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Application Of Generalized Geometric Programming In Preliminary Plant Design

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$$T_{lm} = -(1/\alpha_{lm}) \ln A_{lm}$$

$$\ln \gamma_i^S = \ln D_i + 1 - D_i$$

D_i is defined as in the ASOG equation.

(4) EWG Equation (according to Bruin, 1970)

$$\ln \Gamma_k = \sum_i \left\{ \frac{X_i \ln (A_{ki} A_{lk})}{(\sum_r A_{kr} X_r)(\sum_r A_{lr} X_r)} C_{kl} \right\} - \sum_{\substack{m \\ k \neq l \neq m \\ l < m}} \sum_l \left\{ \frac{X_l X_m \ln (A_{lm} A_{mi})}{(\sum_r A_{lr} X_r)(\sum_r A_{mr} X_r)} C_{klm} \right\}$$

$$C_{kl} = 1 + X_k [1 - 1/(\sum_r A_{kr} X_r) - A_{lk}/(\sum_r A_{lr} X_r)]$$

$$C_{klm} = 1 - A_{lk}/(\sum_r A_{lr} X_r) - A_{mk}/(\sum_r A_{mr} X_r)$$

Nomenclature

a_{mi} = binary interaction parameter between molecules

A_{mi} = binary interaction parameter between groups

f = function in eq 1

f_G = function in eq 4

f_S = function in eq 6

q_i = pure component area parameter

Q_k = group area parameter

r_i = pure component volume parameter

R_k = group volume parameter

R = gas constant

T = temperature, K

u_{ij} = molar interaction energy between molecules

x_i = liquid phase mole fraction

\bar{X}_k = liquid phase group fraction

Greek Letters

α_{mi} = nonrandom factor in NRTL and NRTL equation

γ_i = activity coefficient of component i

γ_i^G = contribution to γ_i determined mainly by the interaction between groups

γ_i^S = contribution to γ_i due to differences in size and shape of the molecules

Γ_k = group-activity coefficient of group k

Γ_k^i = group-activity coefficient of group k in the pure component i

θ_i = area fraction of component i

Θ_k = area fraction of group k

ν_{ki} = number of groups of kind k in a molecule of component i

Φ_i = segment fraction of component i

Superscript

∞ = infinite dilution

Subscripts

i, j = component i and j

k = group k

l, m, r = running index

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Application of Generalized Geometric Programming in Preliminary Plant Design

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This study utilizes a primal based generalized geometric programming algorithm for the optimal design of a model absorber-stripper process. The GGP algorithm reduces the generalized geometric program to a convex, linear program by two sequential condensation procedures and a logarithmic transformation. Although inactive inequality constraints and arbitrary variable bounds were easily accommodated by the algorithm, considerable effort was required to activate the inequality constraints which required an equality condition. The GGP algorithm converged to a local minimum from arbitrary starting points for approximately 60% of the trials.

Introduction

Geometric programming was developed by Duffin et al. (1967). This early development was based on a strong

duality theory that transformed the nonlinear primal problem into a convex, linear dual problem. However, this strong duality theory only held for regular geometric

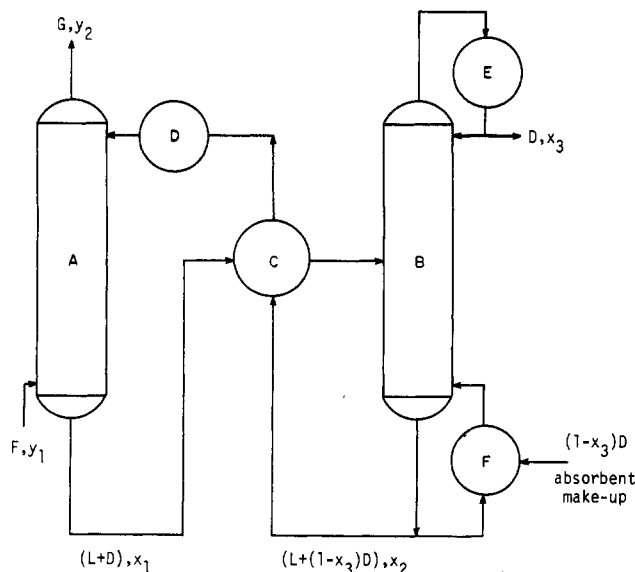


Figure 1. Absorber-stripper process flowsheet: A, absorption column; B, stripping column; C, feed heater; D, absorbent recycle cooler; E, distillate condenser; F, reboiler.

programming problems (GP) where all terms are positive. Subsequent algorithms were developed for generalized geometric programs (GGP) by Blau and Wilde (1969) and Avriel et al. (1975) which allow both positive and negative terms. Most engineering design problems can be transformed into a form compatible with GGP. Blau and Wilde (1969) used a Newton-Raphson method to solve the dual problem. They presented a general solution procedure which, however, can have difficulties with the behavior of redundancies and inactive constraints (for example variable bounds) in the dual space. In contrast, Avriel et al. (1975) provided a general procedure for solving the primal problem which directly accommodated redundancies, inactive constraints, and primal variable bounds.

The application of GGP solution methods has been extensively discussed in a number of recent publications: Dembo and Avriel (1978), Dembo (1978), Ecker and Wiebking (1978), Rijckaert and Martens (1978a,b). The most direct example with theoretical details is that of Rijckaert and Martens (1974), based upon the originating work of Passy and Wilde (1967).

Rijckaert and Martens (1978) compared the available dual and primal GGP algorithms on a set of test problems. The primal codes are favored for their ability to handle inequality constraints, their ability to handle large problems more efficiently, and their speed. This study used the primal GGP algorithm developed by Avriel et al. (1975), as coded by Dembo (1975).

The absorber-stripper plant of Umeda (1969) provided the optimization model. The plant was chosen because of its presence in the literature and representative nature. The model contains chemical process equipment units typically encountered in preliminary process design studies. The purpose of this study was to evaluate the convenience, effectiveness, and accuracy of the GGP approach to preliminary process design problems.

