.5 Scope

The scope of this project include development and testi of a CAD module for design of a packed absorption column in order to determine the pertinent design parameters of the column and to use the CAD module to optimize the design with respect to operating temperature, pressure drop, packing size and type, percent flooding velocity, and gas flow rate. The program will be developed in Visual Basic because of its user- friendliness, easier comprehension, and faster application development. The software (CAD module) is practically useful to the industry as it can be used for design and optimization of packed gas absorption column.

CHAPTER TWO

LITERATURE REVIEW

2.1 System Efficiencies and Performance

Removal efficiencies for gas absorbers vary for each solute-solvent system and with the type of absorber used. Most absorbers have removal efficiencies in excess of 90 percent, and packed tower absorbers may achieve efficiencies as high as 99.9 percent for some solute-solvent system(Treybal, 1980).

The suitability of gas absorption as a pollution control method is generally dependent on the following factors:

1. Availability of suitable solvent
2. Required removal efficiency
3. Solute concentration in the inlet vapour.
4. Capacity required for handling gas, and
5. Recovery value of the solute(s) or the disposal cost of the spent solvent (Treybal., 1980)

Physical absorption depends on properties of the gas stream and solvent, such as density and viscosity, as well as specific characteristics of the solute(s) in the gas and the liquid stream (e.g. diffusivity, equilibrium solubility). These properties are temperature dependent, and lower temperatures generally favour absorption of gases by the solvent. Absorption is also enhanced by greater contacting surface, higher liquid-gas ratios, and higher concentrations in the gas stream.

The solvent chosen to remove the solute(s) should have a high solubility for the gas, low vapour pressure, low viscosity, and should be relatively inexpensive (Treybal, 1980). Water is the most common solvent used to remove inorganic solute; it is also used to absorb organic compounds having relatively high water solubilities. For organic compounds that have low water solubilities, other solvents such as hydrocarbon oils are used, though only in industries where large volumes of these oils are available (i.e. petroleum refineries and petrochemical plants) (Jack D. Brady, personal communication June 9, 1992).

Solute removal may also be enhanced by manipulating the chemistry of the absorbing solution so that it reacts with the solute(s), e.g. caustic solution for acid-gas absorption vs. pure water as a solvent. Chemical absorption may be limited by the rate of reaction, although the rate limiting step is typically the physical absorption rate, not the chemical reaction rate.

2.2 Process Description

Absorption is a mass transfer operation in which one or more soluble compounds of a gas mixture are dissolved in a liquid that has low volatility under the process condition. The solute diffuses from the gas into the liquid when the liquid contains less than the equilibrium concentration of the gaseous component.

A properly designed gas absorber will provide thorough contact between the gas and the solvent in order to facilitate diffusion of the solute(s). It will perform much better that a poorly designed absorber (S Raymond Woll, personal communication June 25, 1992). The rate of mass transfer between the two phases is largely dependent on the surface area exposed and the time of contact. Other factors governing the absorption rate, such as the solubility of the gas in the particular solvent and the degree of the chemical reaction, are characteristics of the constituents involved and are relatively independent of the equipment used.

2.2.1 Absorber System Configuration

Gas and liquid flow through an absorber may be countercurrent, crosscurrent, or concurrent. The most commonly installed designs are countercurrent, in which the waste gas stream enters at the bottom of the absorber column and exits at the top. Conversely, the solvent stream enters at the top and exits at the bottom. Countercurrent designs provide the highest theoretical removal efficiency because gas with the lowest solute concentration contacts liquid with the lowest solute concentration. This serves to maximize the average driving force for absorption throughout the column (Mclnnes et al., 1990). Moreover, countercurrent designs usually require lower liquid to gas ratios than cocurrent and are more suitable when the solute loading is higher (Jose L. Bravo, personal communication June 8, 1992)

In a crosscurrent tower, the waste gas flows horizontally across the column while the solvent flows vertically down the column. As a rule, crosscurrent designs have lower pressure drops and require lower liquid-to-gas ratios than both cocurrent and countercurrent designs. They are applicable when gases are highly soluble, since they offer less contact time for absorption (Mclnnes et al., 1990).

In concurrent towers, both the gas and solvent enter the column at the top of the tower and exit at the bottom. Concurrent designs have lower pressure drops, are not subject to flooding limitations and are more efficient for fine (i.e. submicron) mist removal. Cocurent designs are only efficient where large absorption driving forces are available. Removal efficiency is limited since the gas-liquid system approaches equilibrium at the bottom of the tower (Mclnnes et al., 1990).

2.2.2 Types of Absorption Equipment

Devices that are based on absorption principles include packed tower, plate (or tray) columns, venturi scrubbers, and spray chambers. Packed towers are the most commonly used gas absorbers for pollution control. Packed towers are columns filled with packing materials that provide a large surface area to facilitate contact between the liquid and gas. Packed absorbers can achieve higher removal eficiencies, handle higher liquid rates, and have relatively lower water consumption requirements than other types of gas absorbers (Mclnnes et al., 1990). However, packed towers may also have high system pressure drops, high clogging and fouling potential, and extensive maintenance costs due to the presence of packing materials. Installation, operation, and spent solvent disposal costs may also be higher for packed bed absorbers than for other absorbers (Mclnnes et al., 1990). In addition to pump and fan power requirements and solvent costs, packed towers have operating costs associated with replacing damaged packing (Mclnnes et al., 1990).

Plate, or tray, towers are vertical cylinders in which the liquid and gas are contacted in stepwise fashion on trays (plates). Liquid enters at the top of the column and flows across each plate and through a downspout (downcomer) to the plates below. Gas moves upwards through openings in the plates, bubbles into the liquid, and passes to the plate above. Plate towers are easier to clean and tend to handle large temperature fluctuations better than packed towers do (Treybal., 1980). However, at high gas flow rates, plate towers exhibit larger pressure drops and have larger liquid holdups. Plate towers are generally made of materials such as stainless steel, that can withstand force of the liquid on the plates and also provide corrosion protection. Packed columns are preferred to plate towers when acids and other corrosive materials are involved because tower construction can then be of fiber glass, polyvinylchloride, or other less costly, corrosive-resistant materials. Packed towers are also preferred for columns smaller than two feet in diameter when pressure drop is an important consideration (Perry and Chilton, 1984).

Spray towers operate by delivering liquid droplets through a spray distribution system. The droplets fall through a countercurrent gas stream under the influence of gravity and contact the solute(s) in the gas (Perry and Chilton, 1984). Spray towers are simple to operate and maintain, and have relatively low energy requirements. However, they have the least effective mass transfer capability of the absorbers discussed and are usually restricted to particulate removal and control of highly soluble gases such as sulfur dioxide and ammonia. They also require higher water recirculation rates and are inefficient at removing small particles (Mclnnes et al., 1990).

2.2.3 Packed Tower Internals

A packed tower unit is comprised of a column shell, mist eliminator, liquid distributors, packing materials, packing support and may include a packing restrainer. Corrosion resistant alloys or plastic materials such as polypropylene are required for column internals when highly corrosive solvents or gases are used. A schematic drawing of a countercurrent packed tower is shown in Figure 1.1. In this figure, the packing is separated into two sections. This configuration is more expensive than designs where the packing is not so divided (Jack D. Brady, personal communication June 9, 1992).

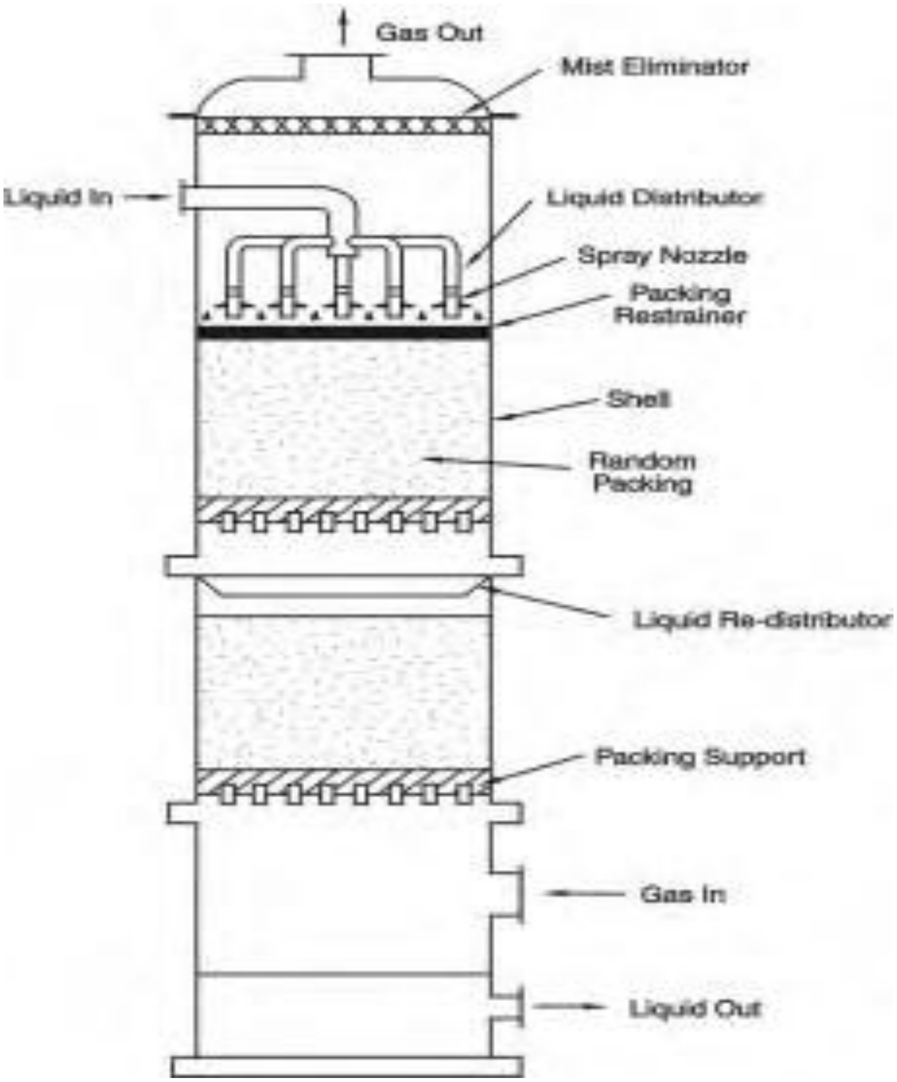


Figure 2.1: Packed Tower for Gas Absorption

The tower shell may be made of steel or plastic, or a combination of these materials depending on the corrosiveness of the gas and liquid streams, and the process operating conditions. One alloy that is chemical and temperature resistant or multiple layers of different, less expensive materials may be used. The shell is sometimes lined with a protective membrane, often made from a corrosion resistant polymer. For absorption involving acid gases, an interior layer of acid resistant brick provides additional chemical and temperature resistance (Crowe et al., 1988).

At high gas velocities, the gas exiting the top of the column may carry off droplets of liquid as a mist. To prevent this, a mist eliminator in the form of corrugated sheets or a layer of mesh can be installed at the top of the column to collect the liquid droplets, which coalesce and fall back into the column.

A liquid distributor is designed to wet the packing bed evenly and initiate uniform contact between the liquid and the vapour. The liquid distributor must spread the liquid uniformly, resist plugging and fouling, provide free space for gas flow, and allow operating flexibility (Harrison et al., 1989). Large towers frequently have a liquid redistributor to collect liquid off the column wall and direct it toward the centre of the column for redistribution and enhanced contact in the lower section of packing (Treybal, 1980). Liquid redistributors are generally required for every 8 to 20 feet of random packing depth (Coker, 1991).

Distributors fall into two categories: gravitational types, such as orifice and weir types, and pressure-drop types, such as spray nozzles and perforated pipes. Spray nozzles are the most common distributors, but they may produce a fine mist that is easily entrained in the gas flow. They also may plug and usually require high feed rates to compensate for poor distribution. Orifice-type distributors typically consist of flat trays with a number of risers for vapour flow and perforations in the tray floor for liquid flow. The trays themselves may present a resistance to gas flow (Harrison et al.,1989). However, better contact is generally achieved when orifice distributors are used.

Packing materials provide a large wetted surface for the gas stream maximizing the area available for mass transfer. Packing materials are available in a variety of forms, each having specific characteristics with respect to surface area, pressure drop, weight, corrosion resistance, and cost. Packing life varies depending on the application. In ideal circumstances, packing will last as long as the tower itself. In adverse environments packing life may be as short as 1 to 5 years due to corrosion, fouling and breakage (Roy Oommen, personal communication April 4,1992). Packing materials are categorized as random or structured. Random packings are usually dumped into an absorption column and allowed to settle. Modern random packings consist of engineered shapes intended to maximize surface-to-volume ratio and minimize pressure drop (Mclnnes et al., 1990). Examples of different random packings are presented in Figure 2.

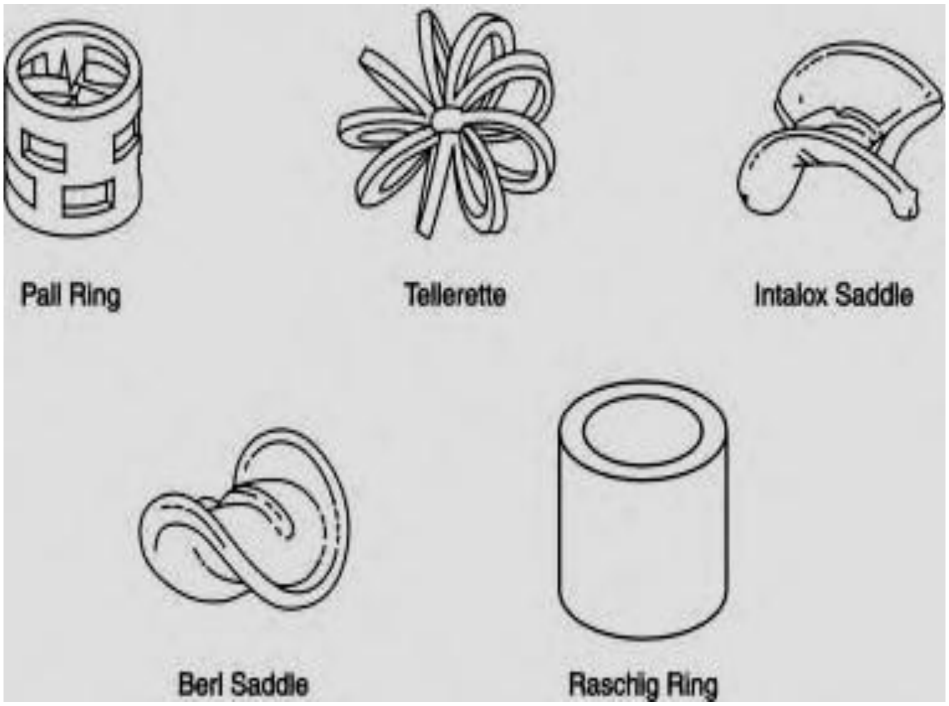


Figure 2.2: Various Forms of Random Packing Materials

The first random packings specifically designed for absorption towers were made of ceramic. The use of ceramic has declined because of their brittleness, and the current markets are dominated by metal and plastic. Metal packings cannot be used for highly corrosive pollutants, such as acid gas, and plastic packings are not suitable for high temperature applications. Both plastic and metal packings are generally limited to an unsupported depth of 20 to 25 feet. At higher depths the weight may deform packing (Coker, 1991).

Structured packing may be random packings connected in an orderly arrangement, interlocking grids, or knitted or woven wire screen shaped into cylinders or gauze like arrangements. They usually have smaller pressure drops and are able to handle greater solvent flow rates than random packing (Treybal, 1980). However, structured packings are more costly to install and may not be practical for smaller columns. Most structured packings are made from metal or plastic.

In order to ensure that the gas is well distributed, an open space between the bottom of the tower and the packing is necessary. Support plates hold the packing above the open space. The support plates must have enough strength to carry the weight of the packing, and enough free area to allow solvent and gas to flow with minimum restrictions (Treybal, 1980).

High gas velocities can fluidize packing on top of a bed. The packing could then be carried into the distributor, become unlevel, or be damaged (Harrison et al., 1989). A packing restrainer may be installed at the top of the packed bed to contain the packing. The packing restrainer may be secured to the wall so that column upsets will not dislocate it, or a "floating" unattached weighted plate may be placed on top of the packing so that it can settle with the bed. The latter is often used for fragile ceramic packing.

2.2.4 Packed Tower Operation

The most common packed tower designs are countercurrent. As the waste gas flows up the packed column it will experience a drop in its pressure as it meets resistance from the packing materials and the solvent flowing down. Pressure drop in a column is a function of the gas and liquid flow rates and properties of the packing elements, such as surface area and free volume in the tower. A high pressure drop results in high fan power to drive the gas through the packed tower and consequently high costs. The pressure drop in a packed tower generally ranges from 0.5 to 1.0 in.H_2O/ft of packing (Perry and Chilton,1984).

For each column, there are upper and lower limits to solvent and vapour flow rates that ensure satisfactory performance. The gas flow rate may become so high that the drag on the solvent is sufficient to keep the solvent from flowing freely down the column. Solvent begins to accumulate and blocks the entire cross section for flow, which increases the pressure drop and prevents the packing from mixing the gas and solvent effectively. When all the free volume in the packing is filled with liquid and the liquid is carried back up the column, the absorber is considered to be flooded (Treybal, 1980). Most packed towers operate at 60 to 70 percent of the gas flooding velocity, as it is not practical to operate a tower in a flooded condition (Perry and Chilton, 1984). A minimum liquid flow rate is also required to wet the packing materials sufficiently for effective mass transfer to occur between the gas and liquid (Perry and Chilton, 1984).

