Solving problems in packed absorption using Mathcad®

E.N. Bart, J. Kisutcza
NJIT, Department of Chemical Engineering, University Heights, Newark NJ 07102-1982

The techniques for solving problems in packed tower absorption are very dated. These techniques have been subjected to a host of different approximations. Much of these calculations are very slow and tedious. The procedures dated back to the time when the primary means of computation was by slide rule and mechanically drawn graphs. Engineering students were well versed in the use of the slide rule and were taught engineering drawing. The present age is the age of the computer and the old techniques are no longer needed. The computations for packed tower design are an enigma and are very difficult for the modern engineering student. Most of the procedures that were used to determine the required height of a column packing required some form of graphical integration. The curves that were plotted often have great curvature at some location and it was often extremely difficult to obtain any accurate results.

The concept of two film theory made it possible to deal with four different rate equations. These were based on conditions within the gas film or the liquid film. In addition it might be possible to work with overall coefficients for gas or liquid. It was often difficult to transfer between the systems except by making certain assumptions which were usually only valid if the systems involved were extremely dilute.

The rigorous equations were known for some time and one of these is as follows:

$$Z = \int_{y_1}^{y_2} \frac{V\,dy}{\dfrac{k_y\,a\,S}{(1-y)_{ilm}}(1-y)(y-y_i)} \tag{1}$$

Three additional equations could be written to accomplish the same result. Z is the necessary height of packing. Since some of the terms did not change greatly in a dilute system it was common practice to remove some of these from under the integral sign and making use of an average value between the top of the column and the bottom. The result was:

$$Z = \left[\frac{V}{k_y\,a\,S} \frac{(1-y)_{ilm}}{(1-y)} \right]_{av} \int_{y_1}^{y_2} \frac{dy}{y-y_i} \tag{2}$$

The first term would be calculated at the top and at the bottom of the column and averaged. The first term had units of height and was often referred to as the height of a transfer unit. The second term was dimensionless and had to be evaluated by graphical integration. It was often referred to as the number of transfer units. The term y_i is an interfacial value of mole fraction in the vapor associated with the vapor composition y at some location in the column.

With Mathcad® it is now possible to obtain a regression fit equation for the equilibrium data. All of the various terms in the rigorous equation above can be readily obtained as a

function of y and the result rigorously integrated on the computer in an instant. The author is considering using this technique as means of designing packed distillation columns where a modified procedure would be used to find the height of packing for both the enriching and exhausting sections of the column.

The procedure as outlined above has a number of far reaching implications. The often used method of designing packed distillation equipment is to use the McCabe-Thiele[1] procedure used to design tray towers. A calculation of something called the "height equivalent to a theoretical plate" is then used to obtain the height of packing for the packed tower. The procedure is not rigorous in a true sense but it will roughly obtain the packed height desired. A modified procedure can be developed that can obtain the necessary height of packing in a rigorous procedure for both the enriching and exhausting section of a distillation column. Additional work will be necessary to achieve this goal since the procedure hinges on the type of packing used in the column. Many new packing's have become available in recent years. Equilibrium data for distillation is widely available from numerous sources.

An example of the current technique for dealing with packed absorbers or strippers is available from several textbooks[2,3]. One of these, is the coverage given by Giankoplis[4] (See example 10.7-1 starting on page 681). An equation for the operating line is based on the assumption that the carrier gas and the solvent liquid are non-diffusing. Only the solute in this example, SO_2 is diffusing. The solvent liquid, water and the carrier gas, air, are non-diffusing. The equilibrium information is generated by some Henry's law type correlation which is available from numerous sources. All necessary material balances are performed so that all input and output molar flow rates and compositions are known. It is then necessary to find the interfacial composition at various locations in the column. Equations for the mass transfer coefficients are known for the packing used. In the cited example the packing is 1 inch ceramic raschig rings. Several points along the operating line are chosen. From each of the points chosen straight lines are drawn whose slopes are:

$$-\frac{k_x'a \cdot (1-y)_{ilm}}{k_y'a \cdot (1-x)_{ilm}} \tag{3}$$

This procedure is often difficult because the y_i and the x_i are unknown, so that the procedure is by trial. Furthermore if the compositions become concentrated the flow rates may change from location to location sufficiently, so that the mass transfer coefficients can change from location to location. The intersections of these lines (nearly parallel) locates the values of x_i and y_i corresponding to a point on the operating line having coordinates x and y. This procedure is performed for all of the points used and the calculations for the values of