Experimental Section

A. Process Description. The plant used in this study (the process equations) is essentially that of Umeda (1969) shown in Figure 1. Symbols used in Figure 1 are in the nomenclature and the process parameters and physical properties are presented in Hoerner (1979).

The feed gas (60 kg-mol/h, $y_1 = 0.40$) to the process is composed of a solute gas (molecular weight = 58, normal

boiling point = 41.42 °C) and a nonabsorbed waste gas. The molecular weight of the waste gas is needed to determine the flooding velocity in the absorber; its molecular weight was set equal to that of the solute gas. The solute gas is preferentially absorbed by an oil absorbent (molecular weight = 100, normal boiling point = 77.65 °C) in an isothermal (30 °C) packed-bed absorber (pressure = 760 mmHg). The enriched absorbent stream leaving the absorber is preheated to its bubble point by the absorbent recycle stream before it enters the stripping column (pressure = 760 mmHg). The product is recovered as a saturated liquid ($x_3 = 0.99$) from the stripping column. The absorbent recycle stream is cooled to the absorber operating temperature (30 °C) by a trim cooler before re-entering the absorption column.

Some of the physical properties of Umeda's plant have been altered. The density of the absorbent was changed to 1000 kg/m³, density of the gas to 2.6 kg/m³, molecular weight of the absorbent to 100, and the molecular weight of the product to 58.42. The cost functions used for this study are based on recent cost data (Guthrie, 1970). As a result of these changes, no direct comparison between the optimal policy for this plant and that of Umeda is possible.

B. Optimization Method. A generalized geometric program (GGP) is defined as the following nonlinear mathematical programming problem

$$\begin{aligned} &\text{minimize} && P_0(\bar{x}) - Q_0(\bar{x}) \\ &\text{subject to} && P_k(\bar{x}) - Q_k(\bar{x}) \leq 1 \quad k = 1, \dots, K \\ &&& 0 \leq x_j^{lb} < x_j^{ub} \quad j = 1, \dots, N \end{aligned}$$

where

$$\begin{aligned} \bar{x} &= (x_1, \dots, x_N) \\ P_k(\bar{x}) &= \sum_{i=1}^{J_k} c_i \prod_{j=1}^N x_j^{a_{ij}} \quad k = 0, \dots, K \\ Q_k(\bar{x}) &= \sum_{i=1}^{L_k} d_i \prod_{j=1}^N x_j^{a_{ij}} \quad k = 0, \dots, K \end{aligned}$$

$c_i, d_i > 0$ for all $i \in J_k$ and $i \in L_k$ where J_k and L_k are sets of integers numbering the positive and negative terms, respectively, of the k th constraint. The values x_j^{lb} and x_j^{ub} are specified lower and upper bounds on the variable x_j .

A generalized geometric program can always be transformed into an equivalent problem, with a linear objective function, by the addition of one variable and one constraint equation. Therefore, the standard GGP form becomes

$$\begin{aligned} &\text{minimize} && x_0 \\ &\text{subject to} && P_k(\bar{x}) - Q_k(\bar{x}) \leq 1 \quad k = 0, 1, \dots, K \\ &&& 0 \leq x_j^{lb} \leq x_j \leq x_j^{ub} \quad j = 0, 1, \dots, N \end{aligned}$$

where

$$\begin{aligned} \frac{P_0(\bar{x})}{x_0} - \frac{Q_0(\bar{x})}{x_0} &= P_0(x) - Q_0(x) \leq 1 \\ x &= (x_0, x_1, \dots, x_N) \end{aligned}$$

The constraints of the standard GGP problems are rearranged to yield

$$\frac{P_k(x)}{1 + Q_k(x)} \leq 1 \quad k = 0, 1, \dots, K$$

The denominator $(1 + Q_k(x))$ for each constraint is approximated with a monomial by using the condensation procedure. This yields an associated problem that is a regular geometric programming problem (GP). This associated problem contains no negative terms. Any point

Table I. Starting Points

starting point	G	L	X ₂	R	cost	convergence
1	55.00	45.00	0.050	15.00	513217.435	no
2	50.00	60.00	0.050	15.00	495410.137	yes
3	45.00	55.00	0.050	10.00	361406.177	no
4	40.00	60.00	0.075	7.00	216414.171	yes
5	38.00	50.00	0.050	5.00	121818.323	yes

x' , satisfying the constraints of the GP problem will satisfy the constraints of the GGP problem. Therefore, the optimal solution to the GP problem will be a feasible (but not necessarily optimal) point for the GGP problem.

The constraints of the GP problem are then condensed to monomials. Any point, x' , satisfying the GP constraints will also satisfy the condensed GP (GP). However, the feasible set for the GP problem is contained in that for the GP problem; therefore, the solution to the GP will not, in general, be feasible for the GP.

A logarithmic transformation of the GP problem yields a convex, linear programming problem (LP). The lower bounds on the variables are included during the logarithmic transformation. The LP problem is solved using a modified version of the dual simplex method, which accounts for upper bounded variables implicitly. The solution space for the LP problem is reduced by the Kelly cutting-plane technique which adds a recondensed form of the most violated constraint to the LP problem. The solution space for the LP problem is reduced until the LP optimum is feasible for the GGP problem.

A GGP constraint is considered feasible if

$$G_i \leq 1 + \text{EPSCON}$$

where G_i is the numerical value of the i th constraint and EPSCON is the constraint tolerance. The convergence criterion is defined as

$$\frac{|x_0^i - x_0^{i+1}|}{x_0^i} \leq \text{EPSCGP}$$

where x_0^i is the value of the objective function at the i th iteration and EPSCGP is the convergence criterion for the objective function.

