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COMPUTER SIMULATION OF H_2S AND CO_2 ABSORPTION PROCESSES

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Abstract—A new computer program has been developed for the simulation of chemical absorption of H_2S and CO_2 using MEA, DEA or hot potassium carbonate. The program can calculate either tray or packed columns. The material and energy balances, and equilibrium relationship are solved using the Naphtali-Sandholm method and the stage to stage method complementarily. The packed column is divided into a number of sections. Each section is treated as a tray, but with a different method of efficiency calculation. The enhancement factor was incorporated to reflect the enhancement of absorption rate which is an inherent nature of chemical absorption. Using this program named as AGRES, 20 sample problems were solved for absorption and stripping and the results were compared with those of other competing programs of AMSIM, PROCESS, ASPEN PLUS and DESIGN II. In the calculation of ideal stages, all the programs gave similar results. In the calculation of real stages, however, only AMSIM and AGRES were effective. AMSIM could not calculate packed columns and tray columns having more than 22 stages. While, AGRES could overcome this limitation of AMSIM, providing a broader application.

Key words: Hydrogen Sulfide, Carbon Dioxide Absorption, Simulation

INTRODUCTION

Gases from chemical plants contain acidic components such as H_2S and CO_2 which must be removed before they are subsequently processed to form chemicals or discharged to the atmosphere. A variety of processes are available to remove H_2S and CO_2: physical absorption, chemical absorption, direct conversion and dry bed processes [1]. Among them, the chemical absorption has been most widely used. The chemical absorption process employs a chemical solvent in an aqueous solution; the H_2S and CO_2 are removed through reaction with the solvent. Alkanolamines including MEA(mono-ethanolamine), DEA(di-ethanolamine), and MDEA (methyldiethanolamine), and potassium carbonate solutions with additives are well-known chemical solvents. Fig. 1 shows a typical flow diagram for chemical absorption processes. The feed gas is fed to the bottom of absorber and flows upward countercurrent to the descending solvent. The rich solvent in which the acidic components are dissolved leaves the bottom of the absorber and is sent to the stripper and regenerated there. The regenerated solvent is recycled back to the top of the absorber.

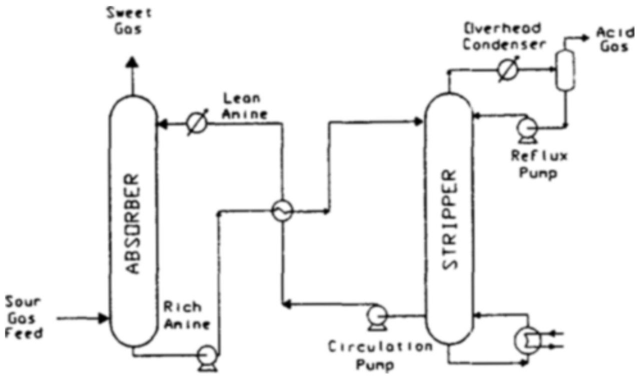

Fig. 1. Conventional alkanolamine treating process.

In the chemical absorption, the vapor-liquid equilibrium is highly nonlinear, a considerable amount of heat is generated due to heat of reaction and the absorption efficiency of a stage is much lower than 100% implying the determination of the absorption efficiency should be a crucial factor in the design of a chemical absorption process. Currently available commercial programs such as PROCESS, ASPEN-PLUS and DESIGN II can not calculate the absorption efficiency [14], and the user must provide it to simulate real columns. While, AMSIM, which was developed by the Robinson and Associates, Ltd., Canada, can calculate the efficiency by itself, and can be directly applied to real columns. However, there is a limitation in AMSIM; its application is limited to tray columns up to 22 trays and moreover it can not calculate packed columns at all [15]. Sivasubramanian [2] developed a program which is applicable to either tray or packed columns. His program was based on the non-equilibrium model due to Krishnamurthy and Taylor [3]. According to their non-equilibrium model, the mass and energy conservation equations are split into two parts, one for each phase, and mass and energy transfer through the interface is modeled by means of rate equations and transfer coefficients. The model, however, has a drawback of the number of equations to be solved being much larger; for c components, the number of equations to be solved per stage is $5c+1$.

