Development of a Computer Software for Optimization of Packed Absorption Column

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Abstract

A Computer Aided-Design module was developed for the 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 cost of the absorber and its annual operation was also done by studying the trend in the operating parameters. The optimum total 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.

Key Words: Packed column, gas absorption, optimization, CAD, visual BASIC

1.0 INTRODUCTION AND BRIEF LITERATURE

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 et al., 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 et al., 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 et al., 2001).

Generally, when setting out to optimize any system, the first step is to identify 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 (Richardson and Coulson, 2004).

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 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 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.

A comprehensive review of absorption and packed columns can be found in many units operations books (Richardson and Coulson, 2009, Brunazziet al., 2002, Perry and Green 1997,Mclnnes et al., 1990,Ayoade 1994, McCabe, Smit and Harriott1993, Coker 1991and Treybal 1981) and that of optimization techniques can be found in many optimization books (Edgar et al.,2001, Richardson and Coulson, 2004 and Peters and Timmerhaus, 1991).

Computer Aided Design (CAD) is a utility that exploits the capabilities provided computers for speedy processing of design procedures. It enables the engineers to solve large and complex design problems much morefaster and accurately than hitherto. The evolution, types structure, components and advantages of CAD are well detailed (Onifade 2000 and Oguntoyinbo 1993).

This work makes use of a CAD module, a high level language program of the procedure required for the optimization of a packed absorption column. Thus it is an assembly of a set of mathematical equations and the techniques for solving them. The main program draws relevant information/data from a database of phase equilibria; and physical, chemical and thermodynamic properties.

The aim of this research work is to develop a computer software foroptimization of packed gas absorption column in terms of the overall cost of the absorber and its operation using a Computer Aided-Design module.

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 cost of the column to the design parameters of the column.
2. Solve the mathematical program obtained from (1) using a program developed in Visual Basic. The solution constitutes the CAD module.
3. Use the CAD module to optimize the design problem

2.0 METHODOLOGY

2.1 Design Module Source Code

The design and optimization procedures implemented in the CAD module are based on the following assumptions:

(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 encountered.

(d) Chemical reaction does not occur.

(e) The system is assumed to be isothermal.

(f) The equilibrium curve is assumed to be linear since the process fluid are dilute.

(e) The molar flow rate of the solute-free gas is assumed to be constant to be constant throughout the column.

The flowchart for implementing CAD module for absorption column design parameters is shown in Figure 1 and the flowchart for implementing the solution of the optimization program is shown in Figure 2. The program was developed using Visual Basic language because of its

user friendliness, easier comprehension, and faster application development.