Detailed discussion and lucid example problems are presented in Avriel et al. (1975). The program code of Dembo (1975) follows the GGP algorithm directly in all details, with the addition of input data checks, feasibility and consistency monitoring, and several levels of printed output to aid in diagnosing difficulties. Documentation included with the program is considered adequate.

C. GGP Model. The transformation from the process model given in Appendix A to a model compatible with the GGP method is a two-step procedure. The equations must first be transformed to the sum of power products. Then, the proper form for the inequality must be determined so the inequality is active for constraints that require an equality condition. The proper form of the inequality is determined by noticing the direction the algorithm moves the variable's value as the objective function is minimized. If the proper form cannot be determined in this manner, the inequality must be written in both senses to ensure activation. In order to hold the degree-of-difficulty of the GGP problem to a minimum, not all design variables will be explicitly calculated.

The details of the difficulties which occur in the reformulation of the plant process equations are described in Hoerner (1979). Term defining equations are added to the set to reduce the degree of difficulty of the GGP, written in both senses to ensure their activation. Material balance

equations are written directly with the form output \leq input and the overall material balance is written in the opposite sense to ensure their activation. The redundancy of this equation is of no importance. The design equations for the height of the absorber were adapted from the usual short cut equations and written in the sense which minimizes the height as the search minimizes the cost. Equations for flooding velocities, number of stages in the stripper, and all the heat transfer areas were written in the same sense.

GGP requires that the objective function remain positive, so a large positive constant is added to the sum of the investment, interest, materials, utilities. The last term, which is negative, is the income provided by the transfer charge for the distillate value.

The original model equations consisted of material balances, energy balances, bubble and dew point correlations, sizing equations for each unit, fluid properties, cost correlations. Proper ordering makes this system of 20 equations acyclic in four independent variables — L , G , X_2 , and R (q was set equal to unity). The conversion to GGP form results in 32 inequality constraints in 40 variables with 37 degrees of difficulty. The objective function contains 12 terms accounting for equipment costs, materials costs, utilities expenses, and product value. Details are available in Hoerner (1979).

Results and Discussion

Five starting points are shown in Table I. Runs initiated from points 2, 4, and 5 converged to an optimum. The optimal policies for the three successful runs are shown in Table II. The policies differ by less than 1%. The GGP optimal policy is taken as the arithmetic average of these three policies: $G = 36.39213082$; $L = 33.26354978$; $x_2 = 0.00502649$; $R = 2.51106827$.

The cost surface for the GGP model was investigated in the area of the GGP optimum. The contours were generated by taking combinations of the four policy variables two at a time, holding those constant at their GGP optimum values, and perturbing the other two policy variables by 10% about their optimum values. The six contour plots generated in this manner verify that this policy defines a local minimum. Although the algorithm converges to the GGP optimum from multiple starting points, this policy can only be considered a local minimum without further investigation of the entire cost surface.

The GGP optimal policy generates design parameters that are consistent with usual preliminary design practice (area of the feed heater $> 5^*$ area of the absorber cooler, number of stages $\approx 2^*$ minimum, $R \approx 1.1^*$ minimum) for this type of process.

Table II shows the values obtained by substituting the GGP optimal policy into the model equations. These values show a deviation of less than 5% from those for GGP in most cases. Larger differences for some variables occurred because of the inability to completely activate the energy balance for the feed preheater.

A random search (500 valid policies) of the cost surface for the Appendix A model in the area of the GGP optimum produced only one better policy. This policy produced a deviation of less than 2% in both the cost function and

Table II

variable name	GGP optimum			original process model design variables using GGP optimal policy, value
	point 2 EPSCON=0.00001	point 4 EPSCON=0.00001	point 5 EPSCON=0.00001	
COST	22 963.8496	22 964.1980	22 964.1762	23 400.1256
G	36.3950	36.3918	36.3895	36.3921
L	33.2640	33.2723	33.2541	33.2635
X2	0.005056	0.005063	0.004961	0.005027
R	2.5084	2.5130	2.5117	2.5110
RMIN	2.3437	2.3439	2.3433	2.3436
X1	0.4163	0.4162	0.4163	0.4163
Y2	0.0108	0.0107	0.0107	0.0107
D	23.8433	23.8466	23.8489	23.8463
T2	54.7487	54.7495	54.7463	54.7473
T4	77.1372	77.1365	77.1465	77.1415
T5	33.8120	33.7857	33.8093	42.2583
AFH	26.9412	27.0157	26.9345	
ADC	42.1581	42.2202	42.2078	
AAC	1.4727	1.4645	1.4714	
ARB	9.0081	9.0213	9.0196	
QR	418 260.9362	418 876.9217	418 753.6280	417 746.7213
VS	2 279.5221	2 282.8792	2 282.2072	2 281.5362
DS	1.0156	1.0164	1.0162	1.0161
DA	0.7646	0.7646	0.7645	0.7021
STGS	34.8064	35.6083	34.7131	36.3044
SMIN	14.2641	14.2623	14.2916	14.2583