In the present study, a new program is developed which can calculate both tray and packed columns while maintaining the number of equations to be solved per stage at $2c+3$. The efficiency for a component at a stage is incorporated into the model equations and updated every iteration using the data of previous step. The packed column is divided into a number of sections. Each section is treated as a stage, but with a different method of efficiency calculation.

PROGRAM DEVELOPMENT

In order to calculate the absorption, the following equations must be satisfied for N stages and C components:

Component mass balances (N×C equations):

$$(L_{n+1}-W^{l}_{n+1})X_{n+1,i}+(V_{n-1}-W^{v}_{n-1})Y_{n-1,i}-L_nX_{n,i}-V_nY_{n,i}$$
$$+F^{v}_{n}Z^{v}_{n,i}+F^{l}_{n}Z^{l}_{n,i}=0 \tag{1}$$

Equilibrium relationships (N×C equations):

$$\eta_{n,i}=\frac{Y_{n,i}-Y_{n+1,i}}{K_{n,i}X_{n,i}-Y_{n+1,i}} \tag{2}$$

Summation of flows (2 N equations):

$$\sum_{i=1}^{C} X_{n,i}=1.0 \tag{3}$$

$$\sum_{i=1}^{C} Y_{n,i}=1.0 \tag{4}$$

Enthalpy balances (N equations):

$$(L_{n+1}-W^{l}_{n+1})H^{l}_{n+1}+(V_{n-1}-W^{v}_{n-1})H^{l}_{n-1}-L_nH^{l}_{n}-V_nH^{v}_{n}$$
$$+F^{v}_{n}H^{vf}_{n}+F^{l}_{n}H^{lf}_{n}+Q_n=0 \tag{5}$$

A total of (2N×C+3N) equations must be solved simultaneously for $X_{n,i}$, $Y_{n,i}$, L_n, V_n and T_n, where $X_{n,i}$ is the liquid mole fraction of component i at stage n, $Y_{n,i}$ is the vapor mole fraction of component i at stage n, L_n is the total liquid flow rate at stage n, V_n is the total vapor flow rate at stage n and T_n is the temperature at stage n. The liquid temperature and the vapor temperature at a stage are assumed to be the same. The above equations are nonlinear, requiring an iterative procedure. The stage efficiency $\eta_{n,i}$ and the vapor-liquid equilibrium constant $K_{n,i}$ in Eq. (2) must be provided; determination of these values is an essence of the simulation. The enthalpies and heats of reaction in Eq. (5) must also be provided.

1. Numerical Method

In order to solve Eqs. (1) to (5), the Naphtali-Sandholm method [4] and the stage to stage method was used complementarily. The Naphtali-Sandholm method, which is based on the Newton-Raphson iteration technique, is known to be the best choice for chemical absorption problems [5]. However, this method has an inherent disadvantage of the convergence being dependent upon the initial values for unknown variables. While, in the stage to stage method, the dependency on the initial values becomes less critical. The stage to stage method, however, has a drawback of the solution being damping between iterations if the heat content of the liquid (product of flow rate and heat capacity of the liquid) is not sufficiently high [6].

In this work, the solution is sought first by using the stage to stage method. If it fails, the Naphtali-Sandholm method is introduced subsequently. In the stage to stage method, a liquid composition at the bottom stage is assumed and the computation moves toward the top stage by stage to obtain the composition of the gas leaving the top stage. Using this composition of the gas a new liquid composition at the bottom stage is determined. Iteration continues until the difference between the old and new liquid composition at the bottom stage becomes smaller than a predetermined value. In the Naphtali-Sandholm method, all the unknown variables are initially assumed and those variables are corrected through the inversion of the Jacobian or the (2C+3)N by (2C+3)N matrix of partial derivatives with respect to all the variables. The correction continues until the variables satisfy the material, energy and equilibrium Eqs. of (1) to (5) within a given tolerance. With the Sivasubramanian model, the Jacobian is (5C+1)N by (5C+1)N matrix and would be 1020 by 1020 for 10 components and 20 stages. It would be reduced to 460 by 460 with the present model which might give a substantial reduction in computational load although comparison of computation time is not available at present.

