Development of a Computer Software for Design of Packed Absorption Column

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Abstract - A Computer Aided-Design (CAD) module was developed for the design of packed gas absorption column. The program was tested using a problem statement by supplying specifications such as operating conditions (pressure, temperature), physical properties (density, viscosity, surface tension), the solute to be absorbed, the solvent selected, gas and solvent mole fractions, percentage flooding velocity, pressure drop, gas flow rate ,packing type and size. The design parameters calculated agreed with those obtained from manual solution, with a correlation coefficient of 1.000. The specifications above were varied to obtain the design outputs within the shortest possible time. For example, operating pressure of 760 mmHg, operating temperature of 30°C, gas flow rate of 0.126kg/s, flooding velocity of 50%, pressure drop of 21 mm H₂O/m of packing, and 0.025m raschig ring ceramic packing gave the following design parameters: cross-sectional area of 0.6209431 m², column diameter of 0.8891045 m, packing height of 2.743771 m, surface area of 22.35612 m², tower height of 7.558167 m, and volume of packing of 1.703726 m³.

Key Words: Packed column, gas absorption, design, software, CAD.

1.0 INTRODUCTION

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. 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 (McInnes et al., 1990). Moreover, countercurrent designs usually require lower liquid to gas ratios than co-current and are more suitable when the solute loading is higher (Jose L. Bravo, personal communication June 8, 1992).

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 (McInnes 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 (http://www.pdnengineers.com Retrieved February, 2011).

The following factors are usually considered for optimum design an absorption column:

- 1. The best solvent for the operation
- 2. The column diameter to handle the gas flow and liquid flow up to flooding point.
- 3. The height of the column and its internal members e.g the height and type of packing.
- 4. Selection of the type and size of packing.
- 5. The optimum operating conditions (temperature and pressure).
- 6. The mechanical accessories of the column, e.g packing support, liquid distributor and re-distributor.
- Economic design specifications include:
- 1. The gas flow rate.
- 2. The gas composition at least with respect to the component to be absorbed.
- 3. Operating pressure, temperature and allowable pressure drop.
- 4. The minimum degree of recovery of one or more solutes.
- 5. The solvent to be used and the type and size of packing.

A comprehensive review of gas absorption and packed column design can be found in many units operations books (Richardson and Coulson, 2004 and 2009; Brunazzi et al., 2002; Perry and Green, 1997; McInnes et al., 1990; Ayoade, 1994; McCabe, Smit and Harriott, 1993; Coker, 1991; Treybal, 1981 and http://www.pdnengineers.com Retrieved February, 2011).

Computer Aided Design (CAD) is a utility that exploits the capabilities provided by computers for speedy processing of design procedures. It enables the engineers to solve large and complex design problems much more faster 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 design of 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 work is to develop a computer software for design of packed gas absorption column using a Computer Aided-Design module and to investigate the effects of the operating variables on the design parameters.

2.0 METHODOLOGY

2.1 Development of program (software)

The design procedure implemented in the CAD module is 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 fluids are dilute.

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

The flowchart for implementing the CAD module for absorption column design is shown in Figure 1. 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 column design

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 labelled appropriately. Command buttons were also placed on the forms for giving appropriate commands for obtaining equilibrium curve equation, calculating the pertinent design parameters of the packed absorption column, generating report, up-dating record, adding record to data base and for exiting the application and were labelled appropriately. All the equations, data and correlations for obtaining equilibrium curve equation and the design parameters of the packed column 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 coded in the code window. A typical graphical user interface (GUI) and an output screen are shown below.

| 5 | 3. Determination of Gas and Liquid | Stream Condition | | | |
|---|---|-----------------------------------|-------------------|-----|----------|
| | Input the Gas flow Rate In | 0.126 | | | |
| | Nilogram Per Second | 0.120 | Flooding Velocity | 0.5 | _ |
| | Select Pressure Drop in Millimeter of Water Per Metre of Packing | 8 | Select Solute Gas | S02 | • |
| | Select Operating Temperature | 30 💌 | Select Solvent | H20 | • |
| | | Obtain Equilibrium Curve Equation | Ē | iit | |

Figure 2: Graphical User Interface for Obtaining Equilibrium Curve Equation.