The gas inlet temperature is another important scrubbing parameter. In general, the higher the gas temperature, the lower the absorption rate, and vice-versa. Excessively high gas temperatures also can lead to significant solvent loss through evaporation. Consequently, precoolers e.g. spray chambers) may be needed to reduce the air temperature to acceptable levels (S Raymond Woll, personal communication June 25, 1992)

For operations that are based on chemical reaction with absorption, an additional concern is the rate of reaction between the solvent and solute(s). Most gas absorption chemical reactions are relatively fast and the rate limiting step is the physical absorption of the solutes into the solvent. However, for solvent-solute systems where the chemical reaction is the limiting step, the rates of reaction would need to be analyzed kinetically.

2.3 Design Procedures

The design of packed tower absorbers for controlling gas streams containing a mixture of solute and air depends on knowledge of the following parameters:

(a) Gas flow rate;
(b) Gas composition and concentration of the solutes in the gas stream;
(c) Required removal efficiency;
(d) Equilibrium relationship between the solute(s) and solvent; and
(e) Properties of the solute(s), gas, and solvent: diffusivity, viscosity, density, and molecular weight.

The primary objectives of the design procedures are to determine column surface area and pressure drop through the column. In order to determine these parameters, the following steps must be performed:

(a) Determine the gas and liquid stream conditions entering and exiting the column.
(b) Determine the absorption factor (AF).
(c) Determine the diameter of the column (D_C).
(d) Determine the tower height (H_{tower}) and surface area (A_S).
(e) Determine the packed column pressure drop (ΔP).

To simplify the sizing procedures, a number of assumptions have been made. For example, the gas is assumed to comprise a two-component gas mixture (solute/air), where the solute consists of a single compound present in dilute quantities. The gas is assumed to behave as an ideal gas and the solvent is assumed to behave as an ideal solution. Heat effects associated with absorption are considered to be minimal for the solute concentrations encountered. The procedures also assume that, chemical reaction does not occur.

The design procedures presented here are complicated, and careful attention to units is required.

2.3.1 Determining Gas and Liquid Stream Conditions

Gas absorbers are designed based on the ratio of liquid to gas entering the column (L/G), slope of the equilibrium curve (m), and the desired removal efficiency (η). These factors are calculated from the inlet and outlet gas and liquid stream variables:

(a) Gas flow rate, in cubic meter per second (m^3/s), entering and exiting column (G_1 and G_2, respectively);

(b) Solute concentration (kg-moles solute per kg-mole of solute free gas) entering and exiting the column in the gas (Y_1 and Y_2, respectively);

(c) Solvent flow rate, in cubic meter per second (m^3/s), entering and exiting the column (L_2 and L_1, respectively); and

(d) Solute concentration (kg-moles solute per kg-mole of solute free solvent) entering and exiting the column in the solvent (X_2 and X_1, respectively).

This design approach assumes that the inlet gas stream variables are known, and that a specific solute removal efficiency has been chosen as the design basis; i.e., the variables G_1, Y_1, and η are known. For dilute concentrations typically encountered in pollution control applications and negligible changes in moisture content, G_1 is assumed equal to G_2. If a once-through process is used, or if the spent solvent is regenerated by an air stripping process before it is recycled, the value of X_i will approach zero. The following procedures must be followed to calculate the remaining stream variables Y_2, L_2 (and L_1), and X_1. A schematic diagram of a packed tower with inlet and outlet flow and concentration variables labeled is presented in Figure 2.3.

The exit solute concentration, Y_2, may be calculated from the following equation:

$$Y_2 = Y_1\left(1 - \frac{\eta}{100}\right) \qquad (2.1)$$

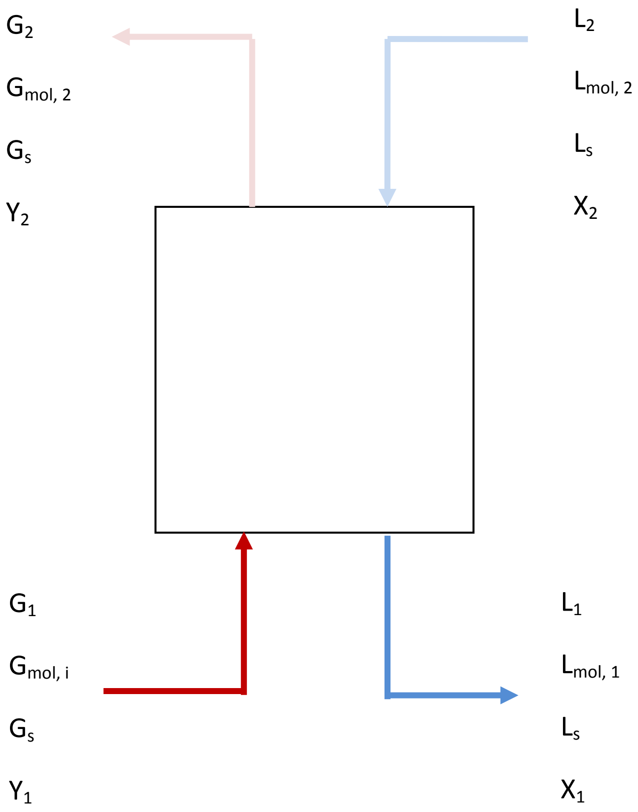


Figure 2.3: Schematic diagram of countercurrent packed bed

The liquid flow rate entering the absorber, L_2 (m^3/s), is then calculated using a graphical method. Figure 2 4 presents an example of an equilibrium curve and operating line. The equilibrium curve indicates the relationship between the concentration of solute in the gas and the concentration of solute in the solvent at a specified temperature. The operating line indicates the relation between the concentration of the solute in the gas and solvent at any location in the gas absorber column. The vertical distance between the operating line and equilibrium curve indicates the driving force for diffusion of the solute between the gas and liquid phases. The minimum amount of liquid which can be used to absorb the solute in the gas stream corresponds to an operating line drawn from the outlet concentration in the gas stream (Y_2) and the inlet concentration in the solvent stream (X_2) to the point on the equilibrium curve corresponding to the entering solute concentration in the gas stream (Y_1). At the intersection point on the equilibrium curve, the diffusional driving forces are zero, the required time of contact for the concentration change is infinite, and an infinitely tall tower results.

The slope of the operating line intersecting the equilibrium curve is equal to the minimum *L/G* ratio on a moles of solute-free solvent (L_s) per moles of solute-free basis G_s, in other words, the values L_s and G_s do not include the moles of solute in the liquid and gas streams. The values of Ls and Gs are constant through the column if a negligible amount of moisture is transferred from the liquid to the gas phase. The slope may be calculated from the following equations:

$$\left(\frac{L_s}{G_s}\right)_{min} = \frac{Y_1 - Y_2}{{X_1}^* - X_2} \tag{2.2}$$

Where ${X_1}^*$ would be the maximum concentration of the solute in the liquid phase if it were allowed to come to equilibrium with the solute entering the column in the gas phase, Y_1. The value of X^*_1 is taken from the equilibrium curve. Because the minimum L_s/G_S, ratio is an unrealistic value, it must be multiplied by an adjustment factor, commonly between 1.2 and 1.5, to calculate the actual L/G ratio (Perry and Chilton, 1984):

$$\left(\frac{L_S}{G_S}\right)_{act} = \left(\frac{L_S}{G_S}\right)_{min} * (adjustment\ factor) \qquad (2.3)$$

The variable Gs may be calculated using the equation:

$$G_S = \frac{\rho_G\, G_1}{MW_G(1 + Y_1)} \qquad (2.4)$$

Where MW_G is the molecular weight of the gas stream (kg/kg-mole), and ρ_G is the density o the gas stream (kg/m^3). For solute concentrations typically encountered, the molecular weight and density of the waste gas are assumed to be equal to that of ambient air.

The variable L_s may be calculated by:

$$L_S = \left(\frac{L_S}{G_S}\right)_{act} * \ G_S \qquad (2.5)$$

The total molar flow rates of the gas and liquid entering the absorber $(G_{mol,1}\ and\ L_{mol,2})$ are calculated using the following equations:

$$G_{mol,1} = G_S\ (1 + Y_1) \qquad (2.6)$$

$$L_{mol,2} = L_S\ (1 + X_2) \qquad (2.7)$$

The volume flow rate of the solvent, L_2, may then be calculated by using the following relationship:

$$L_2 = \frac{L_{mol,2} MW_L}{\rho_L} \qquad (2.8)$$

Where MW_L is the molecular weight of the liquid stream (kg/kg-mole), ρ_L is the density of the liquid stream (kg/m^3). If the volume change in the liquid stream entering and exiting the absorber is assumed to be negligible, then $L_2 = L_1$.

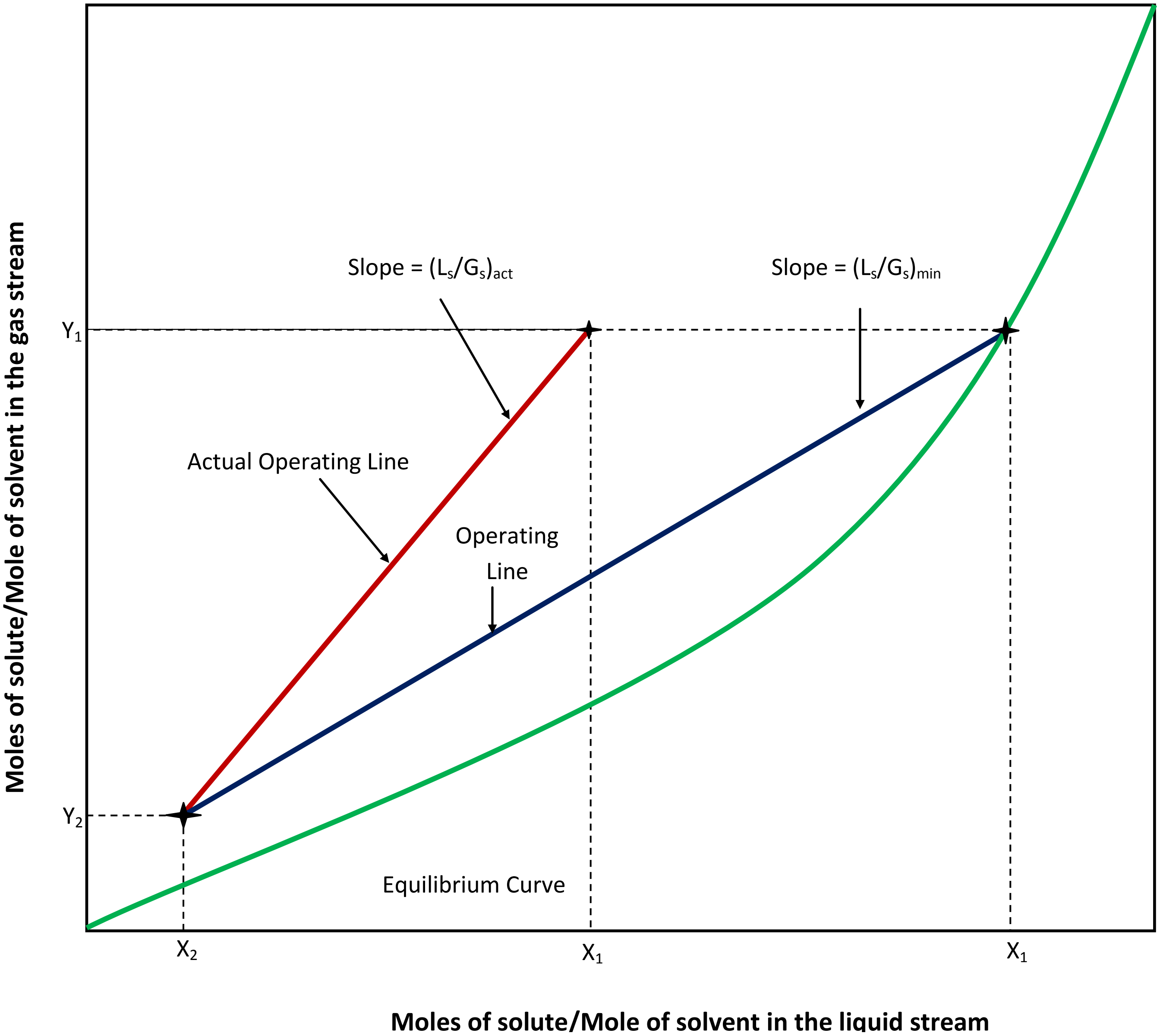


Figure 2.4: Minimum and Actual Liquid-to-Gas Ratio

Finally, the actual operating line may be represented by a material balance equation over the gas absorber (Treybal, 1980):

$$X_2L_s + Y_1G_s = X_1L_s + Y_2G_s \qquad (2.9)$$

Equation (2.9) may then be solved for X_1:

$$X_1 = \frac{Y_1 - Y_2}{\left(\frac{L_S}{G_S}\right)} + X_2 \qquad (2.10)$$

2.3.2 Determining Absorption Factor

The absorption factor (*AF*) value is frequently used to describe the relationship between the equilibrium line and the liquid-to-gas ratio. For many solute-solvent systems, the most economical value for *AF* ranges around 1.5 to 2.0 (Perry and Chilton, 1984). The following equations may be used to calculate *AF* (Perry and Chilton, 1984):

$$AF = \frac{L_{mol,\ 2}}{mG_{mol,1}} \qquad (2.11)$$

Where m is the slope of the equilibrium line on a mole fraction basis. The value m may be obtained from available literature on vapour-liquid equilibrium data for specific systems. Since the equilibrium curve is typically linear in the concentration ranges usually encountered, the slope, m would be constant (or nearly so) for all applicable inlet and outlet liquid and gas streams. The slope may be calculated from mole fraction values using the following equation (Treybal, 1980).

$$m = \frac{y_2^* - y_1^*}{x_1 - x_2} \qquad (2.12)$$

Where y_1^* and y_2^* are the mole fractions of the solute in the vapour phase in equilibrium with the mole fractions of the solute entering and exiting the absorber in the liquid, x_2 and x_1, respectively. The slope of the equilibrium line in Figure 2.4 is expressed in terms of concentration values X_2, X_1, Y_1^* and Y_2^*. These values may be converted to x_2, x_1, y_1^* and y_2^* using the equations:

$$x_2 = \frac{X_2}{1 + X_2} \tag{2.13}$$

$$x_1 = \frac{X_1}{1 + X_1} \tag{2.14}$$

$$y_1^* = \frac{Y_1^*}{1 + Y_1^*} \tag{2.15}$$

$$y_2^* = \frac{Y_2^*}{1 + Y_2^*} \tag{2.16}$$

2.3.3 Determining Column Diameter

Once stream conditions have been determined, the column diameter may be estimated. One of the designs is based on selecting a fraction of gas flow rate at flooding conditions.

Eckert's modification to the generalized correlation for randomly packed towers based on flooding considerations (pdnengineers, 2011) is used to obtain the superficial gas flow rate entering the absorber, g_v *(kg/s-m^2)* or the gas flow rate per cross sectional area based on the L_{mol}/G_{mol} ratio calculated. The cross-sectional area (A) of the column and the column diameter (D_c)

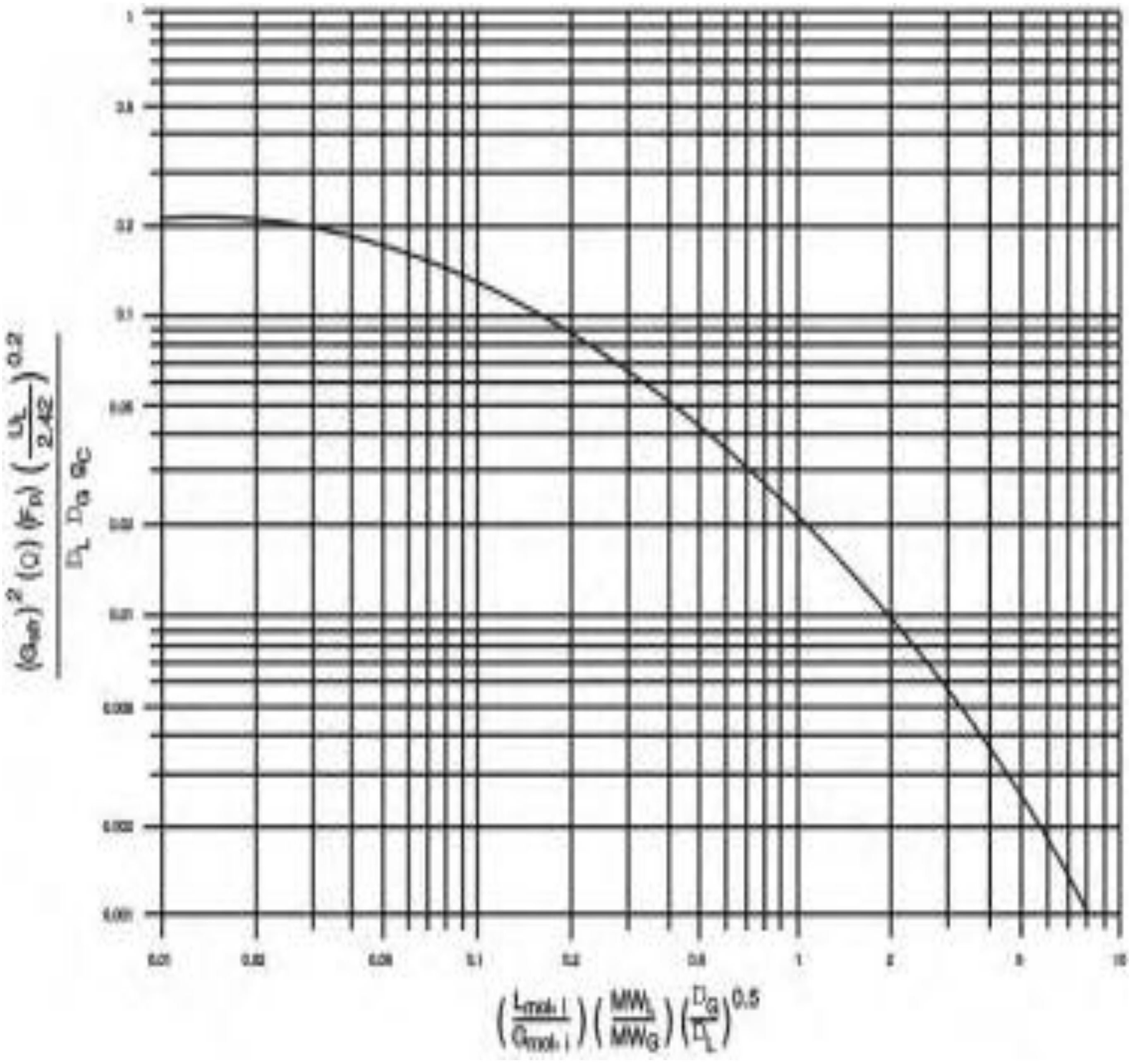


Figure 2.5: Eckert's Modification to the Generalized Correlation at Flooding Rate

can then be determined from g_v. Figure 2.5 presents the relationship between g_v and L_{mol}/G_{mol} ratio at the tower flood point. The x-axis in the graph is expressed as (Coker, 1991):

$$Abscissa = \frac{L_{mol,i}}{G_{mol,i}} \left(\frac{MW_L}{MW_G}\right) \sqrt{\frac{\rho_G}{\rho_L}} \tag{2.17}$$