2. Vapor-Liquid Equilibrium Data

H_2S and CO_2 in the vapor dissolves in the solvent and subsequently react with the solvent to generate ionic species such as HS^-, S^{2-}, HCO_3^-, CO_3^{2-}, and $RR'NCOO^-$ (carbamate ion). The vapor-liquid equilibrium constant for CO_2 is defined as the ratio of the vapor-phase mole fraction of CO_2 to the liquid-phase mole fraction of all carbon-containing species, not only free CO_2 but also HCO_3^-, CO_3^{2-} and $RR'NCOO^-$. Likewise, for the equilibrium constant for H_2S, the liquid mole fraction accounts for total concentration of free H_2S, HS^- and S^{2-}. The presence of ionic species makes it difficult to determine the vapor-liquid equilibrium constants. Activity-coefficient models are available for the equilibrium constants [7]. However, those models may be too complex to be incorporated into the global model for the simulation.

In this work, a simpler method by Kent and Eisenberg [8] was employed. In this method, all the species in the liquid are assumed to behave like ideal liquid. The non-idealities are accounted by fitting two of the equilibrium reaction constants, namely, the carbamate formation and the amine protonation reactions to experimental solubility measurements. This approach of lumping the effects of the non-idealities into two adjustable parameters may be valid only within the range over which those parameters were adjusted. The model of Kent and Eisenberg covers most of operating conditions encountered in real processes.

According to the model of Kent and Eisenberg, the vapor-liquid equilibrium constants for a H_2S-CO_2-amine system are obtained by solving the following elementary reaction equations simultaneously.

$$RR'NH_2^+ \overset{K_1}{\rightleftharpoons} H^+ + RR'NH \tag{6}$$

$$RR'CNOO^- + H_2O \overset{K_2}{\rightleftharpoons} RR'NH + HCO_3^- \tag{7}$$

$$H_2O + CO_2 \overset{K_3}{\rightleftharpoons} H^+ + HCO_3^- \tag{8}$$

$$H_2O \overset{K_4}{\rightleftharpoons} H^+ + OH^- \tag{9}$$

$$HCO_3^- \overset{K_5}{\rightleftharpoons} H^+ + CO_3^= \tag{10}$$

$$H_2S \overset{K_6}{\rightleftharpoons} H^+ + HS^- \tag{11}$$

$$HS^- \overset{K_7}{\rightleftharpoons} H^+ + S^= \tag{12}$$

$$P_{CO_2} = H_{CO_2}[CO_2] \tag{13}$$

$$P_{H_2S} = H_{H_2S}[H_2S] \tag{14}$$

Eqs. (13) and (14) relate the equilibrium partial pressures of H_2S and CO_2 to the free concentrations of H_2S and CO_2 in solution (denoted by brackets) by the Henry Law relationship. All constants, other than K_1 and K_2 were used as found in the literature. K_1 and K_2 are determined by forcing a fit with experimental va-

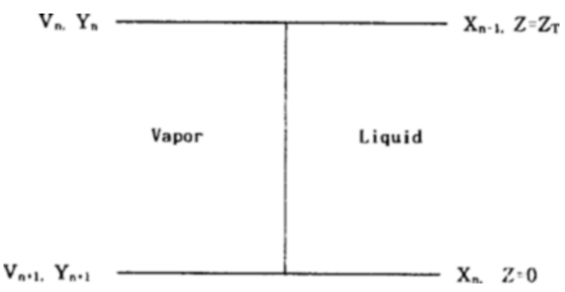

Fig. 2. Vapor-liquid contact in one stage.

por-liquid equilibrium data.

3. Mass Transfer Coefficients

In the absence of chemical reactions, a variety of models are available for the prediction of mass transfer coefficients for gas-liquid contacting devices; the Onda model [9] and the Sharma model [10] have been widely used for packed columns and for tray columns, respectively. However, in the presence of chemical reactions in the liquid, the enhancement of mass transfer rate in the liquid phase due to chemical reaction must be taken into account. The enhancement factor defined by Eq. (15) is introduced to reflect the enhancement.

$$I=\frac{k_l}{k_l^o} \tag{15}$$

where k_l^o is the mass transfer coefficient in the liquid side in the absence of chemical reaction and k_l is the one in the presence of chemical reaction. k_l is obtained by multiplying k_l^o by the enhancement factor. The estimation of the enhancement factor is an essence in determining the mass transfer coefficients. In this work, the Olander model [11] was employed for the calculation of enhancement factor for H_2S and the Decoursey model [12] for CO_2.