$$\frac{V}{\dfrac{k_y\,a\,S}{(1-y)_{ilm}}(1-y)(y-y_i)} \tag{4}$$

are obtained for each of the chosen points. These values are plotted against the values of y and the area under the curve is the desired packing height. As anyone can see this procedure is extremely time consuming and is often difficult to accomplish if the resulting curve necessary to find the height curves greatly. A table of the tabulated values
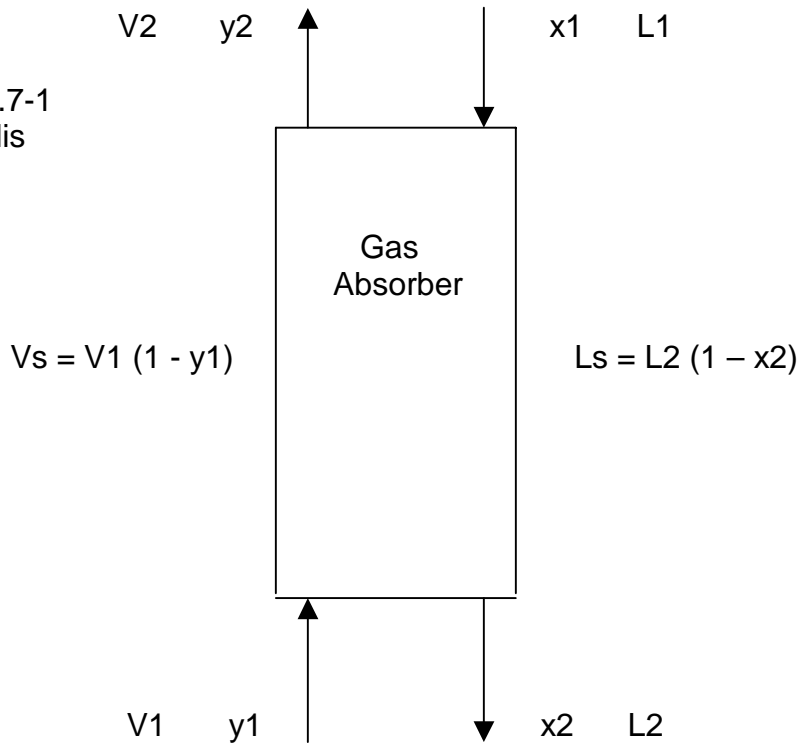
necessary to perform the graphical integration for this problem appears in Giankoplis on page 683.

The procedure proposed here makes use of the fact that the equilibrium data is such that little or no curvature occurs. Mathcad$^{®}$ can readily regress such data for the equilibrium in the form of an equation $xin = f(yin)$. All of the material balances can be performed by machine as a function of y. The mass transfer coefficients can be expressed as a function of y. The interfacial compositions can be expressed as a continuous function of y (not just at 5 or 6 points) and the whole business may be integrated between y in and y out.

The authors have succeeded in performing the same computation by developing $yin = f(xin)$ and developing all variables as function of x. Integration of the numerical results in height almost identical to the integration with y. The approximate solutions using the concepts of H_g and N_g where Z is the product N_g multiplied by H_g have been examined and the results are nearly identical to the rigorous ones. An example calculation is shown in the appendix which follows.