Table III. Process Parameters and Physical Properties

$F = 60 \text{ kg-mol/h}$
$y_1 = 0.400$
$x_3 = 0.990$
$MW_1 = 100$
$MW_g = 58$
$MW_d = 58.42$
$\rho_l = 1000 \text{ kg/m}^3$
$\rho_g = 2.6 \text{ kg/m}^3$
$C_{pi} = 0.20 \text{ kcal/kg}^\circ\text{C} \quad (i = 1, 2, 3, 4, 5)$
$C_{pw} = 1.0 \text{ kcal/kg}^\circ\text{C}$
$h_i = 50 \text{ kcal/kg} \quad (i = 1, 2, 3)$
$h_s = 488 \text{ kcal/kg}$
$A_s = 32.9$
$B_s = 14\,300$
$A_a = 30.4$
$B_a = 13\,800$
$P_t = 760 \text{ mmHg}$
$m = 0.80$
$\alpha \text{ (relative volatility)} = 2.0$
$a/\epsilon^3 = 450 \text{ m}^2/\text{m}^3$
$H_{og} = 1 \text{ m}$
$t_i = 30^\circ\text{C}$
$t_{cwi} = 20^\circ\text{C}$
$t_{cwo} = 25^\circ\text{C}$
$t_s = 170^\circ\text{C}$
$\mu_l = 1 \text{ cP}$
$\mu_w = 1 \text{ cP}$
$U_{dc} = 300 \text{ kcal/m}^2 \text{ h}^\circ\text{C}$
$U_{rb} = 500 \text{ kcal/m}^2 \text{ h}^\circ\text{C}$
$U_{fh} = 100 \text{ kcal/m}^2 \text{ h}^\circ\text{C}$
$U_{ac} = 200 \text{ kcal/m}^2 \text{ h}^\circ\text{C}$
$K_v = 180 \text{ m/h}$

policy. The model seems to be unimodal and shows a local minimum within 2% for both cost and policy.

Runs initiated from starting points 1 and 3 were terminated due to simplex errors. These appear from the dual simplex subroutine which is used to solve the LP subproblem. The solution space for the LP subproblem is a superset of the solution space for the regular geometric program produced by the first condensation procedure. A cutting-plane technique was used to restrict the LP solution space until the optimum for the LP subproblem is feasible for the GP problem. Apparently, in executing the cutting-plane algorithm the program constructs an LP subproblem which is unbounded or one which has no feasible region. This condition can occasionally be cir-

cumvented by changing the value used for EPSCON.

The methods used to arrange the constraint inequalities were successful for all but one constraint equation, the energy balance for the feed heater which defines the value of t_5 . At the optimum, this constraint had a value of 0.98. In general, there is no guarantee this method will force a set of constraints to be active.

Computation time for this problem was a function of the starting point, constraint tolerance, and convergence criterion. To minimize the CPU time, three sequential runs were made from each starting point with EPSCON and EPSCGP set at 0.001, 0.0001, and 0.00001. The optimal policy from the last run was considered the GGP optimum for that starting point. The CPU time time (Amdahl 470) varied between 6 and 120 s.

Conclusions

This model of the absorber-stripper process has a local minimum defined by a policy within the usual range of design practice. The formulation of design equations into GGP form and transformation of these equality conditions into active inequalities is a nontrivial task, but it leads to design parameters within 5% of those from the straightforward process model.

The inability to converge to the optimum from all arbitrary starting points is a shortcoming of this implementation of the GGP algorithm. The cutting-plane subroutine occasionally constructs an LP subproblem that is unbounded or one with no feasible region. This problem has not been reported in previous applications which involved models of significantly smaller size than those typically encountered in preliminary plant design.

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The authors wish to express their thanks for helpful conversation with Professor R. S. Dembo of Yale University, New Haven, Conn.

Appendix A. Process Model

The equations needed to model this plant are presented in this appendix. The process parameters and physical properties are shown in Table III.

A. Material Balance

The steady-state material balance for the process can be adequately represented using the following three bal-

ances. A process flowsheet is given in Figure 1.

1. Absorption Column.

$$Fy_1 + (L + (1 - x_3)D)x_2 = Gy_2 + (L + D)x_1 \quad (\text{A.1})$$

where F = the mass flow rate of the feed gas stream, kg-mol/h; y_1 = the mole fraction of solute in the feed gas stream; $(1 - x_3)D$ = the mass flow rate of the absorbent make-up stream, kg-mol/h; $L + (1 - x_3)D$ = the mass flow rate of the absorbent recycle stream, kg-mol/h; x_2 = the mole fraction of solute in the absorbent recycle stream; G = the mass flow rate of the waste gas stream, kg-mol/h; y_2 = the mole fraction of solute in the waste gas stream; $L + D$ = the mass flow rate of the enriched absorbent stream, kg-mol/h; and x_1 = the mole fraction of solute in the enriched absorbent stream.

2. Stripping Column.

$$(L + D)x_1 = Dx_3 + (L + (1 - x_3)D)x_2 \quad (\text{A.2})$$

where D = the mass flow rate of the product stream, kg-mol/h; x_3 = the mole fraction of solute in the product stream.

3. System.

$$F = G + Dx_3 \quad (\text{A.3})$$

B. Energy Balance

The steady-state energy balance for the process can be adequately represented using the following four balances. The formulation of these balances assumes that the absorption column operates isothermally, all equipment operates adiabatically with respect to the surroundings, and a constant molar overflow in the stripping column.

1. Feed Heater.

$$MW_1(L + D)(C_{p2}t_2 - C_{p1}t_1) = MW_2(L + (1 - x_3)D)(C_{p4}t_4 - C_{p5}t_5) \quad (\text{A.4})$$

where MW_i = the molecular weight of the stream of composition x_i , kg/kg-mol; C_{pi} = the mean specific heat capacity for the stream at temperature t_i , kcal/kg °C; t_1 = the operating temperature for the absorption column, °C; t_2 = the temperature of the enriched absorbent stream entering the stripping column; since $q = 1$, t_2 is the bubble point temperature for composition x_1 , °C; t_4 = the bubble point temperature for the absorbent recycle stream, °C; t_5 = the temperature of the absorbent recycle stream leaving the feed heater, °C.

The Newton-Raphson solution to the bubble point equation used to obtain values for t_2 and t_4 is outlined in Appendix B.

2. Distillate Condenser.

$$Q_{\text{cond}} = MW_3h_3D(R + 1) \quad (\text{A.5})$$

where Q_{cond} = the heat load on the condenser, kcal/h; h_3 = the heat of condensation for the stream with composition x_3 , kcal/kg; and R = the external reflux ratio.

3. Reboiler.

$$Q_r = MW_2h_2D(R + 1) \quad (\text{A.6})$$

where Q_r = the heat load on the reboiler, kcal/h and h_2 = the latent heat of vaporization for the stream with composition x_2 , kcal/kg.