4. Efficiency Calculation

4-1. For Tray Columns

Fig. 2 illustrates a stage, where the vapor flows upward through the liquid of a depth, Z_T. The liquid comes in from the upper stage, flows across the stage perpendicular to the flow of vapor, and down to the lower stage. The present model assumes thermal equilibrium and complete mixing of the liquid on the stage. As the vapor passes through the liquid, H_2S or CO_2 in the vapor is absorbed into the liquid according to

$$\frac{d(VY)}{dZ}=K_{og}(aAP)(Y^*-Y) \tag{16}$$

at $Z=0$, $Y=Y_{n+1}$

With a few steps of mathematical manipulations, we end up with the following equation.

$$Y_n=\frac{a_1Y_n^*}{a_1+a_2}+\left(Y_{n+1}-\frac{a_1}{a_1+a_2}Y_n^*\right)\left(\frac{V_{n+1}}{V_n}\right)^{(a1+a2)/a2} \tag{17}$$

$$a_1=K_{og}(aAP),\quad a_2=\frac{(V_n-V_{n+1})}{Z_T}$$

where V is the molar flow rate of vapor at any point, Y is the mole fraction of vapor, Y* is the mole fraction of vapor in equilibrium with the liquid composition, K_{og} is the overall gas-phase mass-transfer coefficient, a is the interfacial surface area available for mass transfer per unit volume and P is the column pressure. Using Y_n (mole fraction of vapor leaving the plate of n) calculated from Eq. (17), the stage efficiency is calculated as follows.

$$\eta_{n,i}=\frac{Y_{n,i}-Y_{n+1,i}}{Y^*_{n,i}-Y_{n+1,i}} \tag{18}$$

In the iterative calculation of material and energy balances, Eqs. (1) to (5), the stage efficiency is updated using the data at the previous iteration step.

4-2. For Packed Columns

A packed column is divided into a number of equal sections. Eq. (16) can be applied to each section. However, in packed columns, Y* , equilibrium mole fraction of vapor is not constant but varies along the coordinate of Z because the liquid mole fraction varies between the upper and lower ends of a section. The variation of Y* is taken into account by a linear interpolation represented by Eq. (19). The error brought by this approximation may depend on the number of sections employed; the error will decrease as the number increases, and vice versa. There should be a trade-off between the error and the computational load. By substituting Eq. (19) into Eq. (16), Eq. (20) is finally obtained through mathematical manipulations similar to those made for the tray columns. Finally, the efficiency at a section can be calculated using Eq. (18).

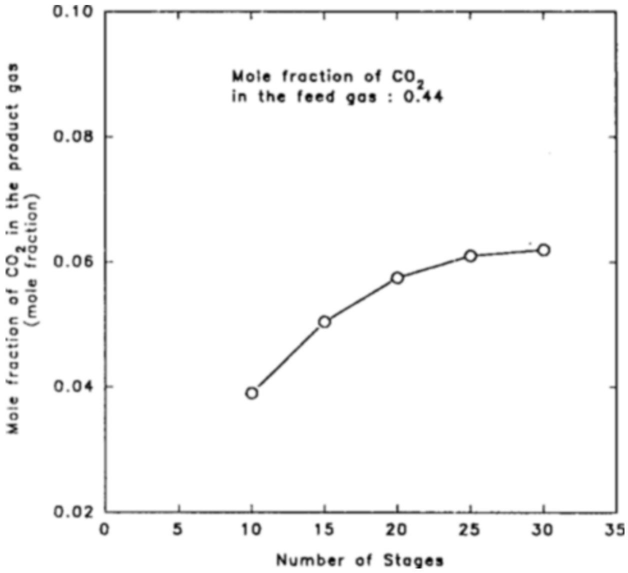

Fig. 3. CO_2 Concentration in the product gas vs. number of stages for example 12.