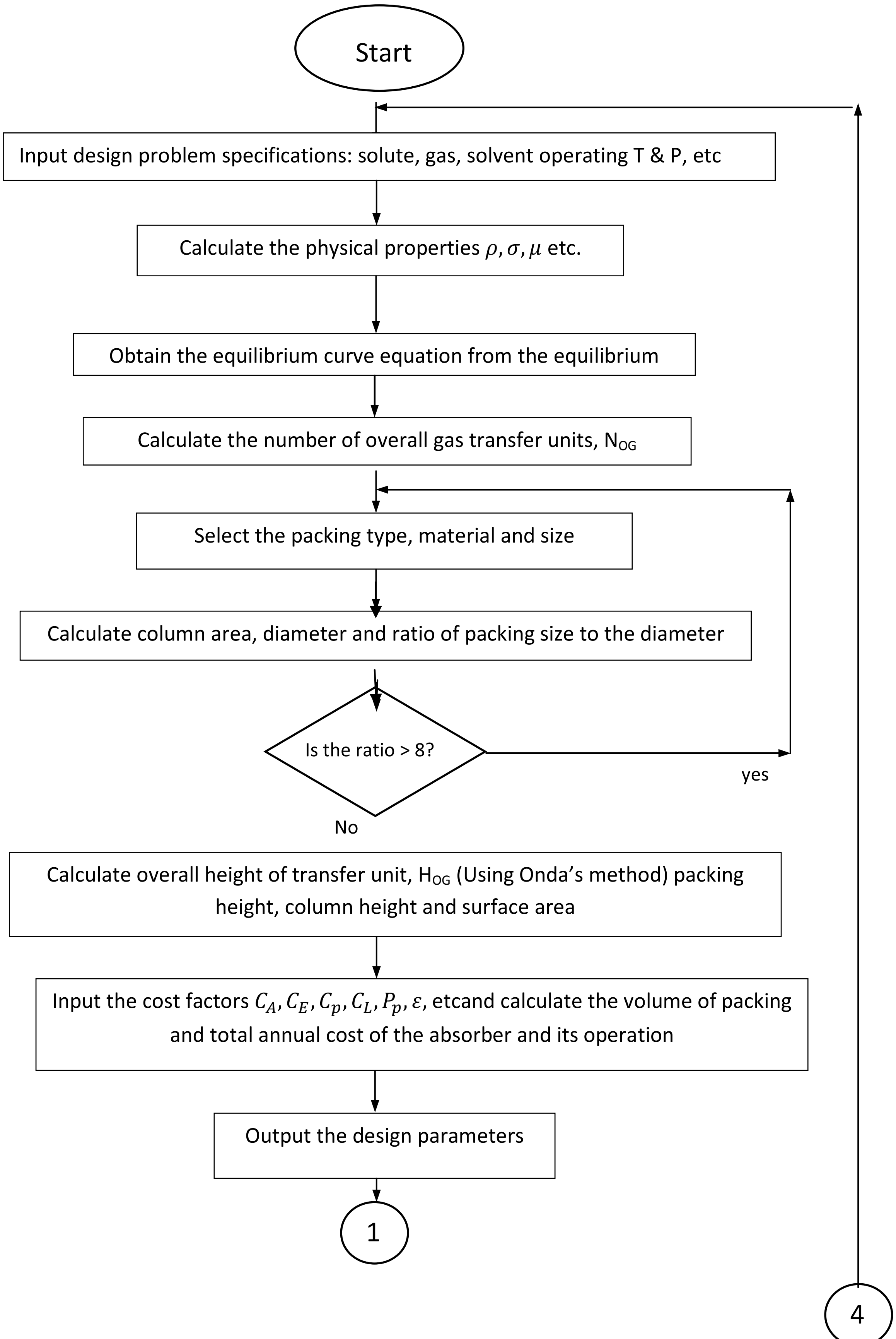


Figure 1: Flowchart for implementing CAD module for absorption

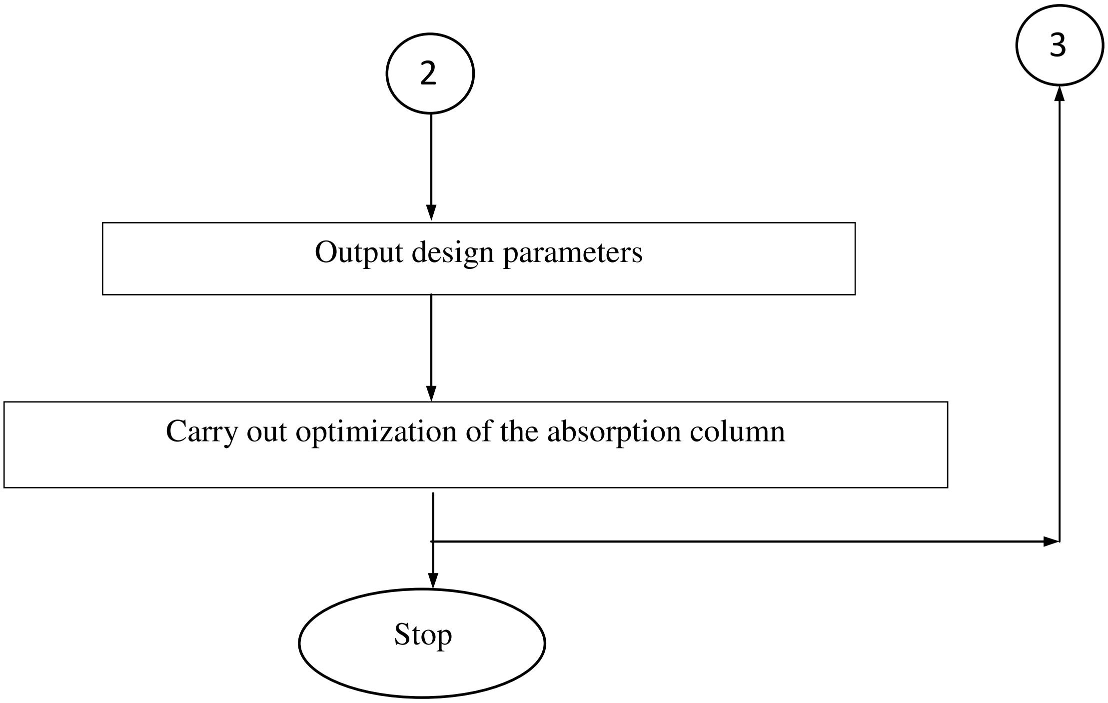


Figure 2: Flowchart for implementing the solution of the optimization program

The Visual Basic 6.0 program Icon was double clicked to open new forms. Text boxes and combo boxes were laid out on the screens for imputing and selecting the design specifications and were labeled appropriately. Command buttons were also placed on the forms for giving appropriate commands for calculating the pertinent design parameters of the packed column, the total annual cost of the absorber and its operation, generating report, updating record, adding record to data base and for exiting the application. All the equations, data and correlations for obtaining the design parameters of the packed column and the total annual cost of the absorber and its operation were then coded in the code window. The codes for generating report, updating record, adding record to data base and for exiting the application were also codedin the code window.A typical graphical user interface (GUI) and output screen are shown below.