APPENDIX

V2   y2   ↑   ↓   x1   L1

Prob. 10.7-1
Giankoplis

```
┌─────────────┐
│             │
│    Gas      │
│  Absorber   │
│             │
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Vs = V1 (1 - y1)   Ls = L2 (1 − x2)

V1   y1   ↑   ↓   x2   L2

$j := 0..11$

Ls := 0.0420 $\dfrac{\text{kgmoles}}{s}$ Vs := 0.000653 $\dfrac{\text{kgmoles}}{s}$

y1 := 0.20   molefraction   y2 := 0.02   molefraction

x1 := 0   molefraction

Msolute := 64.1   MLs := 18   MVs := 29

Sulfur dioxide   Water   Air

S := 0.0929 m^2

$$Y1 := \frac{y1}{1 - y1}$$

$$Y2 := \frac{y2}{1 - y2}$$

$$X1 := \frac{x1}{1 - x1}$$

$$X2 := \frac{Vs}{Ls} \cdot (Y1 - Y2) + X1$$

$$x2 := \frac{X2}{1 + X2}$$

$$Y(y) := \frac{y}{1 - y}$$

$$X2 = 3.57 \times 10^{-3}$$

$$x2 = 3.557 \times 10^{-3}$$

$$X(y) := \frac{Vs \cdot (Y(y) - Y2) + Ls \cdot X1}{Ls}$$

$$x(y) := \frac{X(y)}{1 + X(y)}$$

$$Gy(y) := \frac{Vs \cdot (MVs + Y(y) \cdot Msolute)}{S}$$

$$Gx(y) := \frac{Ls \cdot (MLs + X(y) \cdot Msolute)}{S}$$

$$kya(y) := 0.0594 \cdot Gy(y)^{0.7} \cdot Gx(y)^{0.25}$$

$$kxa(y) := 0.152 \cdot Gx(y)^{0.82}$$

$$\lambda(y) := \frac{kxa(y)}{kya(y)}$$

At a t of 293 k
& a P of 101.3 kPA.

$xxi_j :=$	$yyi_j :=$
0	0
0.0000562	0.000658
0.0001403	0.00158
0.000280	0.00421
0.000422	0.00763
0.000564	0.01120
0.000842	0.01855
0.001403	0.0342
0.001965	0.0513
0.00279	0.0775
0.00420	0.121
0.00698	0.212

$$vs := regress(yyi, xxi, 4)$$

$$xin(yin) := interp(vs, yyi, xxi, yin)$$

$i := 0..4$

$$\Delta y := \frac{y1 - y2}{4} \qquad \Delta y = 0.045 \qquad yy_i := y2 + i \cdot \Delta y \qquad xx_i := x(yy_i)$$

$$yyin_i := \begin{vmatrix} a \leftarrow yy_i \\ b \leftarrow \lambda(a) \\ xb \leftarrow 1 - xx_i \\ yb \leftarrow 1 - a \\ yin \leftarrow a \\ c \leftarrow root\left[yin - 1 + yb \cdot \left(\frac{xb}{1 - xin(yin)} \right)^b, yin \right] \end{vmatrix}$$

$$yyin = \begin{pmatrix} 8.851 \times 10^{-3} \\ 0.044 \\ 0.083 \\ 0.124 \\ 0.165 \end{pmatrix} \qquad yy = \begin{pmatrix} 0.02 \\ 0.065 \\ 0.11 \\ 0.155 \\ 0.2 \end{pmatrix}$$