$$Y^*=Y^*_n+\frac{Y^*_{n-1}-Y^*_n}{Z_T}Z \tag{19}$$

$$\begin{aligned}Y_n={}&Y_{n+1}\left(\frac{V_{n+1}}{V_n}\right)^{(a1+a2)/a2}+\left\{1-\left(\frac{V_{n+1}}{V_n}\right)^{(a1+a2)/a2}\right\}\frac{a_1Y^*_n}{a_1+a_2}\\&+\frac{a_1a_3}{a_2(a_1+2a_2)}\left\{V_n-V_{n+1}\left(\frac{V_{n+1}}{V_n}\right)^{(a1-a2)/a2}\right\}\\&+\frac{a_1a_3V_{n+1}}{a_2(a_1+2a_2)}\left\{\left(\frac{V_{n+1}}{V_n}\right)^{(a1+a2)/a2}-1\right\}\end{aligned} \tag{20}$$

$$a_3=\frac{Y^*_{n-1}-Y^*_n}{Z_T}$$

Table 1. Simulation results for absorption

Input data \ Problem no.	1	2	3	4	5	6	7	8	9	10	11	12
Input												
type of solvent	DEA	MEA	K_2CO_3	MEA	DEA	MEA	DEA	DEA	MEA	MEA	MEA	DEA
H_2S vol% in sour gas	1.66	6.0	0.138	-	-	0.0037	1.999	5.34	-	23.7	6.4	-
CO_2 vol% in sour gas	11.94	10.0	35.34	16.8	7.56	0.1549	12.995	-	17.9	2.3	-	44.0
number of stages	5	3	5	21	20	22	25	20	-	-	-	-
height of packing, cm	-	-	-	-	-	-	-	-	910.0	1220.0	944.8	1380.7
Output												
-H_2S, ppm in product gas												
AGRES	0.36	5.77%	0.05			6.77	6.09	7.2		0.98	16.0	
AMSIM	0.78	5.83%	x			18.5	x	13.0		x	x	
PROCESS	3.37	6.17%										
ASPEN PLUS	3.34	6.17%										
DESIGN II	0.12											
PLANT DATA								<10		nil	nil	
-CO_2, ppm in product gas												
AGRES	2.4	9.05%	10.7	3.06	1.93%	101.6	6.4%		3.43	3.9		6.20%
AMSIM	6.6	9.26%	x	2.65	0.25%	18.8	x		x	x		x
PROCESS	3.55	10.17%										
ASPEN PLUS	4.83	10.17%										
DESIGN-II	0.67											
PLANT DATA				8.0	0.33%				100.0	4.0		1.99%

RESULTS AND DISCUSSION

The present program has been tested on 20 example problems. Examples 1, 2 and 3 represent equilibrium stage calculations for three different solvents of MEA, DEA and K_2CO_3 (potassium carbonate). The other examples refer to data from commercial plants; examples 4 to 12 are for absorption of H_2S and/or CO_2 using MEA or DEA (examples 4 to 8 for tray columns and examples 9 to 12 for packed columns) and examples 13 to 20 are for stripping of the acid gases using external reboilers (examples 13 to 16 for tray columns and examples 17 to 20 for packed columns). The number of sections used in the calculation of those packed columns is 25; according to the test with example (Fig. 3), this number may be good enough. As the number of sections increase the CO_2 concentration in the product gas in Fig. 3 will approach to an asymptotic value, which we believe is the solution in search. At the number of 25, we can see the predicted value is quite close to the asymtote. The computation time for the same example was about 5 minutes using a personal computer with 80486 main processor.