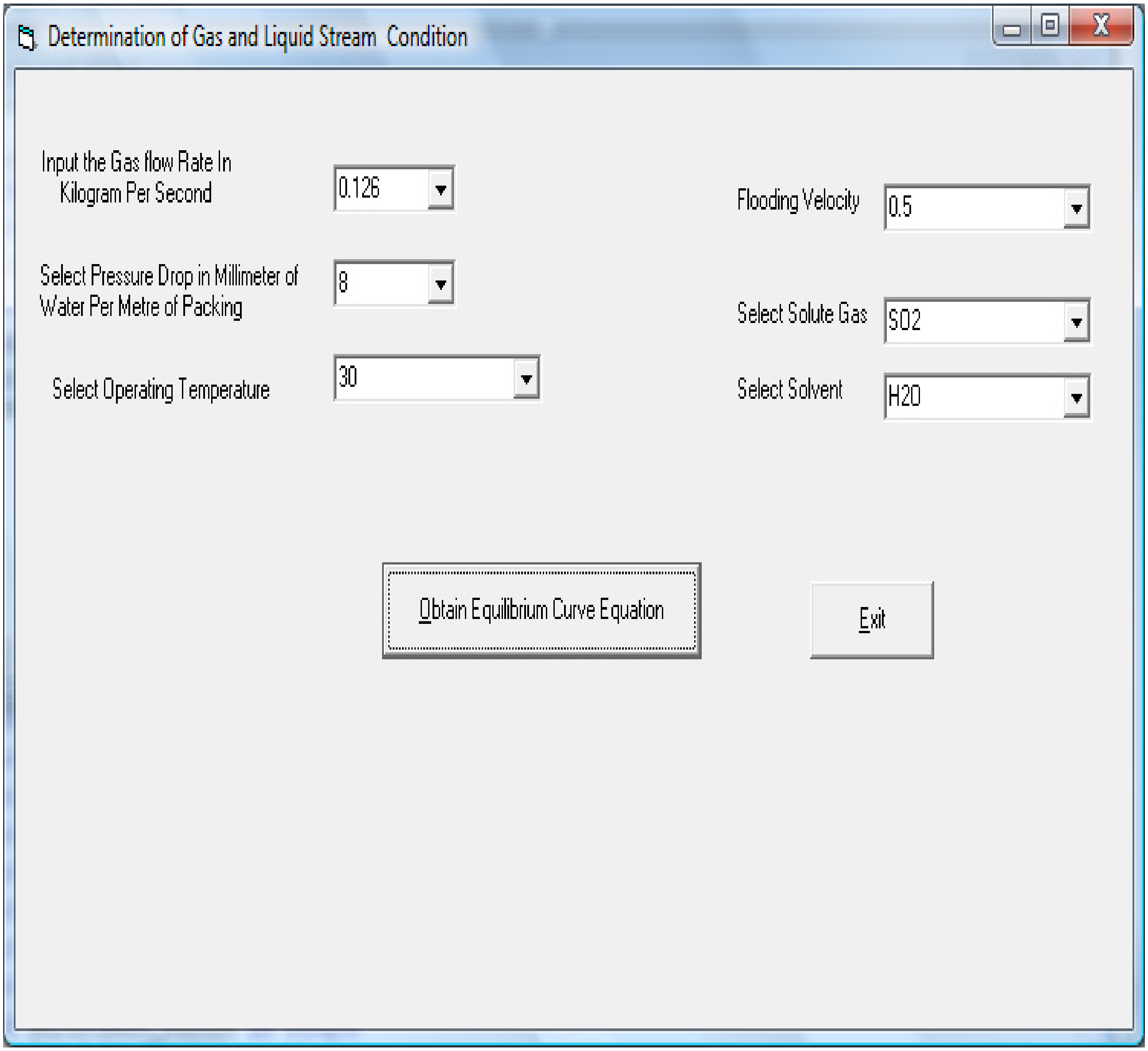