The ordinate value (y-axis) in the graph is expressed as (Coker, 1991):

$$Ordinate = \frac{(g_v)^2 \, \varphi \, F_p \, (\mu_L)^{0.2}}{\rho_L \rho_G \, g_c} \tag{2.18}$$

Where F_p is a packing factor, g_c is the gravitational constant, μ_L is the viscosity of the solvent in centipoise, and φ is the ratio of density of the scrubbing liquid to water. The value of F_p may be obtained from packing vendors (Appendix B, Table B.1). After the Abscissa value is calculated, a corresponding ordinate value may be determined from the flooding curve. The ordinate may also be calculated using the following equation (Coker, 1991):

$$Ordinate = 10^{[-1.668-1.085 \ (\log Abscissa) - \ 0.297 \ (\log A)^2]} \tag{2.19}$$

Equation 2.18 may then be rearranged to solve for g_v.

$$g_v = \frac{\rho_L \, \rho_g \, g_c \, (ordinate)}{F_p \, \varphi \, (\mu_L)^{0.2}} \tag{2.20}$$

The cross-sectional area of the tower (m^2) is calculated as:

$$A_c = \frac{G_{mol} \, MW_G}{g_v F_v} = \frac{G}{g_v F_v} \tag{2.21}$$

Where F_v is the flooding factor. To prevent flooding, the column is operated at a fraction of g_v. The value of F_v typically ranges from 0.50 to 0.75 (Perry and Chilton, 1984).

The diameter of the column (D_c) can be calculated from the cross-sectional area by:

$$D_c = \sqrt{\frac{4}{\pi} A_c} \qquad (2.22)$$

The superficial liquid flow rate entering the absorber, $G_L(\frac{kg}{m^2 s})$ based on the cross-sectional area determined in equation (2.21) is calculated from the equation:

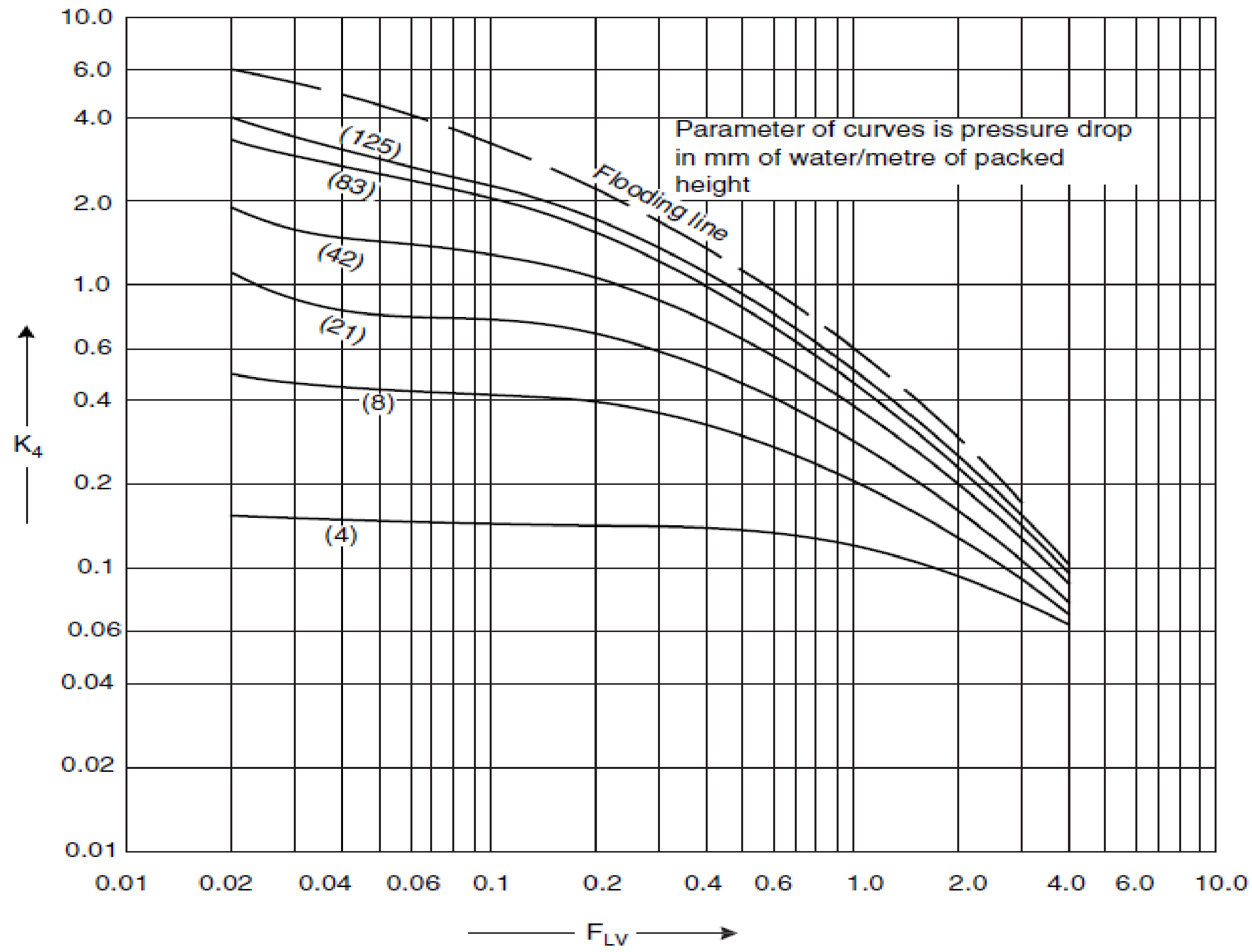
$$G_L = \frac{M_L MW_L}{A_c} \qquad (2.23)$$

The diameter of a column can be designed for a specific pressure drop rather than being determined based on a fraction of the flooding rate. Figure 2.6 presents the relationship between g_v and L_{mol}/G_{mol} ratio. In this case, liquid-gas flow rate (x-axis of the correlation chart) is given by (Coulson and Richardson, 1991):

$$Lgr = \frac{L_{mol\,2}\, MW_L}{G_{mol\,1}\, MW_G} \left(\sqrt{\frac{\rho_G}{\rho_L}}\right) \qquad (2.24)$$

Therefore, the superficial gas flow rate entering the absorber is given by (Coulson and Richardson, 1991):

$$g_v = \left[\frac{k_4 \rho_G (\rho_L - \rho_G)}{13.1 * F_p \left(\frac{\mu_L}{\rho_L}\right)^{0.1}}\right]^{1/2} \qquad (2.25)$$



$$F_{LV} = \frac{L_W^*}{V_W^*}\sqrt{\frac{\rho_V}{\rho_L}}$$

Figure 2. 6 : Generalised Pressure Drop Correlation

Where k_4 is the packing characteristics at the liquid-gas flow rate ratio, F_p is the packing factor. μ_L is the liquid viscosity. The remaining calculations to estimate the column diameter and G_L are the same as in the first method except the flooding factor F_v is not used in the equations. The flooding factor is not required because an allowable pressure drop that will not cause flooding is chosen to calculate the diameter rather than designing the diameter at flooding conditions and then taking a fraction of that value.

2.3.4 Determining Tower Height and Surface Area

Tower height is primarily a function of packing depth. The required depth of packing (*Z_c*) is determined from the theoretical number of overall transfer units N_{OG} needed to achieve a specific removal efficiency, and the height of the overall transfer unit (*H_{OG}*) (Treybal, 1980).

$$Z_c = N_{OG} H_{OG} \qquad (2.27)$$

The number of overall transfer units may be estimated graphically by stepping off stages on the equilibrium-operating line graph from inlet conditions to outlet conditions, or by the following equation (Treybal, 1980):

$$N_{OG} = \frac{Ln\left[\left(\frac{y_1 - mx_2}{y_2 \;\; mx_2}\right)\left(1 - \frac{1}{AF}\right) + \frac{1}{AF}\right]}{1 - \frac{1}{AF}} \qquad (2.28)$$

Where *AF* is the absorption factor, ln is the natural logarithm of the quantity indicated. *N_{OG}* can also be estimated by the following equation:

$$N_{OG} = \frac{y_1 - y_2}{\Delta y_{lm}} \qquad (2.29)$$

$$\Delta y_{lm} = \frac{\Delta y_1 - \Delta y_2}{ln\frac{\Delta y_1}{\Delta y_2}} \qquad (2.30)$$

$$\Delta y_1 = y_1 - y_1^* \qquad (2.31)$$

$$\Delta y_2 = y_2 - y_2^* \qquad (2.32)$$

There are several methods that may be used to calculate the height of the overall transfer unit, all based on empirically determined packing constants. One commonly used method involves determining the overall gas and liquid mass transfer coefficient (*K_G*, *K_L*). A major difficulty in using this approach is that the values of K_G and K_L are frequently unavailable for the specific solute-solvent systems of interest. The method that will be used in this work is based on estimating the height of the gas and liquid film transfer units, H_L and H_G, respectively (Treybal, 1980).

$$H_{OG} = H_G + \frac{1}{AF} H_L \tag{2.33}$$

$$AF = \frac{M g_v F_v}{G_L} \tag{2.34}$$

The following correlations may be used to estimate values for H_L and H_G.

$$H_G = \frac{g_v F_v}{m_A K_G a_w P} \tag{2.35}$$

Where m_A is the molecular weight of the non-diffusing gas, K_G is the gas phase mass transfer coefficient, a_w is the wetted surface area, P is the operating pressure. K_G is given by:

$$K_G = \left[\frac{aD_v}{RT}\right] C_1 \left[\frac{g_v}{a\mu_v}\right]^{0.7} \left[\frac{\mu_v}{\rho_v D_v}\right]^{\frac{1}{3}} [a * dp]^{-2.0} \tag{2.36}$$

Where C_1 = 5.23 for packing size above 15 mm and 2.00 for sizes below 15 mm. D_v is gas diffusivity and is given by:

$$D_v = \frac{1.103\ x\ 10^{-7} * (T+273)^{1.75} (\frac{1}{mA} + \frac{1}{mB})^{0.5}}{P\left[(\Sigma_A V_i)^{\frac{1}{3}} + (\Sigma_B V_i)^{\frac{1}{3}}\right]} \tag{2.37}$$

$$\frac{a_w}{a} = 1 - exp\left[-1.45 \left(\frac{\sigma_c}{\sigma}\right)^{0.75} \left(\frac{G_L}{a\mu_L}\right)^{0.1} \left(\frac{G_L^2\, a}{\rho_L^2 g}\right)^{-0.05} \left(\frac{G_L^2}{\rho_L \sigma_a}\right)^{0.2}\right] \tag{2.38}$$

Where σ is the surface tension and is given by:

$$\sigma = \left[\frac{P_c h * \rho_L}{ms}\right]^4 * 10^{-15} \tag{2.39}$$

σ_c is the critical surface tension.

$$K_L \left[\frac{\rho_L}{\mu_L g}\right]^{\frac{1}{3}} = 0.0051 \left(\frac{G_L}{a_w \mu_L}\right)^{\frac{2}{3}} \left(\frac{\mu_L}{\rho_L D_L}\right)^{\frac{-1}{2}} (a * dp)^{0.4} \tag{2.40}$$

Where D_L is the liquid diffusivity and is given by:

$$D_L = \frac{1.173 * 10^{-3} (AF * ms)^{0.5} * T}{\mu_L * V_m^{0.6}} \tag{2.41}$$

T is the temperature of the solvent in Kelvin.

$$H_L = \frac{G_L}{(K_L * a_w * \rho_L)} \tag{2.42}$$

The height of the column may be calculated from the following correlation (M.W.Vatavuk, personal communication March 27, 1992):

$$H_{tower} = 1.40\, Z_C + 1.02\, D_C + 2.81 \tag{2.43}$$

The surface area of the gas absorber can be calculated using the equation (M.W.Vatavuk, personal communication March 27, 1992):

$$A_S = \pi D_C \left(H_{tower} + \frac{D_C}{2}\right) \tag{2.44}$$

2.4 General Design Information and Data

Information on manufacturing processes, equipment parameters, cost and physical properties of process materials are needed at all stages of design (Richardson and Coulson, 1991). The information on manufacturing processes available in the general literature can be used at the initial stages of process design, for screening potential process, it is usually mainly descriptive, and too superficial to be of much use for detailed design and evaluation.

Chemical process industries are competitive and the information that is published on commercial processes is restricted. The article on particular processes published in technical literatures and in textbooks invariably gives only superficial account of the chemistry and unit operation used. They lacked the detailed information needed on reaction kinetics, process conditions, equipment parameters, and physical properties needed for the process design. The most comprehensive collection of information on manufacturing processes is found in the Kirk Orthman Encyclopedia of Chemical Technology (1991), which covers the whole range of chemical and associated products. Another encyclopedia covering manufacturing processes is the Ketta encyclopedia (1977). Several books have also been published which give brief summaries of the production processes used for the commercial chemicals and chemical products. The most well known of these is Shreve's Book on the Chemical Process Industries, now updated by Austin (1984). More up to date descriptions of the processes in current use can be found in the technical journal such as Hydrocarbon Processing, which publishes an annual review of petrochemical processes, which was entitled Petrochemical Development and is now called Petrochemical Notebook. This publication gives flow-diagrams and brief process descriptions of new process developments. Patents are useful source of information but it should be remembered that the patentee will try to write the patent in a way that protects his invention, by disclosing the least amount of useful information because of the competitors.

2.4.1 Source of Physical Properties

International Critical Tables (1933) is still probably the most comprehensive compilation of physical properties, and is available in most reference libraries (Richardson and Coulson, 2004). Though it was first published in 1933, physical properties do not change except in as much as experimental techniques improve, and ICT is still a source of engineering data.

Tables and graphs of physical properties are given in many handbooks and textbooks on chemical engineering and related subjects. Many of the data given are duplicated from book to book, but the various handbooks provide quick, easy access to data on the more commonly used substances.

An extensive compilation of thermo-physical data has been published by Plenum Press, Touloukian (1970-77). This multiple volume work covers conductivity, specific heat, thermal expansion, viscosity and radiation properties (emittance, reflectance, absorptance and transmittance). Elsevier publishing company have published a series of volumes on physical properties and thermodynamic data.

The Engineering Science Data Unit (ESDU) was set up to provide authenticated data for engineering design. Its publications include some physical property data and other design data and method of interest to chemical engineering designers. They also cover data and methods used in the mechanical design of the equipment, caution should be exercised when taking data from the literature, as topographical errors often occur. If a value looks doubtful it should be cross-checked in an independent reference, or by estimation.

The results of research work on physical properties are reported in the general engineering and scientific literature. The Journal of Chemical Engineering Data specialized in publishing physical property data for use in chemical engineering design. A quick search of the literature for data can be made by using the abstracting journals, such as Chemical Abstracts (America Chemical Society) and engineering index (Engineering Index Incorporated New York).

Computerized physical property data banks have been set up by some organizations (Richard and Coulson, 2004) to provide a service to the design engineers. They can be incorporated into computer aided design programs and are increasingly being used to provide reliable, authenticated, design data.

2.4.2 Prediction of Physical Properties

Whenever possible, experimentally determined values of physical properties should be used. If reliable values cannot be found in the literature and if time or facilities are not available for their determination, then in order to proceed with the design, the designer must resort to estimation. Techniques are available for the prediction of most physical properties with sufficient accuracy for use in process and equipment design (Richardson and Coulson, 2004).

Group contribution techniques, which are based on the concept that a particular physical property of a compound can be considered to be made up of contributions from the constituent atoms, groups and bonds, the contribution being determined from experimental data, provide the designer with simple, convenient methods for physical property estimation, requiring only a knowledge of the structural formula of the compound.

Also useful and convenient to use, are prediction methods based on the use of reduced properties (corresponding states); provided that values for critical properties are available or can be estimated with sufficient accuracy.

The property program developed by the Design Institute for Physical Properties of the American Institute of Chemical Engineers known as DIPPR is widely known and used (Peters and Timmerhaus 1991). The personal computer (PC) version of DIPPR contained twenty six (26) constants and thirteen (13) temperature dependent, pure component properties for seven hundred and sixty six (766) common industrial chemicals. There are at least twenty (20) physical property databases commercially available as online data services (Richardson and Coulson, 1991).