1. Ideal Stage Calculations

Table 1 shows simulation results for absorption along with operating conditions. In example 1, H_2S and CO_2 concentrations in the feed gas are 1.66 vol% and 11.94 vol%, respectively, the solvent is DEA, the number of stages is five, and the stage efficiency is assumed to be 100%. The present program, named as AGRES was run against the data of example 1. For comparison, existing commercial programs of PROCESS, ASPEN PLUS, DESIGN II and AMSIM were also applied to the same problem. The concentration of CO_2 in the product gas was calculated to be 2.4 ppm by AGRES, 6.6 ppm by AMSIM, 3.55 ppm by PROCESS, 4.83 ppm by ASPEN PLUS, and 0.67 ppm by DESIGN II. All the programs gave similar results. The slight differences may be due to differences in vapor-liquid equilibrium data between programs. The differences in the prediction of H_2S concentration in the product gas could be explained by the same reasoning. Example 2 is another problem to which those five programs were applied. AGRES and AMSIM gave values very close to each other, and ASPEN PLUS and PROCESS gave the same values. ASPEN PLUS and PROCESS predicted a slight stripping rather than absorption. In example 2, the concentrations of H_2S and CO_2 in the feed gas must be almost in equilibrium with those in the solvent, resulting in such a low mass transfer between the gas and the solvent. The present program was applied to an absorption using potassium carbonate (example 3), and the result is shown in Table 1. AMSIM could not solve this problem because it dose not have database for potassium carbonate solvent. PROCESS and ASPEN PLUS are known to handle this problem, but it was not attempted at the moment.

2. Simulation of Plant Operation

2-1. Absorbers

For examples 3 and on, PROCESS, ASPEN PLUS and DESIGN II can not be applied since they have no function of calculating the stage efficiency. While, AGRES and AMSIM can calculate the stage efficiency. AMSIM, however, can not calculate packed column, and its application is limited to tray columns having less than 22 stages. In contrast, AGRES can calculate packed columns as well as tray columns. For examples 4, 5 and 8, both AGRES and AMSIM gave good agreement with plant data. For examples 6 and 7, unfortunately no plant data were available on H_2S and CO_2 concentrations in the product gas, and the comparison was made only between the two programs. In example 6, the feed gas containing 37 ppm of H_2S and 1549 ppm of CO_2 is passed through a column of 22 stages with MEA as solvent. AGRES gave 6.77 ppm of H_2S and 101.6 ppm of CO_2 in the product gas. In comparison, AMSIM gave 18.5 ppm of H_2S and 18.8 ppm of CO_2. AMSIM could not solve example 7 since the number of stages exceeds the allowable limit of 22 stages. While, AGRES could

Table 2. Simulation results for stripping

Problem no. Input data	13	14	15	16	17	18	19	20
Input								
type of solvent	MEA	DEA	DEA	MEA	MEA	MEA	MEA	DEA
number of stages	19	20	26	24	-	-	-	-
height of packing, cm	-	-	-	-	762.0	1220.0	1220.0	1195.0
weight % solvent	32.0	27.0	21.5	20.0	16.5	16.2	14.7	50.0
H_2S loading in the feed	-	-	0.3	0.36	-	0.4833	0.4973	-
CO_2 loading in the feed	0.54	0.6418	-	-	0.44	0.079	0.0671	0.60
Output								
-H_2S loading in the regenerated solvent								
AGRES			0.0358	0.015		0.125	0.13	
AMSIM			x	x		x	x	
PLANT DATA			0.0187	0.0744		0.0154	0.018	
regeneration factor for H_2S								
AGRES			0.88	0.96		0.74	0.74	
AMSIM			-	-		-	-	
PLANT DATA			0.94	0.79		0.97	0.99	
-CO_2 loading in the regenerated solvent								
AGRES	0.24	0.072			0.17	0.032	0.0247	0.059
AMSIM	0.21	0.035			-	-	-	-
PLANT DATA	0.18	0.156			0.11	0.032	0.021	0.1164
regeneration factor for CO_2								
AGRES	0.56	0.89			0.61	0.59	0.63	0.90
AMSIM	0.60	0.95			-	-	-	-
PLANT DATA	0.67	0.76			0.75	0.59	0.69	0.81