4. Absorbent Recycle Cooler.

$$Q_{\text{cooler}} = MW_2(L + (1 - x_3)D)(C_{p5}t_5 - C_{p1}t_1) \quad (\text{A.7})$$

where Q_{cooler} = the heat load on the absorbent recycle cooler, kcal/h.

C. Equipment Design Equations

1. Height of a Packed Bed Absorption Column. The height of a packed bed absorption column can be deter-

mined using the following design equation (Perry and Chilton, 1973, p 14-11)

$$z = H_{og}N_{og} = H_{og} \int_{y_2}^{y_1} \frac{(1 - y)_{lm}}{(1 - y)(y - y^*)} dy$$

where H_{og} = the height of a transfer unit in meters and N_{og} = the number of transfer units.

In this study, H_{og} will be given a constant value. If Henry's law is valid over the concentration range and there is no heat of absorption, the more rigorous design equation can be approximated by the equation

$$z = H_{og}N_{og} = \frac{H_{og}}{1 - \frac{mG}{L}} \ln \left[\left[1 - \frac{mG}{L} \right] \left[\frac{y_1 - mx_2}{y_2 - mx_2} \right] + \frac{mG}{L} \right] \quad (\text{A.8})$$

where m = slope of the equilibrium line for the absorbent-solute binary.

2. Diameter of the Absorption Column. The diameter of the packed bed can be calculated by determining the flooding velocity for a given set of operating conditions. The diameter of the bed is then calculated based on a vapor velocity that is 75% of the flooding velocity. The flooding velocity can be determined using the correlation (Sawistowski, 1957)

$$\ln \left[G_f^2 \left(\frac{a}{\epsilon^3} \right) \left(\frac{1}{\rho_l \rho_g g} \right) \left(\frac{\mu_l}{\mu_w} \right)^{0.20} \right] = -4 \left(\frac{L'}{G'} \right)^{0.25} \left(\frac{\rho_g}{\rho_l} \right)^{0.125} \quad (\text{A.9})$$

where G_f = the flooding rate expressed as mass flow of the gas phase per unit area of column, kg/s m²; a = the specific surface of the packing, m²/m³; ϵ = the percent void volume for the packing; a/ϵ^3 = the packing factor, m²/m³; ρ_l = the density of the liquid, kg/m³; ρ_g = the density of the gas, kg/m³; g = the acceleration of gravity, m²/s; μ_l = the viscosity of the liquid, cP; μ_w = the viscosity of water at 20 °C, cP; G' = the mass flow rate of the gas phase, kg/h; and L' = the mass flow rate of the liquid phase, kg/h.

Having calculated the flooding velocity, the column diameter is given by

$$DA = \left[\frac{4G'}{0.75\pi G_f} \right]^{1/2} \quad (\text{A.10})$$

where DA = the diameter of the absorption column in meters.

3. Number of Stages in the Stripping Column. Assuming a constant relative volatility, the number of stages required for a binary separation can be determined using Smoker's Method (Smith, 1963, p 155-160)

$$STGS = f(x_1, x_2, x_3, q, R)$$

4. Diameter of the Stripping Column. The flooding velocities for plate columns can be approximated by using the Sounders-Brown equation (Smith, 1963, p 544)

$$U_f = K_v \left(\frac{\rho_l - \rho_g}{\rho_g} \right)^{1/2}$$

where U_f = the flooding velocity for the vapor, m/h and K_v = a constant that is a function of tray spacing and liquid seal depth. For this study a spacing of 24 in. and a liquid seal of 2 in. were used.

The vapor load in the stripping column is based on constant molar overflow. A mean molar volume is deter-

mined by assuming ideal gas behavior and approximating the top and bottom temperatures as 42 and 75 °C, respectively. The vapor load can then be approximated by the equation

$$V = 27.25D(R + 1)$$

where V = the vapor load in the stripping column, m^3/h . The required stripping column diameter is expressed by

$$DS = \left[\frac{109D(R + 1)}{U_f} \right]^{1/2} \quad (\text{A.11})$$

where DS = the diameter of the stripping column in meters.

5. Distillate Condenser. The log-mean temperature driving force in the condenser is given by the equation

$$\Delta T_{\text{lm}dc} = \frac{(t_3' - t_{\text{cwo}}) - (t_3 - t_{\text{cwi}})}{\ln \frac{(t_3' - t_{\text{cwo}})}{(t_3 - t_{\text{cwi}})}} \quad (\text{A.12})$$

where t_3' = the dew point temperature for composition x_3 , °C; t_3 = the bubble point temperature for composition x_3 , °C; t_{cwi} = the inlet temperature for the cooling water, °C; and t_{cwo} = the outlet temperature for the cooling water, °C.

The heat transfer area required for the distillate condenser can be calculated from the equation

$$ADC = \frac{Q_{\text{cond}}}{U_{\text{dc}} \Delta T_{\text{lm}dc}} \quad (\text{A.13})$$

where ADC = the surface area for the distillate condenser, m^2 ; U_{dc} = the overall heat transfer coefficient for the distillate condenser, $\text{kcal}/\text{m}^2 \text{ h } ^\circ\text{C}$; and $\Delta T_{\text{lm}dc}$ = the log-mean temperature driving force in the distillate condenser, °C.

6. Reboiler. Sufficient steam will be supplied such that the inlet and outlet temperature of the steam will be equal. Therefore, the only heat supplied by the steam will be the heat of condensation. The temperature driving force for the reboiler is given by the equation

$$\Delta T_{\text{rb}} = t_s - t_4 \quad (\text{A.14})$$

where t_s = temperature of the steam, °C.