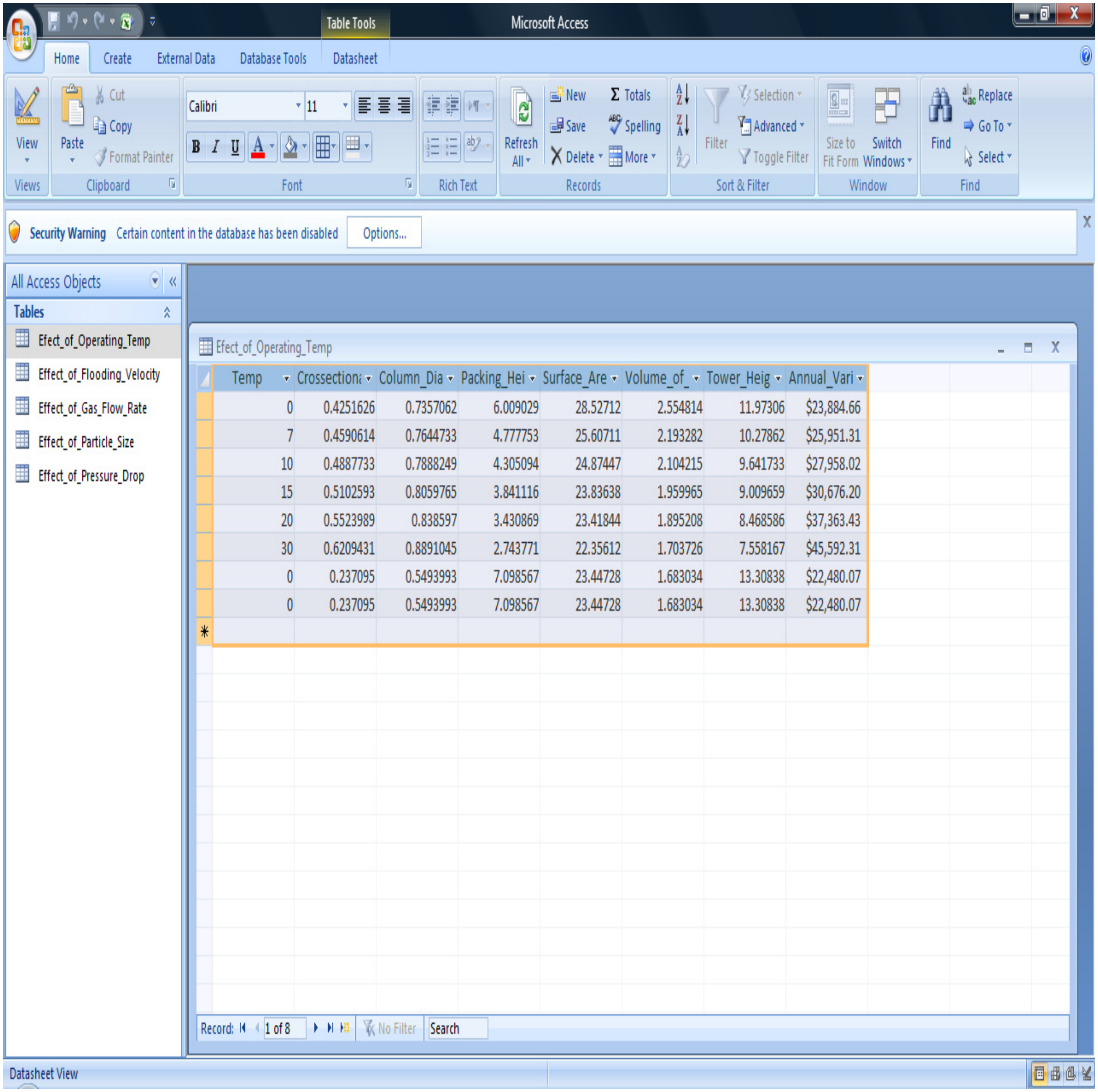