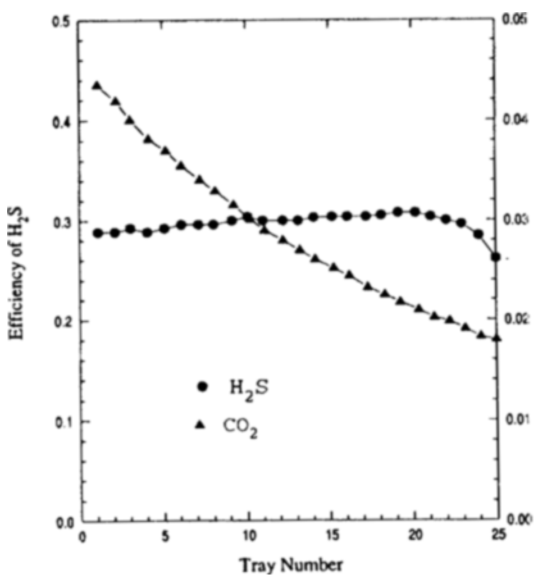

Fig. 4. Efficiencies of H_2S and CO_2 absorption in tray column.

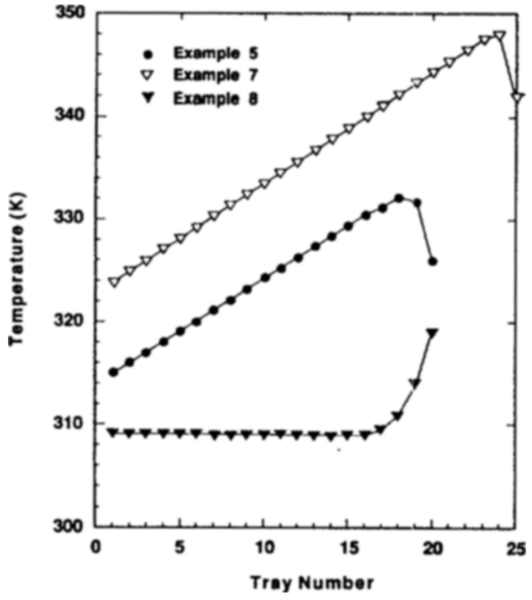

Fig. 5. Temperature distribution in tray column.

successfully solved the problem, although at present no data are available to verify the predicted values.

For examples 9 to 12 which are packed-column absorption problems, only the simulation results of AGRES were compared with plant data, since AMSIM is not applicable to packed columns. Simulated results gave relatively good agreement with plant data, considering that there are so many uncertainties involved in determining the stage efficiency.

2-2. Strippers

The simulation results for stripping columns, where the solvents are regenerated, are shown in Table 2. The regeneration factor in Table 2 is defined as (loading in the feed-loading in the regenerated solvent)/loading in the feed. For the stripping with tray columns (examples 13 to 16), the deviation of predicted regeneration factor from plant data was 6.0 to 20.7% with AGRES and 10.0 to 24.8% with AMSIM. AMSIM could not solve examples 15 and 16 due to the limit in allowable number of stages. For examples 17 to 20, packed column stripping problems. AGRES gave the deviation ranging 6.0 to 25.5%.; AMSIM could not solve

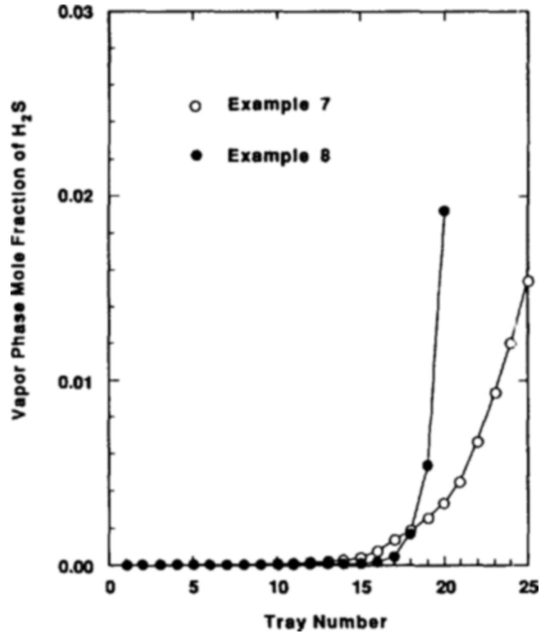

Fig. 6. Composition of H_2S and CO_2 in tray column.

these examples.