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|--|------------|---------------------|-----------|---------------|------------------|------------------------|---|--|---|--|------|---|------------------|-----|
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| All Access Objects 💿 « Tables 🌣 | | | | | | | | | | | | | | |
| Efect_of_Operating_Temp | | Efect_of_Op | erating_ | Temp | | | | | | | | - | = X | |
| Effect_of_Flooding_Velocity | | Temp | | rossectiona 🔻 | Column_Dia 🔻 | Packing_Hei 🗸 S | Surface_Are - V | /olume_of_ 🗸 | Tower_Heig 🔻 | Annual_Vari 🗸 | | | | 1 |
| Effect_of_Gas_Flow_Rate | | | 0 | 0.4251626 | 0.7357062 | 6.009029 | 28.52712 | 2.554814 | 11.97306 | \$23,884.66 | | | | |
| Effect_of_Particle_Size | | | 7 | 0.4590614 | 0.7644733 | 4.777753 | 25.60711 | 2.193282 | 10.27862 | \$25,951.31 | | | | |
| Effect_of_Pressure_Drop | | | 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 | 0.838397 | 3.430809 | 23.41844 | 1.895208 | 8.408380 7.558167 | \$37,303.43 \$45 592 21 | | | | |
| | | | 0 | 0.237095 | 0.5493993 | 7.098567 | 22.33012 | 1.683034 | 13,30838 | \$22,480.07 | | | | |
| | | | 0 | 0.237095 | 0.5493993 | 7.098567 | 23.44728 | 1.683034 | 13.30838 | \$22,480.07 | | | | |
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| Datasheet View | | | | | | | | | | | | | <mark>⊡</mark> ₿ | 8 ¥ |

Figure 3: A Typical Output Screen

2.2 The Test Problem

The CAD module was tested using the following problem. A gas mixture containing 6% SO₂ and 94% dry air is to be scrubbed with fresh water in a tower packed with 0.025m ceramic raschig rings to remove the SO₂ so that the exit will contain no more than 0.1 mole percent SO₂, 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° C and 760mmHg or 1 atm. Determine the tower diameter, cross-sectional area, packing height, volume of packing, column height and surface area.

2.3 Program run

The following important set of screens were 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^{0} C- 30^{0} C)
 - 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, crosssectional area, packing height, surface area, and height) of the absorption column.

After a series of screens which include one for generating the result, updating record and adding record to data base, the final output screen is displayed. A typical output screen is shown in figure 3.

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 3-7 summarise 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 ₂ O /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 statements.

| 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 |
| Correlation coefficient | 1 | 1 |

| operating variable | | | Design Parameters | | | | | | | | |
|------------------------|--|------------------------|-----------------------|-----------------------------------|--|---------------------|--|--|--|--|--|
| varied | | Design Farameters | | | | | | | | | |
| 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) | | | | | |
| 0 | 0.4251626 | 0.7357062 | 6.009029 | 28.52712 | 2.554814 | 11.97306 | | | | | |
| 7 | 0.4590614 | 0.7644733 | 4.777753 | 25.60711 | 2.193282 | 10.27862 | | | | | |
| 10 | 0.4887733 | 0.7888249 | 4.305094 | 24.87447 | 2.104215 | 9.641733 | | | | | |
| 15 | 0.5102593 | 0.8059765 | 3.841116 | 23.83638 | 1.959965 | 9.009659 | | | | | |
| 20 | 0.5523989 | 0.838597 | 3.430869 | 23.41844 | 1.895208 | 8.468586 | | | | | |
| 30 | 0.6209431 | 0.8891045 | 2.743771 | 22.35612 | 1.703726 | 7.558167 | | | | | |

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 21 mm H₂O/m of Packing, 0.025m raschig ring ceramic packing with varying operating temperature.

Table 7: Output from the program using operating pressure of 760 mmHg, operating temperature of 30^oC, gas flow rate of 0.126kg/s, flooding velocity of 50%, pressure drop of 21 mm H₂O/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) | | |
| Rachig Ring | 0.013 | 1.241886 | 1.257384 | 2.450342 | 32.20492 | 3.043046 | 7.52301 | | |
| Ceramic | 0.025 | 0.6209431 | 0.8891045 | 2.743771 | 22.35612 | 1.703726 | 7.558167 | | |
| | 0.038 | 0.4771479 | 0.7793875 | 3.59763 | 22.11629 | 1.716601 | 8.641657 | | |
| Intallox saddle | 0.016 | 0.4847827 | 0.7855982 | 2.68203 | 19.15181 | 1.300202 | 7.366153 | | |
| Plastic | 0.025 | 0.3533431 | 0.6706952 | 3.549105 | 18.54067 | 1.254051 | 8.462855 | | |
| | 0.038 | 0.3089896 | 0.6271895 | 4.585599 | 20.06725 | 1.416902 | 9.869572 | | |
| Intallox Saddle | 0.013 | 0.6962162 | 0.9414537 | 2.709471 | 23.76575 | 1.886378 | 7.563542 | | |
| Ceramic | 0.025 | 0.4693888 | 0.7730246 | 2.786514 | 19.15414 | 1.307959 | 7.499605 | | |
| | 0.038 | 0.3533431 | 0.6706952 | 3.833309 | 19.37914 | 1.354473 | 8.860742 | | |