The heat transfer area required for the reboiler can be calculated from the equation

$$ARB = \frac{Q_r}{U_{\text{rb}} \Delta T_{\text{rb}}} \quad (\text{A.15})$$

where ARB = the surface area for the reboiler, m^2 ; U_{rb} = the overall heat transfer coefficient for the reboiler, $\text{kcal}/\text{m}^2 \text{ h } ^\circ\text{C}$; ΔT_{rb} = the temperature driving for the reboiler, °C; Q_r = the heat load on the reboiler, kcal/h .

7. Feed Heater. The log-mean temperature driving force for the feed heater is given by the equation

$$\Delta T_{\text{lm}fh} = \frac{(t_4 - t_2) - (t_5 - t_1)}{\ln \frac{(t_4 - t_2)}{(t_5 - t_1)}} \quad (\text{A.16})$$

The heat load on the feed heater is given by

$$QFH = MW_1(L + D)(C_{p2}t_2 - C_{p1}t_1) \quad (\text{A.17})$$

Therefore, the heat transfer area required for the feed heater can be calculated from the equation

$$AFH = \frac{QFH}{U_{\text{fh}} \Delta T_{\text{lm}fh}} \quad (\text{A.18})$$

where AFH = the heat transfer area for the feed heater, m^2 ; U_{fh} = the overall heat transfer coefficient for the feed heater, $\text{kcal}/\text{m}^2 \text{ h } ^\circ\text{C}$; $\Delta T_{\text{lm}fh}$ = the log-mean temperature driving force for the feed heater, °C; and QFH = the heat load on the feed heater, kcal/h .

8. Absorbent Recycle Cooler. The log-mean temperature driving force for the absorbent recycle cooler is given by the equation

$$\Delta T_{\text{lm}ac} = \frac{(t_5 - t_{\text{cwo}}) - (t_1 - t_{\text{cwi}})}{\ln \frac{t_5 - t_{\text{cwo}}}{t_1 - t_{\text{cwi}}}} \quad (\text{A.19})$$

Therefore, the heat transfer area required for the absorbent recycle cooler can be calculated from the equation

$$AAC = \frac{Q_{\text{cooler}}}{U_{\text{ac}} \Delta T_{\text{lm}ac}} \quad (\text{A.20})$$

where AAC = the heat transfer area of the absorbent recycle cooler, m^2 ; U_{ac} = the overall heat transfer coefficient for the absorbent recycle cooler, $\text{kcal}/\text{m}^2 \text{ h } ^\circ\text{C}$; $\Delta T_{\text{lm}ac}$ = the log-mean temperature driving force for the absorbent recycle cooler, °C; and Q_{cooler} = the heat load on the absorbent recycle cooler, kcal/h .

Bubble Point Determination

Assuming that Henry's law applies, one may express the vapor-liquid equilibrium for each component of the binary mixture by the equations (Foust et al., 1960, p 21)

$$y_s = K_s x_s \quad (\text{B.1})$$

$$y_a = K_a x_a \quad (\text{B.2})$$

where y_s = the mole fraction of the solute in the vapor phase; y_a = the mole fraction of the absorbent in the vapor phase; x_s = the mole fraction of the solute in the liquid phase; x_a = the mole fraction of the absorbent in the liquid phase; K_s = (the vapor pressure of the solute)/(total pressure); and K_a = (the vapor pressure of the absorbent)/(total pressure).

The vapor pressure for each component can be expressed by Antoine's equation

$$p_s = \exp[A_s - B_s/(T + 503)] \quad (\text{B.3})$$

$$p_a = \exp[A_a - B_a/(T + 503)] \quad (\text{B.4})$$

where p_s = the vapor pressure of the solute at temperature T , mmHg; p_a = the vapor pressure of the absorbent at temperature T , mmHg; A_s, B_s, A_a, B_a = published values for experimentally determined vapor pressure constants for the solute and absorbent; and T = the temperature, °C.

At the bubble point the following relationship must hold

$$y_s + y_a = 1 \quad (\text{B.5})$$

The operating pressure for the process is set at 760 mmHg. Substitution into eq B.5 yields

$$K_s x_s + K_a (1 - x_s) = 1 \quad (\text{B.6})$$

where x_s = the mole fraction of solute in the mixture; $K_s = (1/760) \exp[A_s - B_s/(T + 503)]$; and $K_a = (1/760) \exp[A_a - B_a/(T + 503)]$.

Given x_s , application of the Newton-Raphson method to eq B.6 for T yields the bubble point. Solution of eq B.6 at $x_s = x_1$ yields t_2 . Solution of eq B.6 at $x_s = x_2$ yields t_4 .

Appendix B. Rearrangement of Process Model into GGP Form

1. Term Defining Equations. In order to reduce the degree-of-difficulty of the GGP problem, the following term defining equations were included. Since these

equations have no direct effect on the objective function, it is required that they be written in both senses to ensure activation.

$$L*ARG11^{-1} + D*ARG11^{-1} \leq 1 \quad (G.1)$$

$$ARG11L^{-1} + D*L^{-1} \leq 1 \quad (G.2)$$

$$L*ARG12^{-1} + 0.01*D*ARG12^{-1} \leq 1 \quad (G.3)$$

$$ARG12*L^{-1} - 0.01*D*L^{-1} \leq 1 \quad (G.4)$$

where $ARG11 = L + D$ and $ARG12 = L + (1 - x_3)*D = L + 0.01*D$.