3. Profiles of Operating Parameters

Fig. 4 provides for example (7) the detailed stage to stage profiles of the stage efficiencies of H_2S and CO_2. The stage efficiency of H_2S is around 30% and changes little with stage number. While, the stage efficiency of CO_2 is only about one-tenth of that of H_2S, and decreases continuously as the stage number is increased or the bottom of column is approached. Fig. 5 shows the stage to stage temperature profiles for examples 5, 7 and 8. For example 8, the temperature is maximum at the bottom, decreases sharply in 2 to 3 trays from the bottom and remains constant throughout the upper stages. In contrast, for examples 5 and 7, the temperatures reach maxima at the second or the third tray from the bottom. Fig. 6 presents the profiles of vapor phase mole fraction of H_2S for examples 7 and 8. For example 8, we can see that most of the H_2S are absorbed in five stages from the bottom; the column may be over-designed or there may be a room for higher throughput.

CONCLUSION

The present program can calculate chemical absorption of H_2S and CO_2 with either tray or packed columns. The program employs the Kent-Eisenberg model for the vapor-liquid equilibrium data, the Olander model and the Decoursey model for calculating the enhancement factors of H_2S and CO_2, respectively, and the Naphtali-Sandholm method and the stage to stage method complementarily to solve the nonlinear material and energy balances.

This program was tested on 20 example problems of absorption and stripping, most of which deal with actual plant operation. For the ideal stage calculations, this program was found to be comparable to PROCESS, ASPEN PLUS, DESIGN II and AMSIM. For a variety of plant operations, this program gave relatively good agreement with plant data, considering that there are many uncertain factors involved in arriving at the final solution. Compared to AMSIM which is applicable only to tray columns of no more than 22 stages, this program was shown to have wider applicability; it is applicable not only to tray columns but also to packed columns. Using this program, various other information regarding the operation of chemical absorption columns could be obtained. The stage to stage profiles of the temperature, the stage efficiency, and the vapor phase mole fraction of H_2S were demonstrated for a few examples. The present program would be useful for the analysis of existing plants and also provide valuable information for design of a new absorption plant.

NOMENCLATURE

a : vapor-liquid interfacial area per unit volume [cm^2/cm^3]
A : cross sectional area of a column [cm^2]
F_n^l : total liquid flow rate at stage n [gmol/sec]
F_n^V : total vapor feed rate at stage n [gmol/sec]
H_n^l : molar liquid enthalpy at stage n [cal/gmol]
$H_n^{l,f}$: molar liquid enthalpy of feed at stage n [cal/gmol]
H_n^V : molar vapor enthalpy at stage n [cal/gmol]
$H_n^{V,f}$: molar vapor enthalpy at stage n [cal/gmol]
I : enhancement factor
k_l : liquid-side mass transfer coefficient [gmol/cm^2 sec]
k_{l_0} : liquid side mass transfer coefficient in the abscence of chemical reaction [gmol/cm^2 sec]
K_{og} : overall gas-side mass transfer coefficient [gmol/cm^2 sec]
$K_{n,i}$: vapor-liquid equilibrium constant of component i at stage n [gmol/cm^2 sec atm]
L_n : total flow rate of liquid at stage n [gmol/sec]
N : number of stages
P : column pressure [atm]
Q_n : rate of heat added to stage n [cal/gmol sec]
V_n : total flow rate of vapor at stage n [gmol/sec]
W_n^l : rate of liquid drawn as sidestream from the liquid leaving stage n [gmol/sec]
W_n^v : rate of vapor drawn as sidestream from the vapor leaving stage n [gmol/sec]
$X_{n,i}$: liquid mole fraction of component i at stage n
$Y_{n,i}$: vapor mole fraction of component i at stage n
Y^* : equilibrium vapor mole fraction
Z : distance from the bottom of a stage [cm]
Z_T : height defined in Fig. 2 [cm]
$Z^l_{n,i}$: liquid mole fraction of component i in the liquid feed at stage n
$Z^v_{n,i}$: vapor mole fraction of component i in the vapor feed at stage n
$\eta_{n,i}$: stage efficiency of component i at stage n

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