Figure 3: Graphical User Interface for Obtaining Equilibrium Curve Equation.



Temp	Crossectiona	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 4: A Typical Output Screen

The CAD module was tested using the following problems.

2.1 The Test Problem 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.

2.2 The Test Problem 2

Variable operating charges for the absorber including maintenance, solvent, fan power, and pumping power are included in the objective function.

The problem is to optimize the equation (objective function) with respect to gas flow rate, packing size, operating temperature, pressure drop, and percent flooding velocity.

2.3 Program run

The following important set of screens was used.

1. Design specification screens
   These series of screens are used for inputting the following information:
   a. Solute gas
   b. Solvent
   c. Pressure drop (mmH_2O/m of packing)
   d. Percentage of flooding rate (50-75 %)
   e. Gas flow rate (0.126-0.504 Kg/s)
   f. Operating temperature (0^0C-30^0C)
   g. Mole fraction of the solute in the gas entering the column
   h. Mole fraction of the solute in the gas exiting the column
   i. Mole fraction of the solute in the liquid entering the column
   j. Adjustment factor

   At this point the module displays the operating line equation

2. A screen comes up for inputting the packing type, packing material and size. The module calculates the pertinent design parameters (diameter, cross-sectional area, packing height, surface area, and height) of the absorption column.
3. Another screen comes up for inputting the following information:
   a. cost of absorber per unit surface area (\$/m^2)
   b. Solvent make up fraction
   c. Unit cost of electricity (\$/KW-hr)
   d. Cost of packing per unit volume packing (\$/m^3)
   e. Solvent unit cost (\$/m^3)
   f. Pump operating pressure (m of H_2O)
   g. Combined pump and fan motor efficiency (%)
   h. Operating hour per year (hr)

At this point the module calculates the total annual cost of the absorber and its operation.

After a series of screens which include one for generating the result, updating record and adding record, the final output screen is displayed. A typical output screen is shown in figure 4

3.0 RESULTS AND DISCUSSION

3.1 CAD Module Output.

The results of the manual calculations and those from CAD module are shown in Table 2 while the operating variables for obtaining the design parameters are shown in Table 1.Tables 3-8 summarize the various outputs obtained from the program using different specifications.

Table 1: Operating variables for obtaining the design parameters.