2. Material Balance Equations. The two-component material balances are written in the form; output \leq input. To ensure that these equations are active, the overall component balance is included and written in the opposite sense; input \leq output. The overall material balance is written in the form; input \leq output.

$$[ARG11*x_1 + G*y_2 - 24]*ARG12^{-1}*x_2^{-1} \leq 1 \quad (G.5)$$

$$[0.99*D + ARG12*x_2]*ARG11^{-1}*x_1^{-1} \leq 1 \quad (G.6)$$

$$24*G^{-1}*y_2^{-1} - 0.99*D*G^{-1}*y_2^{-1} \leq 1 \quad (G.7)$$

$$60*G^{-1} - 0.99*D*G^{-1} \leq 1 \quad (G.8)$$

3. Absorber Height Equations. The following equations are necessary to determine the height of the absorption column. The form for the inequalities is based on the concept that the algorithm will move to minimize its cost. The natural logarithm is approximated by the technique suggested by Duffin et al. (1967, p 100).

$$0.8*(x_2*y_2^{-1} + (G*L^{-1} + 0.5*y_2^{-1} - x_2*y_2^{-1} - 0.4*G*L^{-1}*y_2^{-1})*ARG1^{-1}) \leq 1 \quad (G.9)$$

$$10000*ARG1^{0.0001}*ARG2^{-1} - 10000*ARG2^{-1} \leq 1 \quad (G.10)$$

$$ARG3 + 0.80*G*L^{-1} \leq 1 \quad (G.11)$$

where $ARG1$ = the argument of the natural logarithm in eq A.8; $ARG2 = \ln(ARG1)$; and $ARG3 = 1 - m*G/L$. Therefore $z = ARG2*ARG3^{-1}$.

This relationship need not be used as a constraint equation to define the value z . The monomial $ARG2*ARG3^{-1}$ can be substituted for z in the objective function.

4. Absorber Diameter Equations. The flooding velocity for the absorption column is approximated by using a one-term expansion for the exponential function (e^z) (Perry and Chilton, 1973, Section 2-35). The form of the following inequalities is based on the concept that the algorithm will minimize the absorber diameter in order to minimize its cost.

$$0.35436*ARG4 + 0.40570*G^{-0.25}*L^{0.25} \leq 1 \quad (G.12)$$

$$0.16538*G^{0.5}*DA^{-1}*ARG4^{-0.5} \leq 1 \quad (G.13)$$

where $ARG4 = G$, the flooding rate expressed as mass flow rate of the gas phase per unit area of column cross section, kg/s m² and DA = the diameter of the absorption column in meters.

5. Number of Stages in the Stripper. Smoker's Method is not easily transformed into GGP form. The Gilliland chart is based on the same assumptions as Smoker's Method and, therefore, will be used in the GPP model. The Gilliland chart (Smith, 1963, p 634, Figure B-8b) can be approximated over the relevant section by a power function. The minimum number of stages can be determined using the Fenske equation (McCabe and Smith, 1976, p 565). The logarithmic approximation of

Duffin et al. (1967, p 100) is used. The form of the inequalities is based on the concept that the algorithm will minimize the number of stages in order to minimize the stripper column cost.

$$14433.581*x_2^{-0.0001}*SMIN^{-1} - 14426.950*SMIN^{-1} \leq 1 \quad (G.14)$$

$$0.99*RMIN^{-1}*x_1^{-1} + x_1 - 1.01*RMIN^{-1} \leq 1 \quad (G.15)$$

$$ARG8*R^{-1} + RMIN*R^{-1} \leq 1 \quad (G.16)$$

$$R*ARG9^{-1} + ARG9^{-1} \leq 1 \quad (G.17)$$

$$ARG10 + 0.373*ARG8^{-0.15}*ARG9^{0.15} \leq 1 \quad (G.18)$$

$$SMIN*STGS^{-1}*ARG10^{-1} \leq 1 \quad (G.19)$$

where $SMIN$ = the minimum number of equilibrium stages for the stripper column; $RMIN$ = the minimum external reflux ratio (established by the slope of the operating line intersecting the equilibrium curve at x_1); $ARG8 = R - RMIN$; $ARG9 = R + 1$; $ARG10 = 1 - 0.373*(ARG8/ARG9)^{-0.15}$; and $STGS$ = the number of equilibrium stages for the stripper column.

6. Stripper Diameter Equations. Two equations are necessary to determine the diameter of the stripping column. The form of the inequalities is based on the concept that the algorithm will minimize the column diameter in order to minimize its cost.

$$27.25*R*D*VS^{-1} + 27.25*D*VS^{-1} \leq 1 \quad (G.20)$$

$$0.0212731*VS^{0.5}*DS^{-1} \leq 1 \quad (G.21)$$

where VS = the vapor load in the stripping column, m³/h and DS = the diameter of the stripping column in meters.

7. Heat Transfer Area for the Feed Heater. The bubble point temperature, t_2 and t_4 , must be determined. The bubble point equation is solved on the interval 0 to 1 and fitted with a polynomial equation (Barr et al., 1976, p 251). The form of the inequalities is based on the concept the algorithm will minimize the area requirement for the heat exchanger in order to minimize its cost.

$$(C_6*x_1^6 + C_5*x_1^5 + C_4*x_1^4 + C_3*x_1^3 + C_2*x_1^2 + C_1*x_1 + C_0)*t_2^{-1} \leq 1 \quad (G.22)$$

$$D_6*x_2^6 + D_5*x_2^5 + D_4*x_2^4 + D_3*x_2^3 + D_2*x_2^2 + D_1*x_2 + D_0*t_4 \leq 1 \quad (G.23)$$

where $C_6 = 612.36588$; $C_5 = -1231.1806$; $C_4 = 1077.6505$; $C_3 = -570.90247$; $C_2 = 231.60646$; $C_1 = -100.89515$; $C_0 = 77.641460$; t_2 = the bubble point temperature for composition x_1 ; $D_6 = -7.8870990$; $D_5 = 15.857257$; $D_4 = -13.879833$; $D_3 = 7.3530620$; $D_2 = -2.9830256$; $D_1 = 1.2995009$; $D_0 = 0.012879717$; and t_4 = the bubble point temperature for composition x_2 .