2.5 Computer Aided-Design (CAD)

Computing hardware and software are tools - of - the trade of engineers (Peters and Timmerhaus, 1991). The capabilities provided by computers for fast calculation, large storage and logical decisions plus the available technical mathematical software permit engineers to solve larger problems and to do it much more rapidly than ever before possible. The engineer’s emphasis can therefore shift from problem solving to planning, conceiving, interpreting and implementing with the information made available. Design is one of the engineering functions that have been enhanced by computer. Chemical engineering stresses the processes for manufacturing chemicals and chemical based products. In this effort, the emphasis of the chemical engineer tends to be on the process rather than on the product. The computer aids most useful to chemical engineers in design are process rather than product - oriented. The more widely known CAD/CAM (Computer-Aided Design/Computer-Aided Manufacturing) software is usually concerned with product-as-object and is highly graphical and spatial. Chemical process computer-aided design, on the other hand is much less graphical. It is more concerned with the performance of process units (such as the classical unit operations of chemical engineering) and the integration of these units into complete, consistent, efficient processes to produce chemical products.

An engineer may write a programming language code to solve a particular design problem. Before the explosive growth of software, this commonly was done. There is still a place for it when appropriate software is not available or as learning and debugging is usually quite time consuming. It is recommended that available software be used and that a specific design program be written only after determining that appropriate software is not available.

Hundreds, even thousands, of programs have been written to solve problems commonly encountered by chemical engineers. Many of these have become available for purchase. In turn, many of these programs are for the design of individual units of chemical process equipment.

2.5.1 Introduction to Computer Programming

A computer program is a series of instructions that is given to the computer to obey. It is usually written in a particular programming language, and named according to the language used in writing it.

A computer language (programming language) is composed of a set of characters, words and rules that can be used to write a computer program. Such programming language can be classified according to their levels as machine language (level 1), symbolic language (level 2), and higher level language (level 3).

Machine language is low level language that is native or natural to the hardware of the computer. It consists of 0s and 1s. Every computer model has its own machine language which is defined by its hardware structure. Thus, this language depends on the particular computer model, for this, it is said to be machine dependent. The early days of computer programming was almost exclusively machine language programming. It was very difficult and tasking in programming computers using machine language. Because of this, advances in programming techniques led to the development of symbolic languages.

Symbolic languages are mnemonic codes to represent machine instructions. The computer does not understand these codes, because of this, they have to be translated to machines language using appropriate translator. To translate an assembly language program into machine language an assembler is needed.

An assembler is a machine language instruction or program that translates symbolic language (such as Assembly Language Instruction) into machine language instructions.

Higher level languages are intermediate codes developed to enable the programmer code computer instructions in a way that resemble his thinking process using English-like expressions. The language is procedure oriented rather than machine oriented. They focus on the data processing procedure to be accomplished and not on the coding requirements of a particular computer machine. Thus, it is machine independent and very easy to use. This means that programs written in higher level language are not restricted to be used with particular computer models. These higher level programming languages are Beginners All-purpose Symbolic Instruction Code (BASIC), Common Business Oriented Language (COBOL), a UNIX based system programming language (C^{++}), PASCAL – named after the French Mathematician, Blaise PASCAL, Formula Translation (FORTRAN), etc.

Programs written in higher level languages must be translated into the machine understandable form using appropriate translators.

A translator is a machine language program that translates source codes written in either symbolic or higher level language to machine language program as the object language.

If the source program (source code) is a higher level language program such as FORTRAN, PASCAL, COBOL, C, the translator that produces the object code in machine understandable form is called compiler. A compiler is a machine language program that translates or compiles the source code to machine language equivalence called the object code.

The compiler reads the source code and generates the machine code (object code), and saves it onto disk file. When the program is to be executed, the computer simply loads the object code into memory and executes it. At the point of execution, the program asks for inputs data or read input data from appropriate file to generate required output.

There is another kind of translator called interpreter. If the source code is a higher level language program such as BASIC, an interpreter is required to translate the source program to machine understandable form. An interpreter is a translator which reads the source program directly, line by line, starting from the beginning of the source program each time it is to be executed and generates machine codes necessary to carry out the instructions as they proceed through the program, without saving it on disk.

Another kind of translator is the assembler. If the source program is a low level language, the translator that produces the object code in machine understandable form is the assembler.

2.6 Optimisation: Historical Perspective

A well-known approach to principle of optimisation was first scribbled centuries ago on the walls of an ancient Roman bathhouse in connection with a choice between two aspirants for emperor of Rome. It read - “De doubus malis, minus est semper aligendum” translated: of two evils, always choose the lesser (Edgar and Himmeblau, 2001).

The existence of optimisation methods can be traced to the days of Newton, Lagrange and Cauchy (Ayoade, 1994). However, very little progress was made until the advent of computers in 1945. It came of age as a subject in the 1950's when the well-established methods of differential calculus were combined with the highly successful new techniques of mathematical programming which were being developed at that time. The term programming by the way is synonymous with optimisation and was originally used to mean optimisation in the sense of optimal planning.

The 1940's and 1950's saw the development of an important branch of the subject known as linear programming. The work of Kuhn and Tucker in 1951 on the necessary and sufficient conditions for the optimal solution of programming problems laid the foundation for a great deal of later research in non linear programming. Also, in the post war period, the "hill-climbing" methods were developed, these methods were at first very crude, insufficient and did not rely on any special structure in the problem. Since that time, the development of the subject has grown at a fast rate and has included methods or a variety of problems.

2.6.1 Optimisation Techniques

Design is optimisation: the designer seeks the best, the optimum, solution to a problem. Much of the selection and choice in the design process will depend on the intuitive judgement of the designer; who must decide when more formal optimisation techniques can be used to advantage. The task of formally optimising the design of a complex processing plant involving several hundred variables, with complex interactions, is formidable, if not impossible. The task can be reduced by dividing the process into more manageable units, identifying the key variables and concentrating work where the effort involved will give the greatest benefit. Sub-division, and optimisation of the sub-units rather than the whole, will not\ necessarily give the optimum design for the whole process. The optimisation of one unit may be at the expense of another. For example, it will usually be satisfactory to optimize the reflux ratio for a fractionating column independently of the rest of the plant; but if the column is part of a separation stage following a reactor, in which the product is separated from the unreacted materials, then the design of the column will interact with, and may well determine, the optimisation of the reactor design. In this work the discussion of optimisation methods will, of necessity, be limited to a brief review of the main techniques used in process and equipment design. The extensive literature on the subject should be consulted for full details of the methods available, and their application and limitations.

2.6.2 General procedure

When setting out to optimise any system, the first step is clearly to identify the objective: the criterion to be used to judge the system performance. In engineering design the objective will invariably be an economic one. For a chemical process, the overall objectivefor the operating company will be to maximise profits. This will give rise to sub-objectives, which the designer will work to achieve. The main sub-objective will usually be to minimise operating costs. Other sub-objectives may be to reduce investment, maximize yield, reduce labour requirements, reduce maintenance, operate safely. When choosing his objectives the designer must keep in mind the overall objective. Minimising cost per unit of production will not necessarily maximise profits per unit time; market factors, such as quality and delivery, may determine the best overall strategy.

The second step is to determine the objective function; the system of equations, and other relationships, which relate the objective with the variables to be manipulated to optimise the function. If the objective is economic, it will be necessary to express the objective function in economic terms (costs). Difficulties will arise in expressing functions that depend on value judgements; for example, the social benefits and the social costs that arise from pollution.

The third step is to find the values of the variables that give the optimum value of the objective function (maximum or minimum). The best techniques to be used for this step will depend on the complexity of the system and on the particular mathematical model used to represent the system. A mathematical model represents the design as a set of equations (relationships) and it will only be possible to optimise the design if the number of variables exceeds the number of relationships; there is some degree of freedom in the system.

2.6.3 Simple models

If the objective function can be expressed as a function of one variable (single degree of freedom) the function can be differentiated, or plotted, to find the maximum or minimum. This will be possible for only a few practical design problems.

2.6.4 Multiple variable problems

The genera] optimisation problem can be represented mathematically as:

$$f = f\,(v_1, v_2, v_3\ldots\ldots\ldots v_n) = 0 \qquad (2.45)$$

where f is the objective function and $v_1, v_2, v_3\ldots\ldots\ldots v_n$ are the variables. In a design situation there will be constraints on the possible values of the objective function, arising from constraints on the variables; such as, minimum flow-rates, maximum allowable concentrations, and preferred sizes and standards.

Some may be equality constraints, expressed by equations of the form:

$$\Phi_n = \Phi_n(v_1, v_2, v_3\ldots\ldots\ldots v_n) = 0 \qquad (2.46)$$

Others as inequality constraints:

$$\Phi_p = \Phi_p(v_1, v_2, v_3\ldots\ldots\ldots v_n) \leq 0 \qquad (2.47)$$

The problem is to find values for the variables v_1 to v_n that optimise the objective function: that give the maximum or minimum value, within the constraints.

2.6.4.1 Analytical methods

If the objective function can be expressed as a mathematical function the classical methods of calculus can be used to find the maximum or minimum. Setting the partial derivatives to zero will produce a set of simultaneous equations that can be solved to find the optimum values. For the general, unconstrained, objective function, the derivatives will give the critical points; which may be maximum or minimum, or ridges or valleys. As with single variable functions, the nature of the first derivative can be found by taking the second derivative. For most practical design problems the range of values that the variables can take will be subject to constraints (equations 2.46 and 2.47), and the optimum of the constrained objective function will not necessarily occur where the partial derivatives of the objective function are zero.

The method of Lagrange's undetermined multipliers is a useful analytical technique for dealing with problems that have equality constraints (fixed design value).

Analytical methods are applicable to subjective functions which are continuous and easily differentiable. Practical usage of this technique is, however, limited in scope since a sizable number of objective functions of practical importance are either not easily differentiable or leads to more complex algebraic equations on differentiation. Nonetheless, it is necessary to understand the principles of this technique since it forms the basis for developing most of the numerical optimisation techniques. In general terms the classical optimisation techniques are used for solving problems in which the objective function and constraints are fairly simple in terms of the decision variables.

2.6.4.2 Search methods

The nature of the relationships and constraints in most design problems is such that the use of analytical methods is not feasible. In these circumstances search methods, that require only that the objective function can be computed from arbitrary values of the independent variables, are used. For single variable problems, where the objective function is unimodal, the simplest approach is to calculate the value of the objective function at uniformly spaced values of the variable until a maximum (or minimum) value is obtained. Though this method is not the most efficient, it will not require excessive computing time for simple problems. Several more efficient search techniques have been developed, such as the method of the golden section. Efficient search methods will be needed for multi-dimensional problems, as the number of calculations required and the computer time necessary will be greatly increased, compared with single variable problems.

In practical terms, one dimensional search techniques are used for line searches within a multi-variable optimisation method. The available methods could be classified into two groups- bracketing and interpolation methods. Bracketing methods include Fibonacci search, golden section search, binary search and the recently developed one-dimensional simplex search. Interpolation techniques include quadratic interpolation and cubic interpolation. It should be noted that all the methods assume that the function is unimodal, that is, it contains one minimum point in the domain of interest. In addition, univariate search techniques can in general, be used for multivariant optimization through successive perturbation of each decision variable. This approach only works if there is no strong interaction between the decision variables.

2.6.4.3 Linear programming

Linear programming is an optimisation technique that can be used when the objective function and constraints can be expressed as a linear function of the variables. The technique is useful where the problem is to decide the optimum utilisation of resources. Many oil companies use linear programming to determine the optimum schedule of products to be produced from the crude oils available. Algorithms have been developed for the efficient solution of linear programming problems and the SIMPLEX algorithm is the most commonly used.

2.6.4.4 Dynamic programming

Dynamic programming is a technique developed for the optimisation of large systems. The basic approach used is to divide the system into convenient sub-systems andoptimise each sub-system separately, while taking into account the interactions between the sub-systems. The decisions made at each stage contribute to the overall systems objective function, and to optimise the overall objective function an appropriate combination of the individual stages has to be found. In a typical process plant system the possible number of combinations of the stage decisions will be very large. The dynamic programming approach uses Bellman's "Principle of Optimality", which enables the optimum policy to be found systematically and efficiently by calculating only a fraction of the possible combinations of stage decisions. The method converts the problem from the need to deal with “N” optimisation decisions simultaneously to a sequential set of “N” problems.

2.7 Estimating Total Capital Investment

Total capital investment, *TCI*, includes equipment cost, *EC*, for the entire gas absorber unit, taxes, freight charges, instrumentation, and direct and indirect installation costs.

2.7.1 Equipment Costs for Packed Towers

Cost estimates for a range of tower dimensions (i.e. height, diameter) to account for the varying needs of different applications are provided by gas absorber vendors. The equipment for which the vendors provide costs consisted of a packed tower absorber made of fiberglass reinforced plastic (FRP), and to include the following equipment components:

(a) Absorption column shell;
(b) Gas inlet and outlet ports;
(c) Liquid inlet port and outlet port/drain;
(d) Liquid distributor and redistributors;
(e) Two packing support plates;
(f) Mist eliminator;
(g) Internal piping;
(h) Sump space; and
(i) Platforms and ladders;

The cost data the vendors supplied were first adjusted to put them on a common basis, and then were regressed against the absorber surface area (A_S). The equation shown below is a linear regression of cost data provided by six vendors (W. M. Vatavuk, personal communication March 27, 1992).

$$\textit{Total tower cost (\$)} = 115\, A_S \qquad (2.48)$$

Where A_S is the surface area of the absorber, in ft^2. This equation is applicable for towers with surface areas from 69 to 1507 ft^2 constructed of FRP. Costs for towers made of materials other than FRP may be estimated using the following equation:

$$TTC_M = CF * TTC \tag{2.49}$$

Where TTC_M, is the total cost of the tower using other materials and TTC is the total tower cost as estimated using Equation (2.48). The variable CF is a cost factor to convert cost of an FRP gas absorber to an absorber fabricated from other materials. Ranges of cost factors provided by vendors are listed for the following materials of construction (Random Corporation, 1991).

304 stainless steel: 1.10 – 1.75

Polypropylene: 0.80 – 1.10

Polyvinyl chloride: 0.50 – 0.90

Auxiliary costs encompass the cost of all necessary equipments not included in the absorption column unit. Auxiliary equipment includes packing materials, instruments and controls, pumps, and fans. Cost ranges for various types of random packings are presented in appendix E. The cost of structured packing varies over a much wider range. Structured packing made of stainless steel range from \$45/ft^3 to \$405/ft^3, and those made of polypropylene range from \$65/ft^3 to \$350/ft^3 (Random Corporation, 1991).

Similarly, the cost of instrument and controls varies widely depending on the complexity required. Gas absorber vendors have provided estimates from \$1,000 to \$10,000 per column. However, cost data for auxiliaries are available from the literature (Vatavuk, 1990).

The total equipment cost (EC) is the sum of the component equipment costs, which includes tower cost and the auxiliary equipment cost.

$$EC = TTC + packing\ cost + auxiliary\ equipment \tag{2.50}$$

The purchased equipment cost (PEC) includes the cost of the absorber with packing and its auxiliaries (*EC*), instrumentation (0.10 *EC*), sales tax (0.03 *EC*), and freight (0.05 *EC*). The PEC is calculated from the factors in Table 2.1.

$$PEC = (1 + 0.10 + 0.03 + 0.05)\, EC = 1.18\, EC \qquad (2.51)$$

2.7.2 Installation Costs

The total capital investment, *TCI*, is obtained by multiplying the purchased equipment cost, *PEC*, by the total installation factor:

$$TCI = 2.20\, PEC \qquad (2.52)$$

The factors which are included in the total installation factor are also listed in Table 2.1 (Vatavuk and Neveril, 1980). The factors presented in Table 2.2 were confirmed from the gas absorber vendors survey.

Table 2.1: Capital Cost Factors for Gas Absorbers [Vatavuk, W.M. and R.B. Neveril, 1991]

Cost Item	**Factor**
<u>Direct Costs</u>	
Purchased equipment costs	
Absorber + packing + auxiliary equipment[a], EC	As estimated, A
Instrumentation [b]	0.10 A
Sales taxes	0.03 A
Freight	0.05 A
Purchased equipment cost, PEC	B = 1.18 A

Direct installation costs	
Foundation & supports	0.12 B
Handling & erection	0.40 B
Electrical	0.01 B
Piping	0.30 B
Insulation	0.01 B
Painting	0.01 B
Direct installation costs	0.85 B
Site preparation	As required, SP
Buildings	As required, Bldg.
Total Direct Costs, DC	1.85 B + SP + Bldg
Indirect Costs (installation)	
Engineering	0.10 B
Construction and field expenses	0.10 B
Contractor fees	0.10 B
Start-up	0.10 B
Performance test	0.10 B
Contingencies	0.03 B
Total Indirect Costs, IC	0.35 B
Total Capital Investment = DC + IC	2.20 B + SP + Bldg.

[a] Includes the initial quantity of packing as well as items normally not included with the unit supplied by vendors, such as ductwork, fan, piping, etc.

. **Table 2.2:** Annual cost factors for gas absorbers.

Cost Item	**Factor**
Direct Annual Costs, DC	
Operating labour [a]	
Operator	½ hour per shift
Supervisor	15% of operator
Operating materials [b]	Application specific
Solvent	(throughput/year) x (waste fraction)
Chemicals	Based on annual consumption
Waste water disposal	(throughput/year) x (waste fraction)
Maintenance [a]	
Labour	½ hour per shift
Material	100% of maintenance labour
Electricity	(consumption rate) x (hours/yr) x (unit cost)
Fan	
Pump	
Indirect Annual Costs, IC	
Overhead	60% of total labour and material costs
Administrative charges	2% of Total Capital Investment

Property tax	1% of Total Capital Investment
Insurance	1% of Total Capital Investment
Capital Recovery [c]	0.1098 x Total Capital Investment
Total Annual Cost	DC + IC

[a] These factors were confirmed by vendor contacts.