Operating Variable	Value
Temperature (^{0}C)	30
Pressure Drop (mm H_2O/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 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

Table 3:Output from the program using operating pressure of 760 mmHg, gas flow rate of 0.126kg/s, flooding velocity of 50%, pressure drop of 21mm H_2O/m of Packing, 0.025m raschig ring ceramic packing with varying operating temperature.

operating variable varied	Design Parameters						
Temp (^{0}C)	Cross-sectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Total Annual 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: Output from the program using operating pressure of 760 mmHg, gas flow rate of 0.126kg/s, flooding velocity of 50%, operating temperature of 30^{0}C, 0.025m raschig ring ceramic packing with varying pressure drop

operating variable varied	Design Parameters						
Pressure Drop (mm H_2O/m of Packing)	Cross-sectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Total Annual 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 5: Output from the program using operating pressure of 760 mmHg, gas flow rate of 0.126kg/s, pressure drop of 21mm H_2O/m of Packing, operating temperature of 30^0C, 0.025m raschig ring ceramic packing with varying flooding velocity.

operating variable varied	Design Parameters						
Flooding velocity (%)	Cross-sectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Total Annual 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 6: Output from the program using operating pressure of 760 mmHg, operating temperature of 30^0C, flooding velocity of 50%, pressure drop of 21mm H_2O/m of Packing, 0.025m raschig ring ceramic packing with varying gas flow rate.

operating variable varied	Design Parameters						
Gas Flow Rate (Kg/s)	Cross-sectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Total Annual 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 7: Output from the program using operating pressure of 760 mmHg, operating temperature of 30^0C, gas flow rate of 0.126kg/s, flooding velocity of 50%, pressure drop of 21mm H_2O/m of Packing, with varying packing type and size.

Operating variable varied		Design Parameters						
Packing Type	Packing Size (m)	Cross-sectional Area (m^2)	Column Diameter (m)	Packing Height (m)	Surface Area (m^2)	Volume of Packing (m^3)	Tower Height (m)	Total Annual Cost ($/year)
Rachig Ring	0.013	1.241886	1.257384	2.450342	32.20492	3.043046	7.52301	48,338.47
Ceramic	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	0.016	0.4847827	0.7855982	2.68203	19.15181	1.300202	7.366153	42,721.68
Plastic	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	0.013	0.6962162	0.9414537	2.709471	23.76575	1.886378	7.563542	43,605.77
Ceramic	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 8: Optimum Design parameters.

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

3.2 Discussion

Table 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 reasonable 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.

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 cost of the packed column.

In Table 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 both phases, density, viscosity and surface tension. For instance, the higher the gas temperature, the lower the absorption rate and vice-versa (Treybal, 1981). This leads to higher solvent requirement. Column diameter and cross-sectional area are directly proportional solvent flow rate. The density of the solvent (water) is inversely proportional to temperature and the height of transfer unit is directly proportional to liquid density. That is, increase in temperature decreases the height of transfer unit and consequently decreases the tower height, height of packing, volume of packing, and surface area. The total annual 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 cost of the absorber and its operation. 0^0C gives the minimum total annual cost for the absorber and its operation.

In Table 4, the variable changed for the purpose of optimization is the pressure drop. Increase in pressure drop increase 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 elements, 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 cost decreases as the pressure drop is increased from 4 mmH_2O/mof packing to 8 mmH_2O/m of packing and then increases as the pressure drop is increased from 8 mmH_2O/mof packing to 125mmH_2O/mof 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/mof 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 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 5, the variable changed for the purpose of optimization is percentage 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 decrease the capital cost of the column hence, decrease in total annual cost of the absorber and its operation. 70 percent flooding velocity gives the best result.

In Table 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 increases. 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 cost also increases as the operating gas flow rate increases.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, 2009). Gas flow rate of 0.126 kg/s gives the minimum total annual cost for the absorber and its operation.

In Table 7, the variable changed for the purpose of optimization is packing type and size.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, 1981).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, deteriorates rapidly. It is recommended that, if possible, the ratio d_p/D_c equals 1:15 (Treybal, 1981). For raschig rings ceramic,andintalox saddle ceramic, 0.025 m packing size gives the minimum total annual 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 total annual 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 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 0.7, gas flow rate of 0.126 Kg/s and 0.016 m polypropylene packing material).

4.0 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 reasonably well with a correlation coefficient of 1.000, which is a very good validation of the module. 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 percentage flooding velocity.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 and the optimum total annual cost for the absorber and its operation is $22,480.07 per year.

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