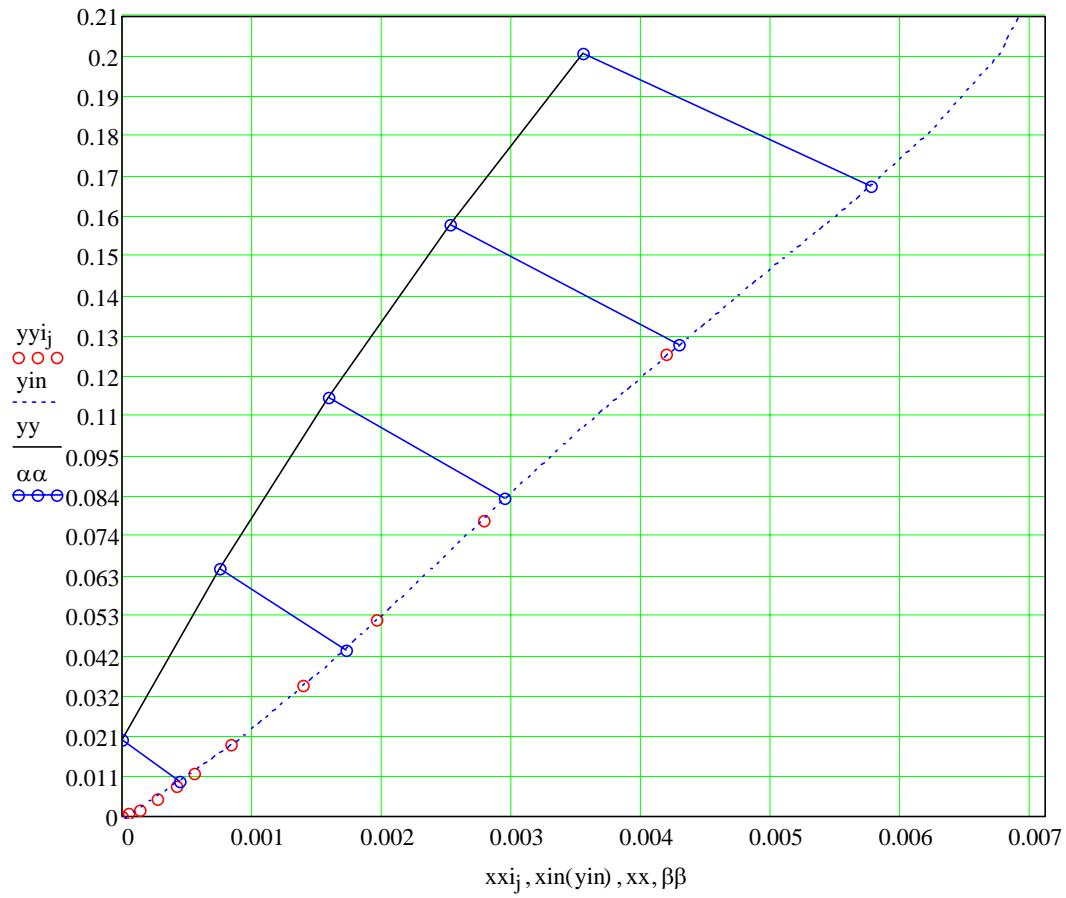$$y\alpha := yyin \qquad x\alpha_i := xin(yyin_i) \qquad slop_i := \frac{y\alpha_i - yy_i}{x\alpha_i - xx_i} \qquad ii := 0..1$$

$$\beta\beta_{ii,i} := xx_i + ii \cdot (x\alpha_i - xx_i) \qquad \alpha\alpha_{ii,i} := yy_i + slop_i \cdot (\beta\beta_{ii,i} - xx_i)$$

This shows the fit of the equilibrium data for the expression yin(xin).

$$vvs := regress(xxi, yyi, 4)$$

$$yin(y) := interp(vvs, xxi, yyi, y)$$

$$\text{yin}(y) := \begin{vmatrix} a \leftarrow y \\ b \leftarrow \lambda(a) \\ xb \leftarrow 1 - x(y) \\ yb \leftarrow 1 - a \\ yin \leftarrow a \\ c \leftarrow \text{root}\left[yin - 1 + yb \cdot \left(\dfrac{xb}{1 - xin(yin)} \right)^{b}, yin \right] \end{vmatrix}$$

$$V(y) := \frac{Vs}{1 - y}$$

$$Z := \int_{y2}^{y1} \frac{V(y)}{\left[\dfrac{kya(y) \cdot S}{\dfrac{(1-y)-(1-yin(y))}{\ln\left(\dfrac{1-y}{1-yin(y)} \right)}} \right] \cdot (1 - y) \cdot (y - yin(y))} \, dy$$

$$\boxed{Z = 1.557} \qquad \text{meters}$$

This result compares favorably with the solution in the text of 1.586 meters. The answer here may actually be better since graphical integration is not used. The computer is used for all computation.

Approximate method 1

This method involves computing H_G at the top of the column and at the bottom. The values are averaged. N_G is obtained by integration. The product of N_G and H_G yields the height of packing.

$$Hg1 := \frac{V(y1)}{kya(y1) \cdot S} \qquad Hg1 = 0.195 \qquad \text{meters}$$

$$Hg2 := \frac{V(y2)}{kya(y2) \cdot S} \qquad Hg2 = 0.211 \qquad \text{meters}$$

$$Hg := \frac{Hg1 + Hg2}{2} \qquad Hg = 0.203 \qquad \text{meters}$$

$$Ng := \int_{y2}^{y1} \frac{\dfrac{(1-y)-(1-yin(y))}{\ln\left(\dfrac{1-y}{1-yin(y)}\right)}}{(1-y)\cdot(y-yin(y))} \, dy \qquad Ng = 7.64$$

$$Zg := Hg \cdot Ng \qquad \boxed{Zg = 1.552} \quad \text{meters} \qquad\qquad Z = 1.557 \qquad \text{meters}$$

This agrees very closely to the rigorous solution.

BIBLIOGRAPHY

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4. Giankoplis, C. J.: "Transport Processes and Separation Process Principles," 4th ed. Prentice Hall, Upper Saddle River, New Jersey, 2003