[b] If system does not use chemicals (e.g., caustic), this quantity is equal to annual solvent consumption.

[c] Assuming a 15-year life at 7%.

2.8 Estimating Annual Cost

The total annual cost (*TAC*) is the sum of the direct and indirect annual costs.

2.8.1 Direct Annual Costs

Direct annual costs (DC) are those expenditures related to operating the equipment, such as labour and materials. The suggested factors for each of these costs are shown in Table 2.2. The annual costs for each item is calculated by multiplying the number of units used annually (i.e., hours, pounds, gallons, kWh) by the associated unit cost.

Operating labour is estimated at ½-hour per 8-hour shift. The supervisory labour cost is estimated at 15 percent of the operating labour cost. Maintenance labour is estimated at ½-hour per 8-hour shift. Maintenance materials costs are assumed to equal maintenance labour costs.

Solvent costs are dependent on the total liquid throughput, the type of solvent required, and the fraction of throughput wasted (often referred to as blow-down). Typically, the fraction of solvent wasted varies from 0.1 percent to 10 percent of the entire total solvent throughput (Random Corporation, 1991).

The total annual cost of solvent (C_s) is given by (www.pdnengineers.com):

$$C_s = L_2 WF\left(60\frac{min}{hr}\right)\binom{annual\ operating}{hours}(solvent\ unit\ cost) \qquad (2.53)$$

Where *WF* is the waste (make-up) fraction, L_2 is the solvent volumetric flow rate in gallons per minutes and the solvent unit cost is expressed in terms of $/gal.

The electricity costs associated with operating a gas absorber derive from fan requirements to overcome the pressure in the column, ductwork, and other parts of the control system, and pump requirements for the solvent. The energy required for the fan can be calculated using equation 51 (www.pdnengineers.com):

$$Energy_{fan} = \frac{1.17 * 10^4\, G_1\, \Delta P}{\varepsilon} \qquad (2.54)$$

Where Energy (in kilowatts) refers to the energy needed to move a given volumetric flow rate of air (ft^3/min), G_1 is the gas flow rate entering the absorber, ΔP is the total pressure drop through the system (in of H_2O) and ε is the combined fan-motor efficiency. Values for ε typically range from 0.4 to 0.7. Likewise, the electricity required by the pump can be calculated using equation 52 (www.pdnengineers.com):

$$Energy_{pump} = \frac{(2.52 * 10^{-1}) L_2 (Pp)}{\varepsilon} \qquad (2.55)$$

Where P_P is the pump operating pressure expressed in feet of water, L_2 is the solvent volumetric flow rate in gallons per minute and ε is the combined pump-motor efficiency.

The cost of electricity (C_e) is then given by (www.pdnengineers.com):

$$C_e = Energy_{fan+pump} \binom{annual\ operating}{hours} (cost\ of\ electricity) \qquad (2.56)$$

Where cost of electricity is expressed in units of \$/kW-hr.

2.8.2 Indirect Annual Costs

Indirect annual costs (IC) include overhead, taxes, insurance, general and administrative (G & A), and capital recovery costs. The suggested factors for each of these items also appear in Table 1.4. Overhead is assumed to be equal to 60 percent of the sum of operating, supervisory, and maintenance labour, and maintenance materials.

The system capital recovery cost, *CRC*, is based on an estimated 15-year equipment life. For a 15-year life and an interest rate of 7 percent, the capital recovery factor is 0.1098. The system capital recovery cost is then estimated by:

$$CRC = 0.1098\ TCI \tag{2.57}$$

G & A costs, property tax, and insurance are factors from total capital investment, typically at 2 percent, 1 percent and 1 percent respectively.

2.8.3 Total Annual Cost

Total annual cost (*TAC*) is calculated by adding the direct annual cost and the indirect annual costs.

$$TAC = DC + IC \tag{2.58}$$

2.9 Review of Related Literature

R .Thiele et al., (2006) designed and optimized industrial reaction absorption processes in sour gas treatment using rigorous modeling and accurate experimentation. The model was successfully validated by vapour-liquid equilibrium data from the literature and by the conducted 10 desorption experiments and 8 absorption experiments in the packed tower in desorption mode. The developed experimental procedure including a data reconciliation method improved the accuracy of the measurement data and also automatically detected gross errors. In addition, the model was used in the commercially available flowsheet simulator CHEMCAD as a User Added Module to simulate for the entire VACASULFw process. The predicted values compare well with the industrial data. It is now being used in industrial practice for the design of the individual units and the overall process and can also be utilised online for model predictive control. Thus, the project allowed for the first time the simulation of the entire process (VACASULFw) with recycles using rigorous models and its application in industrial practice. Furthermore, the industrial process was systematically optimised regarding annual costs using an evolutionary strategy. This resulted in a decrease of 30% in operating costs still complying with the restrictions for the gas outlet concentration. For a new process the heights of the absorber and stripper were significantly reduced resulting also in a decrease in investment costs.

N. J. Suchak and J. B. Joshi (1994) carried out simulation and optimization of NO_X absorption system in nitric acid manufacture. A mathematical model has been developed for the prediction of optimum design of packed and plate columns. The effects of inlet *NOx* composition, temperature, pressure, volume of pre-oxidizer, volume of interstage oxidizers, and extent of absorption per stage have been included in the model. It was found that the concentration of product nitric acid strongly depends upon the inlet NO, composition, temperature, pressure, and excess oxygen. For a given concentration of product nitric acid, the optimum design of pre-oxidizer has been presented. It was also found that the extent of oxidation per stage strongly influences the number of stages. The overall equipment volume was found to increase with an increase in the extent of oxidation. However, the number of stages increases with a decrease in the extent of oxidation. The optimum design depends nominally on the extent of absorption per stage.

Iskandar Halim et al., described a simulation-optimization framework for efficient CO2 capture using amine absorption. The framework has been developed by integrating HYSYS simulator with a jumping gene based multi-objective simulated annealing technique and applied to CO2 capture process from a gas power plant. It has been shown to be capable of generating Pareto optimal solution involving CO2 capture efficiency and operating cost. Such Pareto set will form the basis for comparison with other amine technology.

Chinmay Kale et al., (2012) performed optimization of reactive absorption using an evolutionary algorithm. The process optimization was based on a generic non-equilibrium stage model which considered multicomponent mass and heat transfer, chemical reactions, non-ideal behaviour of the phases and hydrodynamics in the column. The model has been validated using the experimental results from the pilot scale absorption column and it predicts the experimental results with acceptable accuracy. The optimization study was done by assuming 90% removal of CO_2 from feed gas as the design criterion for absorption column. The optimization problem was solved by applying an evolutionary algorithm to minimize the annualized operating costs for absorption of CO_2 as objective function. The optimization variables are mainly column dimensions, flow rates and concentration of absorption solvent. The optimization method mentioned above allows the simultaneous determination of the dimensions of the column and operating conditions required to achieve design criteria with minimum possible operating cost.

E. Brunazzi., (2002) carried out an economical criterion for packed absorption column design. The results show that, in some cases, structured packings can save energy and significantly reduce the operating and investment costs by offering reduced values of pressure drops per transfer unit in comparison to conventional dumped packing. In some other cases columns equipped with random packings give better economical performances than columns equipped with structured packings. The economical analysis has been performed analysing the effects of a number of variables (e.g. column dimensions, working pressure, gas flow-rate, packing or vessel material, absorption efficiency and depreciation period.

U. Wiesner et al., (1996) carried out design and optimization of a nitric acid recovery plant from nitrous waste gases. It was reported that the modelling of the multicomponent absorption with chemical reaction is not a trivial problem due to superposition of many driving forces - multicomponent diffusion, chemical interactions, convective flows, multicomponent thermodynamic interaction etc. Therefore, adequate theoretical description of multicomponent reactive systems calls for the application of the *Maxwell-Stefan equations* and for the use of matrix coupled mass transfer equations together with the relevant reaction kinetics. On this basis, a countercurrent absorption tower for chemisorption of nitrogen oxides (NO_x) to nitric acid was considered and a general non-equilibrium stage model was developed for its design and optimization.

M.A. Olutoye and A. Mohammed (2006) performed Mathematical modeling of a gas absorption packed column for carbon dioxide - sodium hydroxide system. A model equation was developed and tested. The result obtained shows that it can be used to predict the quantity of CO_2 absorbed in a given time.

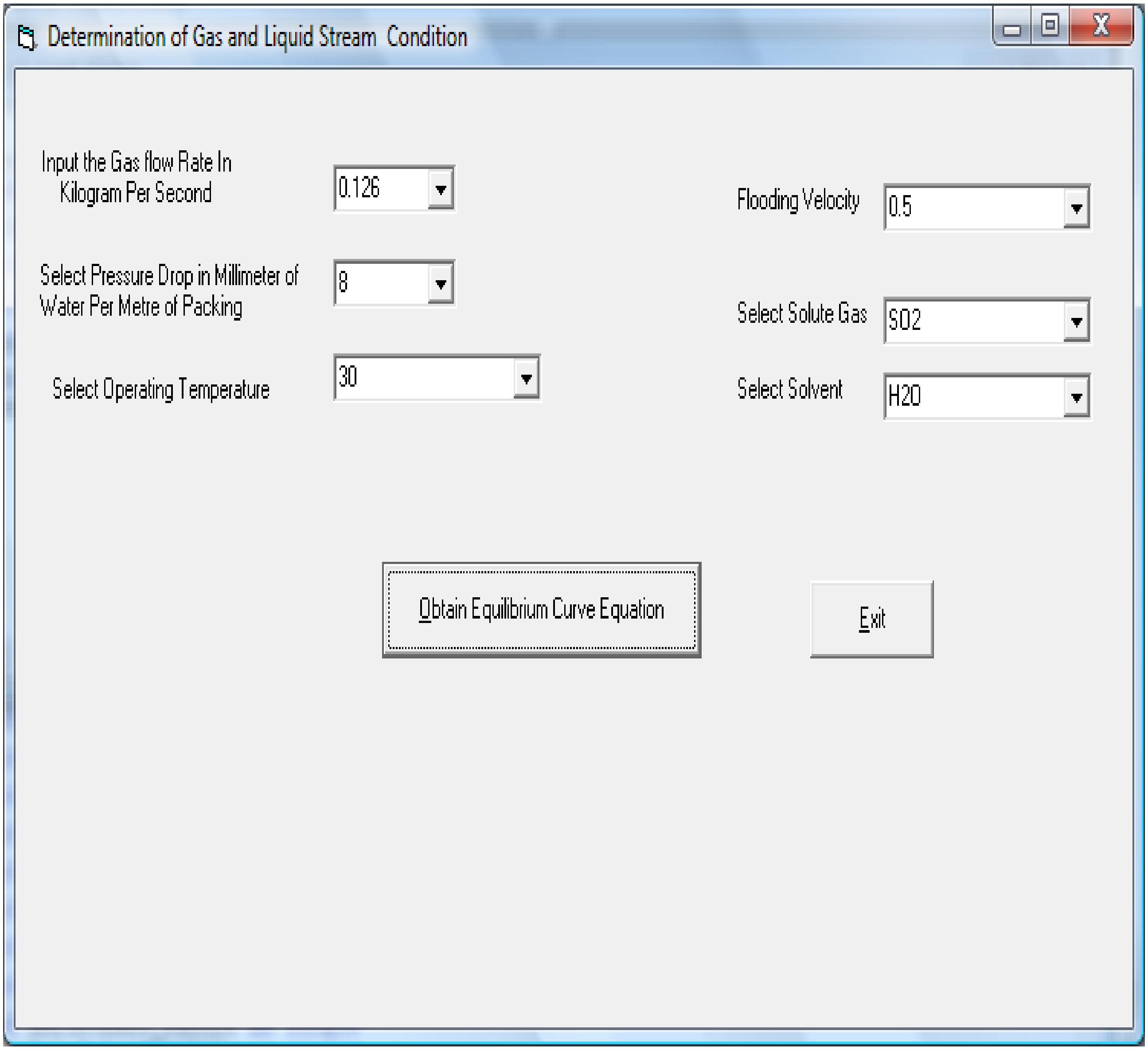
CHAPTER THREE

MATERIALS AND METHODS

This section shows the development of the design and optimization module.

3.1 Development of program, Testing and Application to Problem Statements

The Visual Basic 6.0 program was double clicked to open a new form. Text boxes and combo boxes were laid out on the screen and were labeled as select inlet gas temperature, select pressure drop, select inlet gas flow rate, select flooding velocity, select solute gas and solvent respectively. Command buttons were placed for obtaining equilibrium curve equation and for exiting the application. All the equations, data and correlations for obtaining equilibrium curve equation were then coded in the code window. The codes are shown in appendix F.



Determination of Gas and Liquid Stream Condition

Input the Gas flow Rate In Kilogram Per Second: 0.126

Select Pressure Drop in Millimeter of Water Per Metre of Packing: 8

Select Operating Temperature: 30

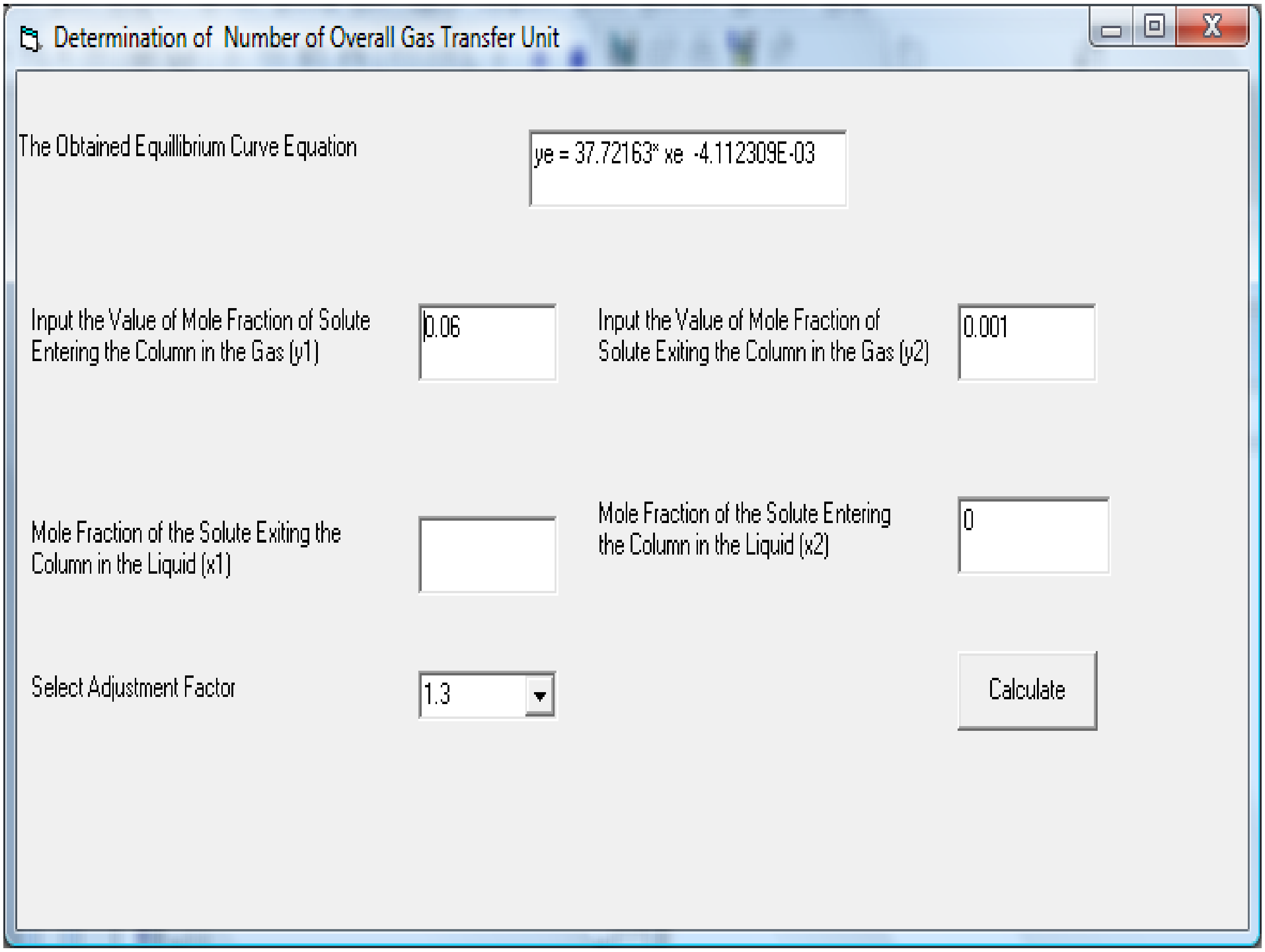
Flooding Velocity: 0.5

Select Solute Gas: SO2

Select Solvent: H2O

Figure 3.1: Graphical User Interface for Obtaining Equilibrium Curve Equation

Starting with a new form, Text boxes and combo boxes were laid out on the screen and were labeled as equilibrium curve equation, input the value of mole fraction of solute entering the column in the gas (y_1), input the value of mole fraction of solute exiting the column in the gas (y_2), input the value of mole fraction of solute entering the column in the liquid (x_2), input the value of mole fraction of solute exiting the column in the gas (x_1), and select adjustment factor respectively. Command button was placed for calculating the number of overall gas transfer units. All the equations, data and correlations for calculating the number of overall gas transfer units were then coded in the code window. The codes are shown in appendix F.