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°C, 0.025m raschig ring ceramic packing with varying pressure drop.

| operating variable varied | Design Parameters | | | | | | | |
|--|---|------------------------|-----------------------|-----------------------------------|--|---------------------|--|--|
| Pressure Drop (mm H ₂ O/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) | | |
| 4 | 0.8781461 | 1.057329 | 2.577494 | 26.66218 | 2.263416 | 7.496967 | | |
| 8 | 0.7271741 | 0.9621574 | 2.665361 | 24.19683 | 1.938181 | 7.522906 | | |
| 21 | 0.6209431 | 0.8891045 | 2.743771 | 22.35612 | 1.703726 | 7.558167 | | |
| 42 | 0.5420035 | 0.8306689 | 2.815053 | 20.91543 | 1.525769 | 7.598356 | | |
| 83 | 0.5141897 | 0.8090746 | 2.843654 | 20.39005 | 1.462178 | 7.616372 | | |
| 125 | 0.4809804 | 0.7825113 | 2.880718 | 19.74892 | 1.385569 | 7.641166 | | |

Table 5: Output from the program using operating pressure of 760 mmHg, gas flow rate of 0.126kg/s, pressure drop of 21 mm H_2O/m of Packing, operating temperature of 30^oC, 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) | | |
| 0.5 | 0.6209431 | 0.8891045 | 2.743771 | 22.35612 | 1.703726 | 7.558167 | | |
| 0.6 | 0.5174525 | 0.8116376 | 3.007907 | 21.051 | 1.556449 | 7.84894 | | |
| 0.65 | 0.4776486 | 0.7797962 | 3.148938 | 20.59033 | 1.504086 | 8.013906 | | |
| 0.7 | 0.4435308 | 0.7514305 | 3.297352 | 20.2301 | 1.462477 | 8.192751 | | |

Table 6: Output from the program using operating pressure of 760 mmHg, operating temperature of 30^{0} C, flooding velocity of 50%, pressure drop of 21 mm H₂O/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) | | | |
| 0.126 | 0.6209431 | 0.8891045 | 2.743771 | 22.35612 | 1.703726 | 7.558167 | | | |
| 0.252 | 1.241886 | 1.257384 | 2.743771 | 33.82787 | 3.407451 | 7.933811 | | | |
| 0.378 | 1.862829 | 1.539974 | 2.743771 | 43.50887 | 5.111176 | 8.222054 | | | |
| 0.504 | 2.483772 | 1.778209 | 2.743771 | 52.26292 | 6.814903 | 8.465053 | | | |

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 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).

Table 3 shows the effect of operating temperature on the design parameters. 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 (http://www.pdnengineers.com Retrieved February, 2011). This leads to higher solvent requirement. Column diameter and cross-sectional area are directly proportional to solvent flow rate. Excessively high gas temperature can also lead to significant solvent loss through evaporation (S Raymond Woll, personal communication June 25, 1992). 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 height of transfer unit

and consequently decreases the tower height, height of packing, volume of packing, and surface area.

Table 4 shows the effect of packing type and size on the design parameters. 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 Generally, as the packing size is increased, the rate. 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 (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 (Treybal, 1981). 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, decreases rapidly. It is recommended that, if possible, the ratio dp/Dc equals 1:15 (Treybal, 1981). Metal packing materials cannot be used for this system because it involves highly corrosive solute (SO₂) (Coker, 1991).

Table 5 shows that 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. 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). Recommended design values for absorbers and strippers is 15-50 mmH₂O/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).

Table 6 shows the effects of percentage flooding velocity on the design parameters. Increase in percentage 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 (Treybal, 1981), interpreted in terms of size of the column.

Table 7 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

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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 (Treybal, 1981). The surface area of the packed column, and column (tower) height, were similarly affected.

4.0 CONCLUSION

A CAD module was developed for implementing the design of a packed absorption column. The program was tested with a design problem by supplying specifications such as operating conditions (pressure, temperature), physical properties (density, viscosity, surface tension), the solute to be absorbed, the solvent selected, gas and solvent mole fractions, percentage flooding velocity, pressure drop, gas flow rate ,packing type and size 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 designer can vary the above specifications to obtain the best design output within the shortest possible time.

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