The Obtained Equilibrium Curve Equation: ye = 37.72163* xe -4.112309E-03

Input the Value of Mole Fraction of Solute Entering the Column in the Gas (y1): 0.06

Input the Value of Mole Fraction of Solute Exiting the Column in the Gas (y2): 0.001

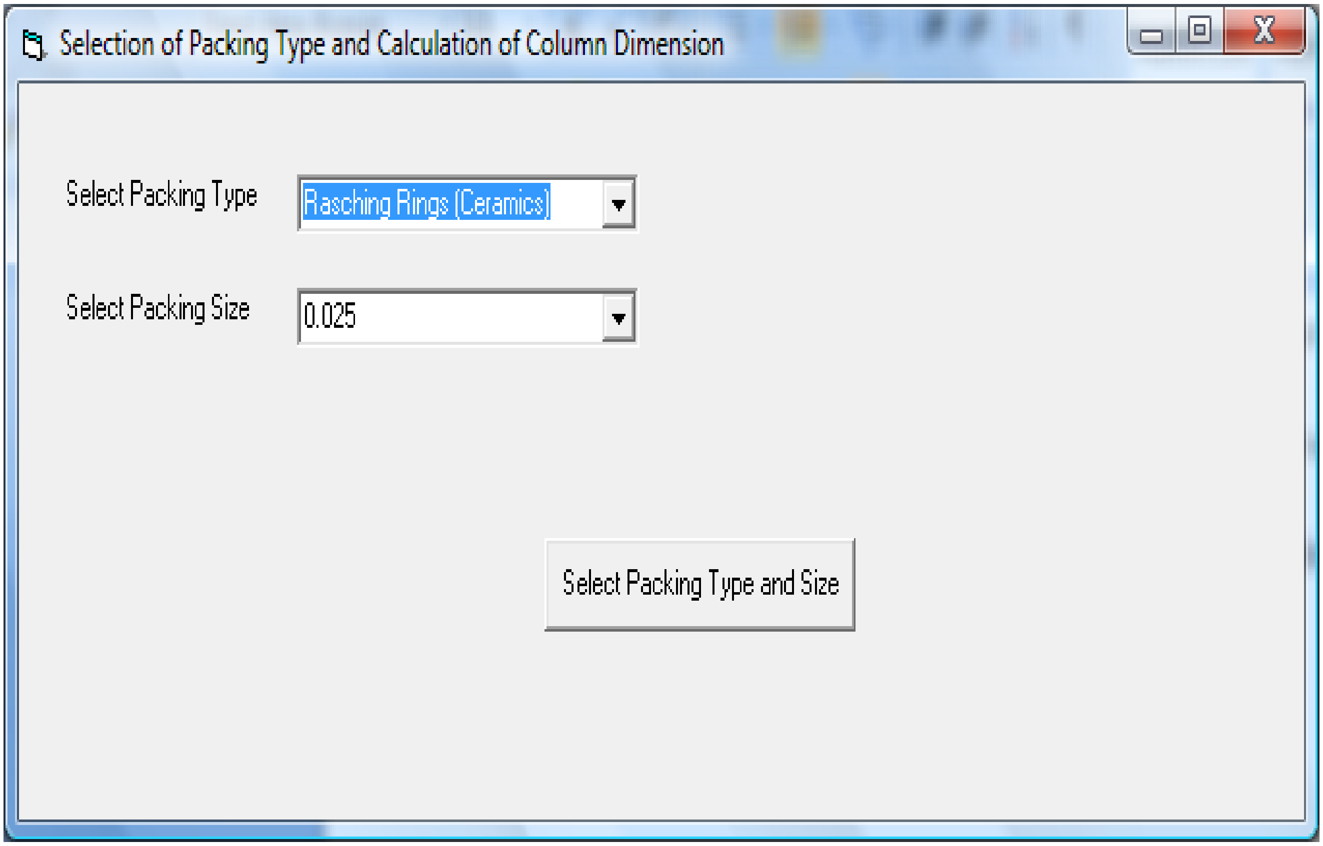
Mole Fraction of the Solute Exiting the Column in the Liquid (x1):

Mole Fraction of the Solute Entering the Column in the Liquid (x2): 0

Select Adjustment Factor: 1.3

Figure 3.2: Graphical User Interface for Determination of Number of Overall Gas Transfer Units

Again starting with a new form, text boxes and combo boxes were laid out on the screen and were labeled as select packing type and size respectively. Command button was then placed for selecting the packing type and size. The various packing materials, their size range, their surface-to-volume ratio and their characteristics were then coded in the code window. The codes are shown in appendix F.

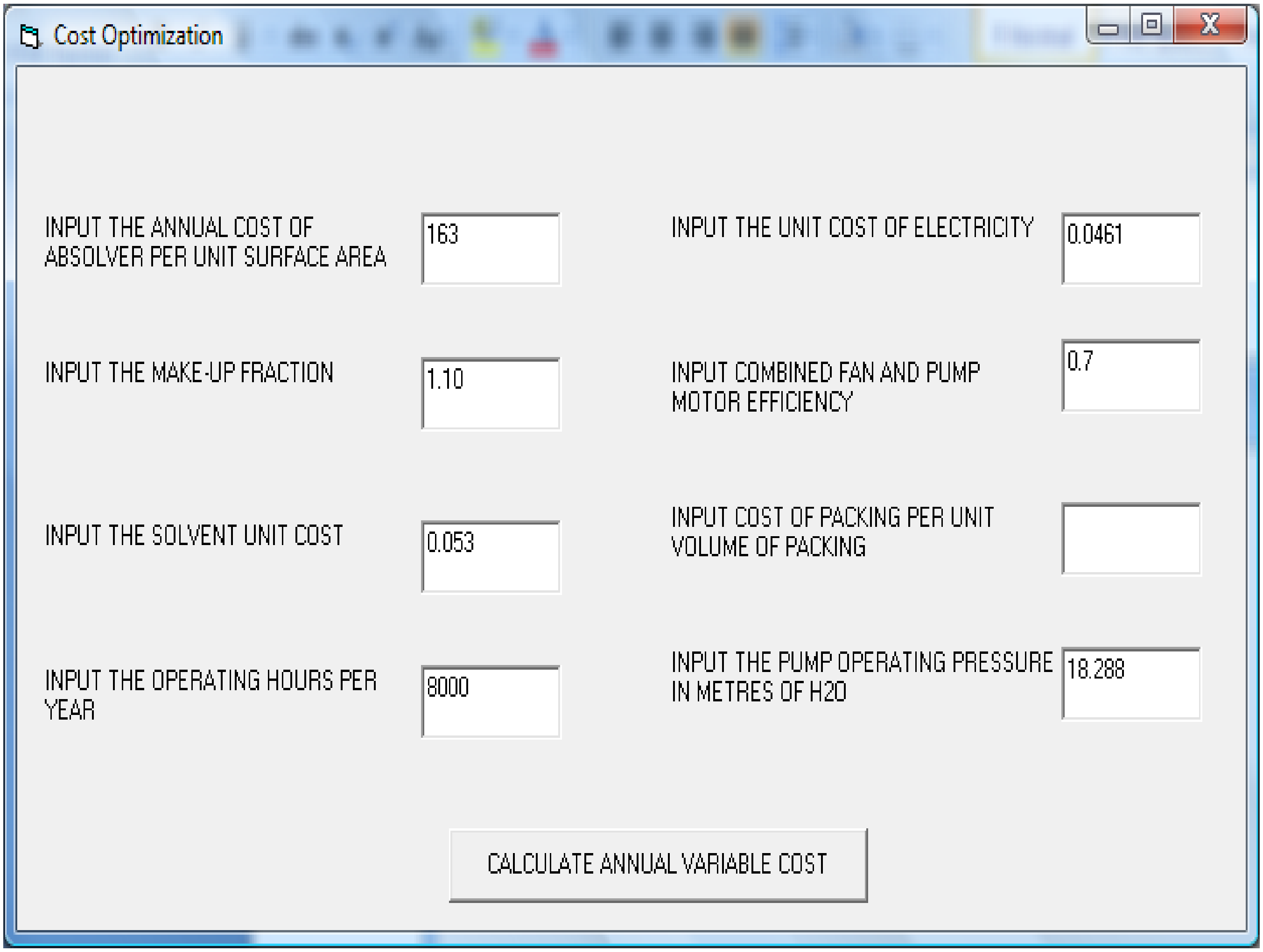


Select Packing Type: Rasching Rings (Ceramics)

Select Packing Size: 0.025

Figure 3.3: Graphical User Interface for Selecting Packing Size and Type and calculation of the column dimensions

A new form was then opened and text boxes were laid out and were labeled as input annual cost of absorber per unit surface area, input the unit cost of electricity, input the make-up fraction, input the combined fan and motor efficiency, input the solvent unit cost, input the cost of packing per unit volume of packing, input the operating hours per year, input pump operating pressure in meters of water. Command button was then placed for calculating the annual variable cost. All the equations, data and correlations for calculating the annual variable cost were then coded in the code window. The codes are shown in appendix F.



INPUT THE ANNUAL COST OF ABSOLVER PER UNIT SURFACE AREA	163
INPUT THE MAKE-UP FRACTION	1.10
INPUT THE SOLVENT UNIT COST	0.053
INPUT THE OPERATING HOURS PER YEAR	8000
INPUT THE UNIT COST OF ELECTRICITY	0.0461
INPUT COMBINED FAN AND PUMP MOTOR EFFICIENCY	0.7
INPUT COST OF PACKING PER UNIT VOLUME OF PACKING	
INPUT THE PUMP OPERATING PRESSURE IN METRES OF H2O	18.288

Figure 3.4: Graphical user Interface for Calculating Total Annual Variable Cost

A new form was then opened and command buttons were laid out for updating record in a database created in Microsoft Access and generating report in a Notepad. Another form was opened and a combo box was laid out and labeled select which database to update. A command button was also laid for adding record to the selected database. All the codes for creating, updating and adding record to the database were coded in the code window. The codes are shown in appendix F.

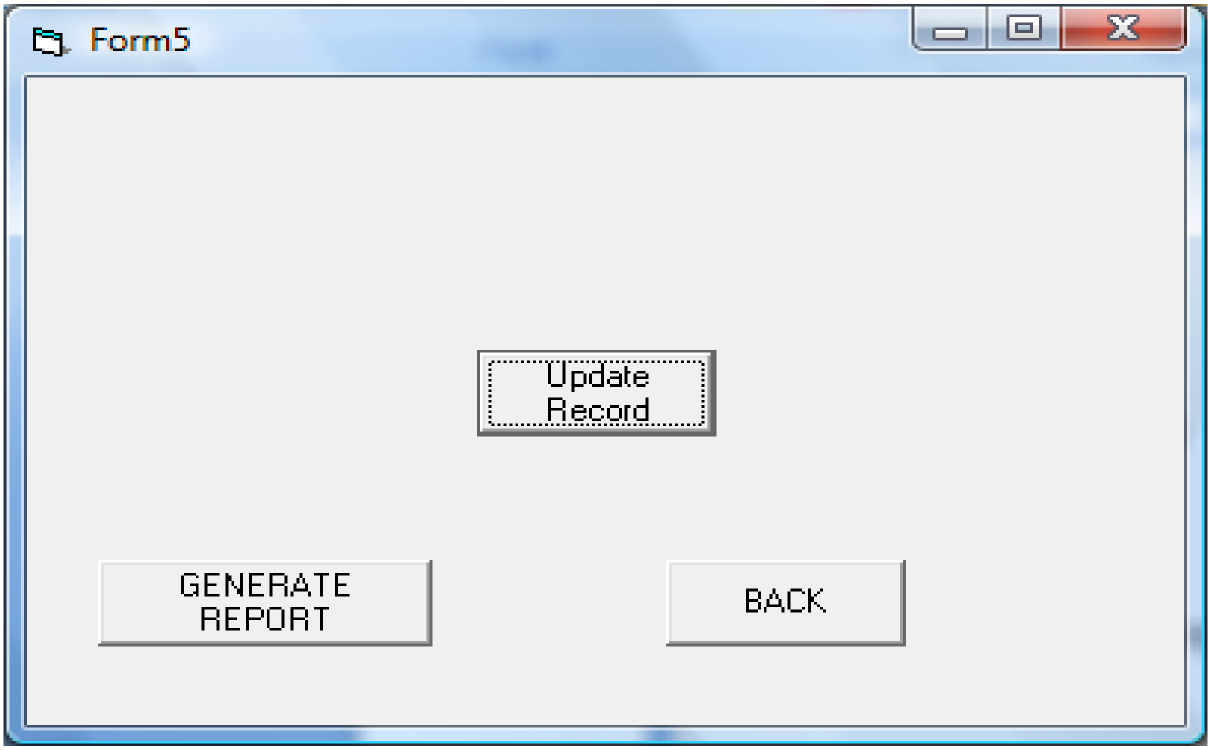
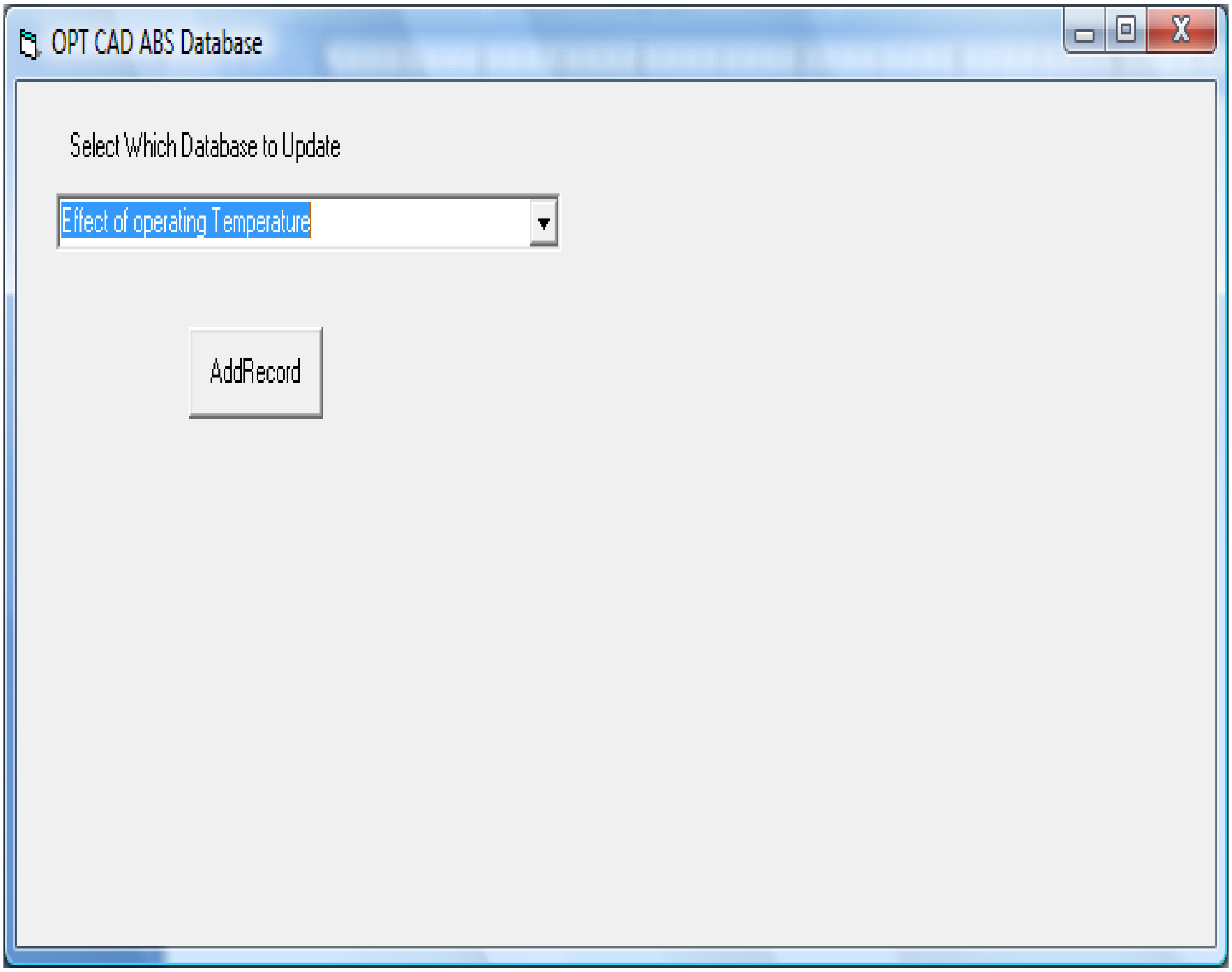


Figure 3.5: Graphical user Interface for Generating Report and Updating Records

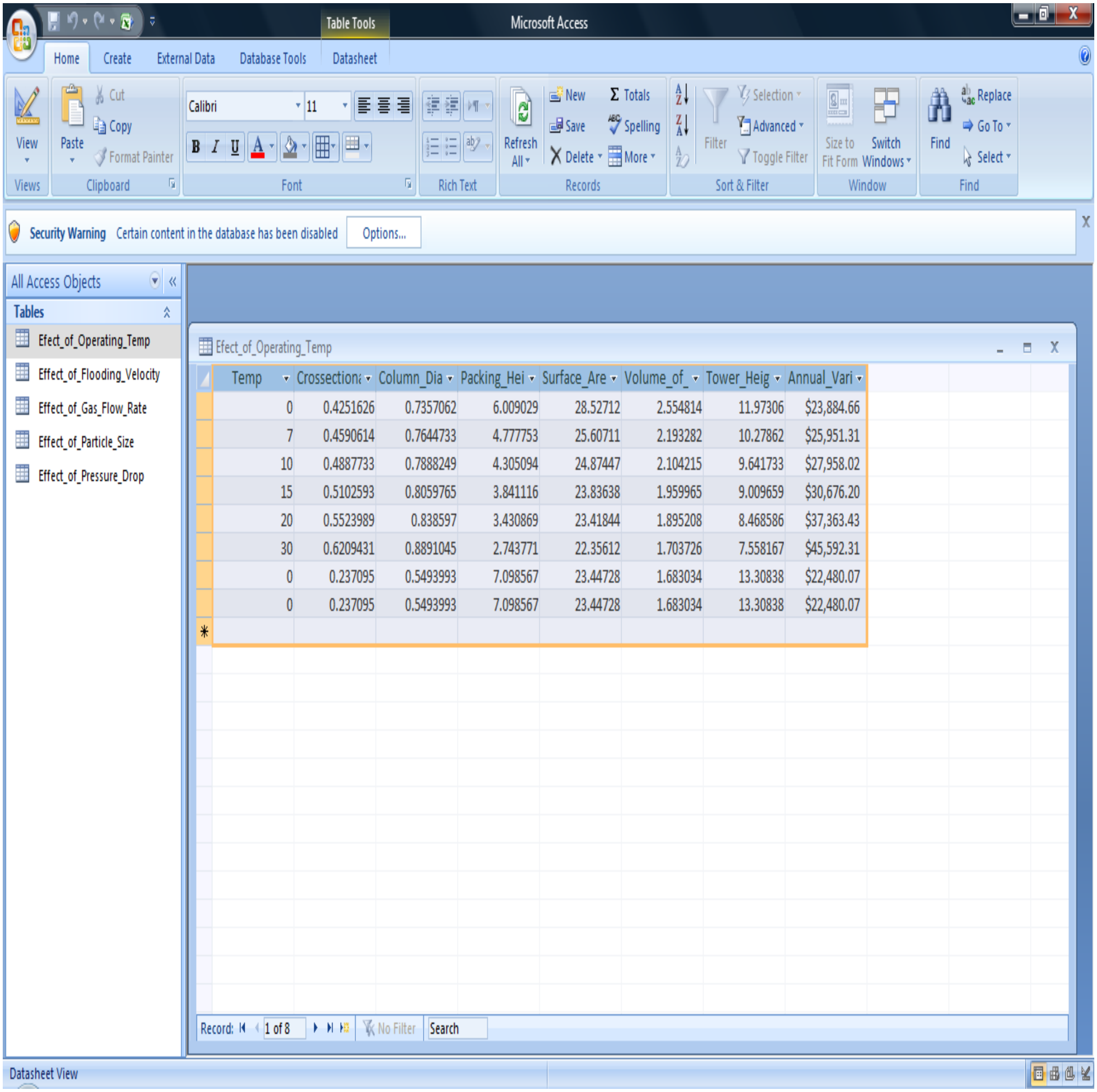


Select Which Database to Update

Effect of operating Temperature

Figure 3.6: Graphical User Interface for adding Records to Database

The final output screen was then displayed. A typical output is shown below.



Security Warning Certain content in the database has been disabled

Temp	Crossection	Column_Dia	Packing_Hei	Surface_Are	Volume_of_	Tower_Heig	Annual_Vari
0	0.4251626	0.7357062	6.009029	28.52712	2.554814	11.97306	$23,884.66
7	0.4590614	0.7644733	4.777753	25.60711	2.193282	10.27862	$25,951.31
10	0.4887733	0.7888249	4.305094	24.87447	2.104215	9.641733	$27,958.02
15	0.5102593	0.8059765	3.841116	23.83638	1.959965	9.009659	$30,676.20
20	0.5523989	0.838597	3.430869	23.41844	1.895208	8.468586	$37,363.43
30	0.6209431	0.8891045	2.743771	22.35612	1.703726	7.558167	$45,592.31
0	0.237095	0.5493993	7.098567	23.44728	1.683034	13.30838	$22,480.07
0	0.237095	0.5493993	7.098567	23.44728	1.683034	13.30838	$22,480.07

Figure 3.7: A Typical Output Screen

3.2 Design Procedures

The design of packed tower absorbers for controlling gas streams containing a solute and air depends on knowledge of the following parameters:

(1) Gas flow rate

(2) Gas composition and concentration of the solutes in the gas stream

(3) Required removal efficiency

(4) Equilibrium relationship between the solute(s) and solvent

(5) Properties of the solute(s), gas, and solvent such as diffusivity, viscosity, density, and molecular weight.

The primary objectives of the design procedures are to determine column surface area and pressure drop through the column. In order to determine these parameters, the following steps must be performed:

(a) Determine the gas and liquid stream conditions entering and exiting the column.

(b) Determine the absorption factor (*AF*).

(c) Determine the diameter of the column (D_C).

(d) Determine packing height (Z_C)

(e) Determine the tower height (H_{tower}) and surface area (A_S).

To simplify the sizing procedures, these assumptions have been made: (a) the gas is assumed to comprise a two-component gas mixture (solute/air), where the solute consists of a single compound present in dilute quantities

(b) The gas is assumed to behave as an ideal gas and the solvent is assumed to behave as an ideal solution.

(c) Heat effects associated with absorption are considered to be minimal for the solute concentrations considered.

(d) chemical reaction does not occur.

The design procedures presented here are complicated, and careful attention to units is required.

3.2.1 Determination of Gas and Liquid Stream Conditions

Gas absorbers are designed based on the ratio of liquid to gas (L/G) flow rate entering the column, slope of the equilibrium curve (m) and the desired removal efficiency (η). These factors are calculated from the inlet and outlet gas and liquid stream variables as follows:

Gas flow rate, in cubic meter per second (m^3/s), entering and exiting column (G_1 and G_2, respectively);

Solute concentration (moles solute per mole of solute free gas) entering and exiting the column in the gas (Y_1 and Y_2, respectively);

Solvent flow rate, in m^3 per second (m^3/s), entering and exiting the column (L_2 and L_1, respectively); and

Solute concentration (moles solute per mole of solute free solvent) entering and exiting the column in the solvent (X_2 and X_1, respectively).

The design in this work assumes that the inlet gas stream variables are known, and that a specific solute removal efficiency has been chosen as the design basis; i.e., the variables G_1, Y_1, and η are known. For dilute concentrations typically encountered in pollution control applications and negligible changes in moisture content, G_1 is assumed equal to G_2. If a once-through process is used, or if the spent solvent is regenerated by an air stripping process before it is recycled, the value of X_i will approach zero. These notions are shown in figure 3.

The following procedures must be followed to calculate the remaining stream variables Y_2, L_2 (and L_1), and X_1.

The exit solute concentration, Y_2, may be calculated from using equation (2.1)

The slope of the operating line may be calculated from equations (2.2) and (2.3).

The variable Gs may be calculated using equation (2.4).

The variable L_s may be calculated by equation (2.5).

The total molar flow rates of the gas and liquid entering the absorber $(G_{mol,1}\ and\ L_{mol,2})$ are calculated using equations (2.6) and (2.7) respectively.

The volume flow rate of the solvent, L_2, may then be calculated by using equation (2.8).

Finally, the actual operating line may be represented by a material balance equation over the gas absorber (Treybal, 1980) and is given by equation (2.9).

Equation (2.9) may then be solved for X_1 as given by equation (2.10).

3.2.2 Determination of Absorption Factor

The absorption factor (*AF*) value is frequently used to describe the relationship between the equilibrium line and the liquid-to-gas ratio. For many solute-solvent systems, the most economical value for *AF* ranges around 1.5 to 2.0 (Perry and Chilton, 1984). Equation (2.11) may be used to calculate *AF*.

Since the equilibrium curve is typically linear in the concentration ranges usually encountered, the slope, m would be constant (or nearly so) for all applicable inlet and outlet liquid and gas streams. The slope was calculated from mole fraction values using the Least square method. First, the equilibrium data was converted to mole fraction units and then the least-square method was used to obtain the equilibrium curve equation. Hence, the slope of equilibrium line (m) is obtained from the equation (since equilibrium curve is assumed linear for dilute absorption process).

$$m = \frac{\sum xy - \bar{y}(\sum x)}{\sum x^2 - \bar{x}(\sum x)} \qquad (3.1)$$

3.2.3 Determination of Column Diameter

Once stream conditions have been determined, the column diameter may be estimated. The diameter of a column was designed for a specific pressure drop rather than being determined based on a fraction of the flooding rate. Figure 6 presents the relationship between g_v and L_{mol}/G_{mol} ratio. In this case, liquid-gas flow rate (x-axis of the correlation chart) is given by equation (2.24)(Coulson and Richardson, 1991).

Therefore, the superficial gas flow rate entering the absorber is given by equation (2.25).

The cross-sectional area of the tower, A_c, (m^2) is calculated by equation (2.21).

The diameter of the column, D_c, (m) can be calculated from the cross-sectional area by equation (2.22).

The superficial liquid flow rate entering the absorber, $G_L(\frac{kg}{m^2 s})$ based on the cross-sectional area determined in Equation (2.21) is calculated from equation (2.23).

3.2.4 Determination of Tower Height and Surface Area

Tower height is primarily a function of packing depth. The required depth of packing (Z_c) is determined from the theoretical number of overall transfer units N_{OG} needed to achieve a specific removal efficiency, and the height of the overall transfer unit (H_{OG}) (Treybal, 1980). This is given by equation (2.27). The number of overall transfer units may be estimated graphically by stepping off stages on the equilibrium-operating line graph from inlet conditions to outlet conditions, or by equation (2.28).

The height of overall gas transfer unit is calculated based on estimating the height of the gas and liquid film transfer units, H_L and H_G, respectively (Treybal, 1980). The height of overall gas transfer unit is given by equation (2.33).

The correlations represented by equations (2.35) to (2.42) may be used to estimate values for H_L and H_G.

The height of the column may be calculated from the correlation given by equation (2.43). The surface area (A_s), (m^2) of the gas absorber can be calculated using equation (2.44)

These equations were used for coding the design module for the absorption column.

3.3 Development of Optimization Equation of a Packed Gas Absorption Column.

The variable annual costs of importance are the charges on the equipment, the cost of solvent, the power cost of pumping the liquid, the power cost for compressing the gas through the absorber and the cost of packing materials (Mclnnes et al., 1990). The annual cost that is to be optimized, therefore can be represented by the following equations (Pdnengineers, 2011):

$$C = F_c C_A A_s + W_F C_L L_2 \left(\frac{3600\ s}{1\ hr}\right) Y + C_E\ Y\ E_{(Fan\ +\ pump)} + C_p V_p \qquad (3.2)$$

E $_{(\text{ Fan } + \text{ Pump})}$ (Power (energy) required by the pump and the fan) is given by (Pdnengineers, 2011):

$$E_{(Fan\ +\ Pump)} = C_E\ Y\ \left\{\frac{\left[1.17 * 10^{-4}\ G_1\left(\frac{3600\ s}{1\ hr}\right)\ \Delta P Z_c * 1.39034\right] + \left[0.746 * 2.52 * 10^{-4} * L_2\left(\frac{3600\ s}{1\ hr}\right) P_p * 866.76\right]}{\varepsilon}\right\} \qquad (3.3)$$

Also, the volume of packing is related to packing height and column diameter by:

$$V_p = \frac{\pi}{4}\ D_c^2\ Z_c \qquad (3.4)$$

Substituting equations (3.33) and (3.34) into equation (3.32) gives

$$\begin{aligned} &C = \\ &F_c C_A A_s + W_F C_L L_2 \left(\frac{3600\ s}{1\ hr}\right) Y + \\ &C_E\ Y\ \left\{\frac{\left[1.17 * 10^{-4}\ G_1\left(\frac{3600\ s}{1\ hr}\right)\ \Delta P Z_c * 1.39034\right] + \left[0.746 * 2.52 * 10^{-4} * L_2\left(\frac{3600\ s}{1\ hr}\right) P_p * 866.76\right]}{\varepsilon}\right\} + \frac{C_p\ \pi\ D_c^2\ Z_c}{4} \qquad (3.5) \end{aligned}$$

Equation (3.5) contains parameters such as surface area of the absorber (A_S), solvent flow rate (L_2), packing height (Z_C),and column diameter (D_C), which have been obtained in equations (2.44), (2.8), (2.27), and (2.22) respectively. Further parameters to be specified are therefore annual cost of absorber per unit surface area (C_A), solvent unit cost (C_L), Waste (make-up) fraction (W_F), operating hours per year (Y), Unit cost of electricity (C_E), Cost of packing per unit volume of packing (C_P), Pressure drop through the system (ΔP), Pump operating pressure(P_p), combined fan and pump motor efficiency (ε) and volumetric flow rate of Gas entering the absorber (G_1). The variables to vary in order to optimize the annual cost are therefore gas flow rate, packing size and type, pressure drop, percent flooding velocity and operating temperature.

3.3.1 Equipment, Packing, Solvent, and Utility (Electricity) Cost.

Equipment, packing, solvent and electricity cost may be obtained by consulting cost texts, journals and extrapolated data using cost indices. Consideration was given to the cost of packed absorber per unit surface area ($/m^2), cost of packing per unit volume of packing ($/m^3), solvent cost per unit volume ($/m^3) and electricity cost per kilowatt-hour ($ /KW-hr).

3.3.2 Problem Statements

There are two problem statements in this work. One is to develop and test the CAD module for calculating the pertinent design parameters of a packed absorption column, while the second is to test the solution of the optimization program.

3.3.2.1 Problem Statement 1

A gas mixture containing 6% SO_2 and 94% dry air is to be scrubbed with fresh water in a tower packed with 0.025m ceramic rasching rings to remove the SO_2 so that the exit will contain no more than 0.1 mole percent SO_2, that is, recovery of about 98.333%. The tower must treat 0.126kg/s of gas and is to be designed using 50% of flooding velocity. The water flow is to be twice the minimum required to achieve this separation in a tower operating at 30^0C and

760mmHg or 1 atm. Determine the tower diameter, cross-sectional area, packing height and surface area.

3.3.2.2 Problem Statement 2

Variable operating charges for the absorber including maintenance, solvent, packing, fan power, and pumping power are represented by equation (3.35) which is the objective function. The problem is to optimize the equation with respect to gas flow rate, packing size, operating temperature, pressure drop, and percent flooding velocity.

3.4 Computer Aided – design module for a packed Absorption column.

This work makes use of a CAD module. It is a high level language program of the procedure required for the design and optimization of a packed absorption column. It is thus an assembly of a set of mathematical equations and techniques for solving them. The main program draws relevant information/data from a database of phase equilibra; and physical, chemical and thermodynamic properties. The computer program was written in visual Basic.

3.4.1 Development of the CAD Module

The flowchart for the source code is shown in Figure 3.8. The computer program was written in visual Basic because its user- friendliness, easier comprehension, and faster application development. However, it can also be run using Qbasic and turbo-Basic compiler.

3.4.2 Solution of the Optimization Objective Function.

The flowchart for the solution of the optimization objective function is shown in Figure 3.9. It is an elongation of Figure 3.8, from output the design parameters. The program was also written in visual Basic.

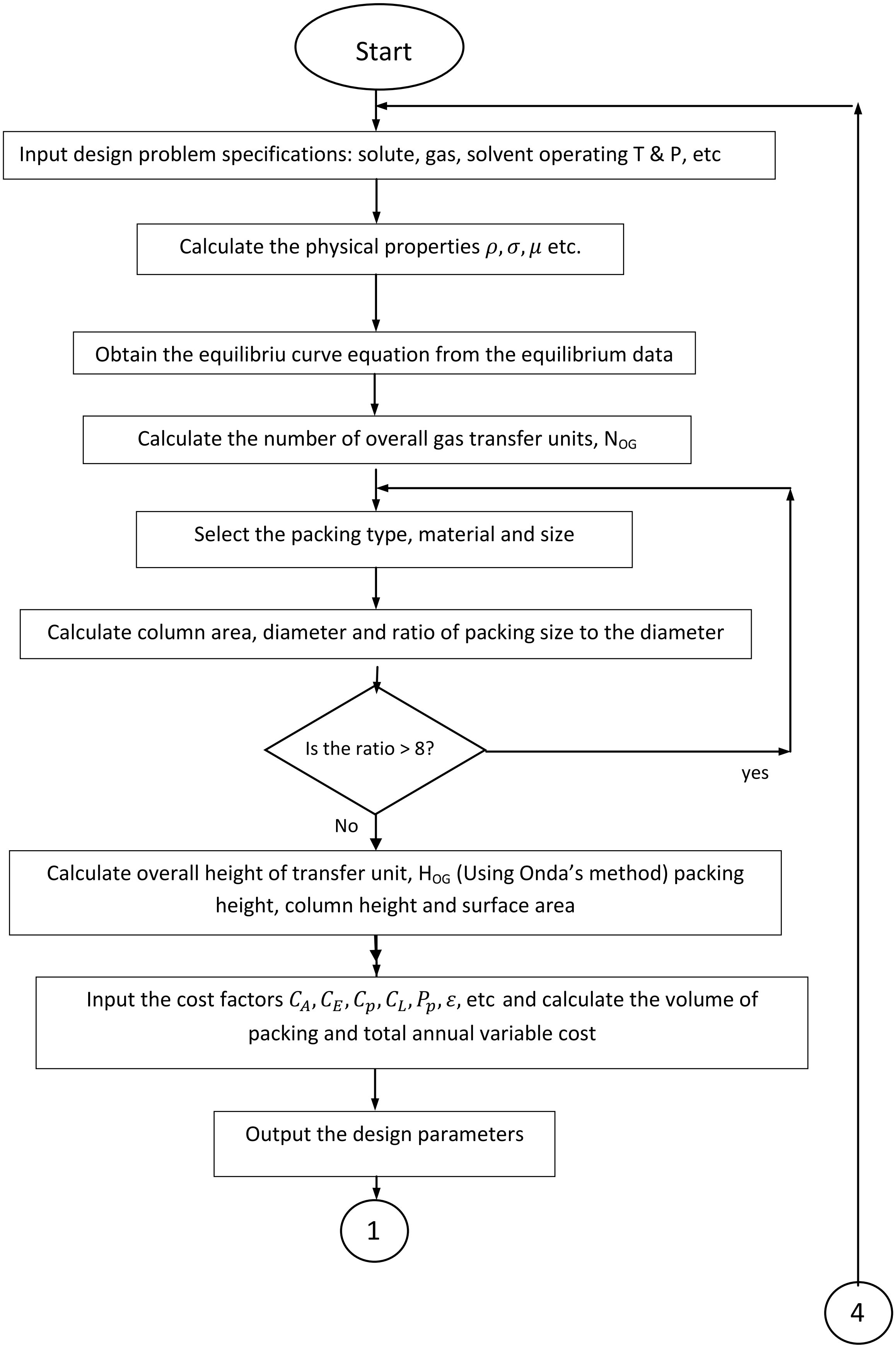


Figure 3.8: Flowchart for implementing CAD module for absorption

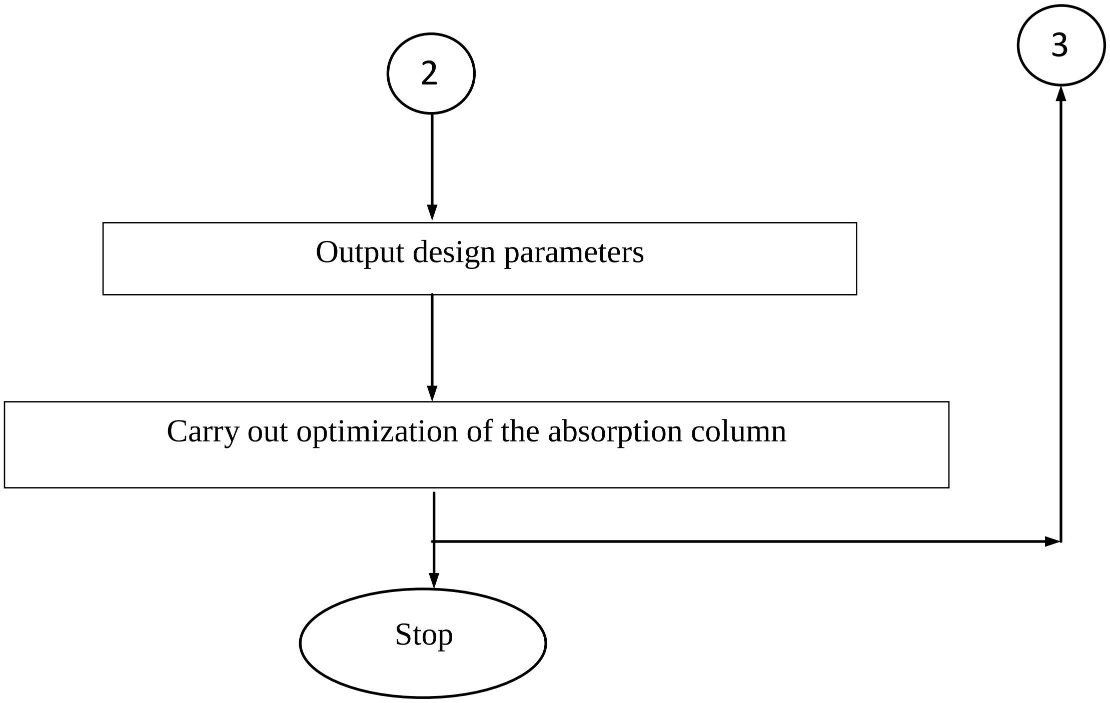


Figure 3.9: Flowchart for implementing the solution of the optimization program

CHAPTER FOUR

RESULTS AND DISCUSSION

4.1 Results

The results of the manual calculations and CAD program for both problem statements are presented below.

4.1.1 Results from Manual Calculations and CAD Program for the Problem Statements.

The manual calculations of the problem statements are shown in Appendix A. The results of these calculations and those from CAD module are shown in Table 4.2 while the operating variables for obtaining the design parameters are shown in Table 4.1.

Table 4.1: Operating variables for obtaining the design parameters.

Operating Variable	Value
Temperature (^{0}C)	30
Pressure Drop (mm HO/m of Packing)	21
Flooding Velocity (%)	0.5
Gas Flow Rate (Kg/s)	0.126
Packing Type and Size(m)	Rachig Ring Ceramic (0.025)

Table 4.2: Results from manual calculations and CAD program for the problem statemen**ts.**

Design parameters	Manual calculations	CAD output
Cross sectional area (m^2)	0.621	0.621
column diameter (m)	0.89	0.889
Packing height (m)	2.73	2.74
Surface area (m^2)	22.3	22.36
Volume of packing (m^3)	1.7	1.7
Tower height (m)	7.54	7.56
Annual Variable Cost($/year)	45,436.91	45,592.31
Correlation coefficient	1.000	1.000

4.1.2 Results of Optimization

The CAD program optimization results at varying operating variables are shown in Tables 4.3-4.8.

Table 4.3: Effects of operating temperature on the packed column dimensions and annual variable cost.

operating variable varied	Design Parameters						
Temp (^0C)	Crossectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Annual Variable Cost ($/year)
0	0.4251626	0.7357062	6.009029	28.52712	2.554814	11.97306	23,884.66
7	0.4590614	0.7644733	4.777753	25.60711	2.193282	10.27862	25,951.31
10	0.4887733	0.7888249	4.305094	24.87447	2.104215	9.641733	27,958.02
15	0.5102593	0.8059765	3.841116	23.83638	1.959965	9.009659	30,676.20
20	0.5523989	0.838597	3.430869	23.41844	1.895208	8.468586	37,363.43
30	0.6209431	0.8891045	2.743771	22.35612	1.703726	7.558167	45,592.31

Table 4.4: Effects of pressure drop on the packed column dimensions and annual variable cost.

operating variable varied	Design Parameters						
Pressure Drop (mm H_2O/m of Packing)	Crossectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Annual Variable Cost ($/year)
4	0.8781461	1.057329	2.577494	26.66218	2.263416	7.496967	45,554.30
8	0.7271741	0.9621574	2.665361	24.19683	1.938181	7.522906	45,034.12
21	0.6209431	0.8891045	2.743771	22.35612	1.703726	7.558167	45,592.31
42	0.5420035	0.8306689	2.815053	20.91543	1.525769	7.598356	47,109.74
83	0.5141897	0.8090746	2.843654	20.39005	1.462178	7.616372	50,853.83
125	0.4809804	0.7825113	2.880718	19.74892	1.385569	7.641166	54,768.35

Table 4.5: Effects of percent flooding velocity on the packed column dimensions and annual variable cost.

operating variable varied	Design Parameters						
Flooding velocity (%)	Crossectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Annual Variable Cost ($/year)
0.5	0.6209431	0.8891045	2.743771	22.35612	1.703726	7.558167	45,592.31
0.6	0.5174525	0.8116376	3.007907	21.051	1.556449	7.84894	45,340.04
0.65	0.4776486	0.7797962	3.148938	20.59033	1.504086	8.013906	45,283.95
0.7	0.4435308	0.7514305	3.297352	20.2301	1.462477	8.192751	45,265.91

Table 4.6: Effects of gas flow rate on the packed column dimensions and annual variable cost.

operating variable varied	Design Parameters						
Gas Flow Rate (Kg/s)	Crosssectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Annual Variable Cost ($/year)
0.126	0.6209431	0.8891045	2.743771	22.35612	1.703726	7.558167	45,592.31
0.252	1.241886	1.257384	2.743771	33.82787	3.407451	7.933811	88,421.97
0.378	1.862829	1.539974	2.743771	43.50887	5.111176	8.222054	131,277.13
0.504	2.483772	1.778209	2.743771	52.26292	6.814903	8.465053	173,958.54

Table 4.7: Effects of packing type and size on the packed column dimensions and annual variable cost.

Operating variable varied		Design Parameters						
Packing Type	Packing Size (m)	Crossectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Annual Variable Cost ($/year)
Rachig Ring Ceramic	0.013	1.241886	1.257384	2.450342	32.20492	3.043046	7.52301	48,338.47
	0.025	0.6209431	0.8891045	2.743771	22.35612	1.703726	7.558167	45,592.31
	0.038	0.4771479	0.7793875	3.59763	22.11629	1.716601	8.641657	46,161.78
Intallox saddle Plastic	0.016	0.4847827	0.7855982	2.68203	19.15181	1.300202	7.366153	42,721.68
	0.025	0.3533431	0.6706952	3.549105	18.54067	1.254051	8.462855	43,213.97
	0.038	0.3089896	0.6271895	4.585599	20.06725	1.416902	9.869572	44,225.55
Intallox Saddle Ceramic	0.013	0.6962162	0.9414537	2.709471	23.76575	1.886378	7.563542	43,605.77
	0.025	0.4693888	0.7730246	2.786514	19.15414	1.307959	7.499605	42,795.24
	0.038	0.3533431	0.6706952	3.833309	19.37914	1.354473	8.860742	$43,570.05

Table 4.8: Optimum Design parameters.

Design Parameters						
Crossectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Annual Variable Cost ($/year)
0.237095	0.5493993	7.098567	23.44728	1.683034	13.30838	22,480.07

4.2 Discussion

The discussion will focus on the comparison between the manual calculations and the CAD program for the problem statements and optimization of the design variables.

4.2.1 Comparison between the Manual Calculations and the CAD Program for the Problem Statements.

Table 4.2 shows that the correlation coefficient between the results obtained from manual calculations and the CAD program is 1.000. This implies that that there is perfect agreement between the two results, which confirms that the programming of the tables, charts, graphs and correlations using appropriate numerical methods and software are accurate. Thus the tedious calculations, iterations, reading of graphs and tables are now eliminated so that quicker and more accurate results can be obtained (Peters and Timmerhaus, 1991). For instance, typical problems in chemical engineering process design or plant operation have many (possibly an infinite number) solutions. The tedious and iterative nature of the procedure lends itself to solution by computers.

4.2.2 Discussion of Optimization Results

The design parameters considered in the optimization of this design were cross sectional area of the packed column, column diameter, surface area of the packed column, column (tower) height, packing height and the total annual variable cost of the packed column.

In Table 4.3, the variable changed for the purpose of optimization is the operating temperature. Comparison of the values show that increase in the operating temperature increase the column diameter and cross-sectional area while tower height, height of packing, volume of packing, and surface area decrease . This could be due to the effect of temperature on the physical properties of the solute gas and solvent such as solubility of the solute gas in the solvent, diffusivity of the solute in both phases, density, viscosity and surface tension. For instance, the higher the gas temperature, the lower the absorption rate and vice-versa (Treybal, 1980). This leads to higher solvent requirement. Column diameter and cross-sectional area is directly proportional to solvent flow rate. Excessively high gas temperature can also lead to significant solvent loss through evaporation. The density of the solvent (water) is inversely proportional to temperature and the height of transfer unit is directly proportional to liquid density (Onifade, 2000). That is, increase in temperature decreases the the height of transfer unit and consequently decreases the tower height, height of packing, volume of packing, and surface area. The total annual variable cost also increases as the operating temperature increases. This is because increasing the column diameter will increase the capital cost (Coulson and Richardson, 2004) and the cost of pumping the solvent through the column increases due to increased solvent flow rate. The overall effect is increase in operating temperature leads to increase in the total annual variable cost of the absorber and its operation. Zero degree celcius (0^0C) gives the minimum annual variable cost for the absorber and its operation.

In Table 4.4, the variable changed for the purpose of optimization is the pressure drop. Increase in pressure drop increased the tower height and height of packing and decrease volume of packing, surface area, column diameter and cross-sectional area. This is attributed to the effect of the properties of the packing materials, such as surface area and free volume in the column. A high pressure drop results in high fan power to drive the gas through the packed column, and consequently high costs. The total annual variable cost decreases as the pressure drop is increased from 4 mmH_2O/m of packing to 8 mmH_2O/m of packing and then increases as the pressure drop is increased from 8 mmH_2O/m of packing to 125mmH_2O/m of packing. This is because the decrease in the capital cost as a result of decrease in column diameter and surface area outweighed the increase in cost of compressing the gas through the column as a result of increase in pressure drop from 4 mmH_2O/m of packing to 8 mmH_2O/m of packing. Normally, the column will be designed to operate at the highest economical pressure drop, to ensure good liquid and gas distribution (Coulson and Richardson, 2004). Though the results show that pressure drop of 8 mmH_2O/m of packing gives the lowest total annual variable cost, recommended design values for absorbers and strippers is 15-50 mmH_2O/m packing (Coulson and Richardson, 2004). This is because it is advantageous to have a reasonable hold-up in the column as this promotes interphase contact (Coulson and Richardson, 2009). Based on this argument, 21 mmH_2O/m packing gives the best result.

In Table 4.5, the variable changed for the purpose of optimization is percent flooding velocity. Increase in percent flooding velocity decreases the column diameter, cross-sectional area, volume of packing, and surface area while tower height and height of packing increase. The results obtained agreed with the theory that higher flooding velocity leads to more efficient separation (Onifade, 2000), interpreted in terms of size of the column. Decrease in the column diameter, volume of packing, and surface area decreased the capital cost of the column hence, decrease in total annual variable cost. Seventy percent (70) percent flooding velocity gives the best result.

In Table 4.6, the variable changed for the purpose of optimization is gas flow rate. The table shows that when the gas flow rate is increased, the packing height does not change. This is due to the fact that the height of gas transfer unit, $H_{G,}$ does not vary with gas flow rate (except at very low gas flow rate, where H_G approaches zero as the gas rate approaches zero). The cross sectional area of the packed column, column diameter, surface area of the packed column and column (tower) height increase as the gas rate increased. This is expected because the cross sectional area of the packed column and column diameter are proportional to gas flow rate. The surface area of the packed column, and column (tower) height, were similarly affected. The total annual variable cost also increases as the operating gas flow rate increased. This is because increasing cross sectional area of the packed column, column diameter, surface area of the packed column, column (tower) height will increase the capital cost of the column (Coulson and Richardson, 1991). Gas flow rate of 0.126 kg/s gives the minimum annual variable cost for the absorber and its operation.

In Table 4.7, the variable changed for the purpose of optimization is the packing type and size. The size of packing used influences the height and diameter of the column, and the pressure drop. Increase in packing size decreases the column diameter and increase tower height. This expected because as the packing size increases, the gas flow rate per unit area decreases. The column diameter is proportional to gas flow rate. Generally, as the packing size is increased, the pressure drop per unit height of packing is reduced and the mass transfer efficiency is reduced. Reduced mass transfer efficiency results in a taller column being needed, so that the overall column cost is not always reduced by increasing the packing size (Coulson and Richardson, 2004). Normally, in a column in which the packing is randomly arranged, the packing size should not exceed one-eight of the column diameter (Coulson and Richardson, 2004). This is because the packing density, that is, the number of packing pieces per unit volume, is ordinarily less in the immediate vicinity of the tower walls, and this leads to a tendency of the liquid to segregate toward the walls and the gas to flow in the centre of the tower (Treybal, 1980).This leads to poor liquid distribution and hence reduced mass transfer efficiency. Above this size, this tendency is much more pronounced, that is, liquid distribution and hence the mass transfer efficiency, decreases rapidly. It is recommended that, if possible, the ratio d_p/D_c equals 1:15 (Treybal, 1980). For raschig rings ceramic,and intalox saddle ceramic, 0.025 m packing size gives the minimum annual variable cost for the absorber and its operation while for polypropylene packing, 0.016 m packing size gives the best results. This may be due to the differences in the properties and costs of the various forms of the packing materials. Of all the packing materials, 0.016 m polypropylene packing gives the minimum annual variable cost for the absorber and its operation followed by 0.025m intalox saddle ceramic packing. 0.016 m polypropylene packing, therefore, gives the best result. Metal packing materials cannot be used for this system because it involves highly corrosive solute (SO_2) (Coker, 1991).

Table 4.8 shows the optimum design parameters obtained at the optimum operating variables (temperature of 0^0C, pressure drop of 8 mm H_2O/ m of packing, flooding velocity of 70 %, gas flow rate of 0.126 Kg/s and 0.016 m polypropylene packing material).

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

A CAD module was developed for implementing the optimization of a packed absorption column. The program was tested with a design problem and the results of the manual calculations and CAD program agree perfectly well. The program can thus be used for hundreds of design specifications and accurate results obtained within the shortest possible time.

The CAD program was also used in optimizing the design by varying the values of certain operating parameters such as gas flow rate, packing type and size, operating temperature, pressure drop, and percent flooding velocity.

From the results obtained, the following conclusions can be made:

1) Increase in operating temperature leads to increase in the total variable cost of the absorber and its operations
2) Increase in flooding velocity leads to decrease in the total variable cost of the absorber and its operations
3) Increase in gas flow rate leads to increase in the total variable cost of the absorber and its operations
4) Increase in pressure drop results in high fan power to drive the gas through the packed tower and hence high costs.

5) The optimum operating parameters are temperature of 0^0C, pressure drop of 21 mm H_2O/ m of packing, flooding velocity of 0.7, gas flow rate of 0.126 Kg/s and 0.016 m polypropylene packing material.
6) The optimum total variable cost for the absorber and its operation is $22,480.07 per year.
7) The results of the manual calculations and CAD program agree reasonably well with a correlation coefficient of 1.000, which is a very good validation of the module.

5.2 Recommendations

The following suggestions can be considered in future work:

(1) The module could be used for determining the optimum operating parameters for other gas-liquid systems.
(2) General purpose engineering software such MathCAD, HYSYS, PROII, OLGA, MATLAB etc., should be explored to optimize the design.
(3) Sensitivity analysis should be carried out on the work.