The energy balance around the feed heater defines the temperature t_5 . For simplicity, the molecular weights MW_1 and MW_2 are assumed to be equal to that of the pure absorbent. The form of this inequality is based on the concept the algorithm will maximize the temperature t_5 in order to maximize the temperature driving force in the feed heater.

$$0.0333*(t_5*ARG12*ARG11^{-1} + t_2 - t_4*ARG12*ARG11^{-1}) \leq 1 \quad (G.24)$$

The following equations are necessary to determine the log-mean temperature difference in the feed heater.

$$DTF1*t_4^{-1} + t_2*t_4^{-1} \leq 1 \quad (G.25)$$

$$DTF2*t_5^{-1} + 30*t_5^{-1} \leq 1 \quad (G.26)$$

$$10000*DTF1^{0.0001}*DTF2^{-0.0001}*ARG5^{-1} - 10000*ARG5^{-1} \leq 1 \quad (G.27)$$

$$DTF*DTF1^{-1}*ARG5 + DTF1^{-1}*DTF2 \leq 1 \quad (G.28)$$

where $DTF1 = t_4 - t_2$; $DTF2 = t_5 - 30$; $ARG5 = \ln(DTF1/DTF2)$; and DTF = the log-mean temperature driving force in the feed heater. The heat transfer area of the feed heater is expressed by the equation

$$(0.20*t_2 - 6.0)*ARG11*DTF^{-1}*AFH^{-1} \leq 1 \quad (G.29)$$

where AFH = the heat transfer area of the feed heater, m^2 .

8. Heat Transfer Area for the Reboiler. Six equations are necessary to determine the heat transfer area for the reboiler. The value of MW_2 is taken to be that of the pure absorbent. The form of the inequalities is based on the concept the algorithm will minimize the heat transfer area in order to minimize its cost.

$$5000*D*QR^{-1}*(R + 1) \leq 1 \quad (G.30)$$

$$0.00588*(DTR + t_4) \leq 1 \quad (G.31)$$

$$0.002*DTR^{-1}*ARB^{-1}*QR \leq 1 \quad (G.32)$$

where QR = the heat load on the reboiler, kcal/h; DTR = the temperature driving force in the reboiler, $^{\circ}C$; and ARB = the heat transfer area for the reboiler, m^2 .

9. Heat Transfer Area for the Distillate Condenser. Since the product purity is set ($x_3 = 0.99$), the bubble point and dew point for the product stream can be calculated. The inlet and outlet temperatures for the cooling water are 20 and 25 $^{\circ}C$, respectively; therefore, the temperature driving force in the distillate condenser is constant. One equation is required to determine the heat transfer area for the distillate condenser. The form of this inequality is based on the concept that the algorithm will minimize the heat transfer area in order to minimize its cost.

$$0.50397*D*ADC^{-1}*(R + 1) \leq 1 \quad (G.33)$$

where ADC = the heat transfer area for the distillate condenser, m^2 .

10. Heat Transfer Area for the Absorbent Recycle Cooler. Five equations are necessary to determine the heat transfer area for the absorbent recycle cooler. The form of the inequalities is based on the concept that the algorithm will minimize the heat transfer area in order to minimize its cost.

$$DTC1*t_5^{-1} + 20*t_5 \leq 1 \quad (G.34)$$

$$0.20*DTC1*ARG6^{-1} \leq 1 \quad (G.35)$$

$$10000*ARG6^{0.0001}*ARG7^{-1} - 10000*ARG7^{-1} \leq 1 \quad (G.36)$$

$$DTC*ARG7*DTC1^{-1} + 5*DTC1^{-1} \leq 1 \quad (G.37)$$

$$(t_5 - 3.0)*ARG12*DTC^{-1}*AAC^{-1} \leq 1 \quad (G.38)$$

where $DTC1 = t_5 - 20$; $ARG6 = 0.20DTC1$; $ARG7 = \ln(ARG6)$; DTC = the log-mean temperature driving force in the absorbent recycle cooler, $^{\circ}C$; and AAC = the heat transfer area for the absorbent recycle cooler, m^2 .

11. Objective Function. The objective function is derived in Appendix C. However, the GGP program requires that the objective function remains positive. Therefore, a constant value of 500000 was added to the function in Appendix C. Substitution of the GGP model variables results in the following objective function. $COST = 500000 + 1889.7*DS^{1.059}*STGS^{0.832} + 45.091*DS^{1.583}*STGS^{0.944} + 2035.8*DA^{1.059}*ARG2^{0.832} + ARG3^{-0.832} + 237.33*DA^2*ARG2*ARG3^{-1} + 710.21*AFH^{0.646} + 710.21*ADC^{0.646} + 710.21*AAC^{0.646} +$

$958.49*ARB^{0.646} + 0.2592*QR + 70.285714*DTC*AAC - 27750.08*D$ where $COST$ = the value of the objective function.

The formulation of these inequalities is a nontrivial task. The success of the algorithm and its machine implementation will be measured by whether or not it converges to a minimum and the computer (CPU-Amdahl 470) time required. The success of the algorithm will also depend on the correspondence of the minimum and policy with the original model equations (Appendix A).

The original model equations were also solved using a direct search procedure. The model equations were arranged for rapid solution using the equation ordering algorithm of Book (1976). After choosing values for the four variables (G, L, x_2, R) the system of equations is acyclic. The value of these four variables will be referred to as the policy for the process.

Appendix C. Objective Function

The objective function to be used in the optimization problem will reflect the yearly cost of the process. The general form of the cost function can be written as

$$COST = F_c C_{inv} + C_{op} - R_p$$

where F_c = the yearly cost factor for the capital investment, 1/year; C_{inv} = the operating cost, dollars/year; and R_p = the yearly revenue received for the product, dollars/year.

A. Yearly Cost Factor

The total investment the company would make in a plant has been referred to as C_{inv} . However, not all the investment will come directly from the company.

Let $0.50C_{inv}$ be the dollar amount actually invested from the company's assets. The required return on investment for this portion will be 15% after taxes. Then $0.50C_{inv}$ is the dollar amount borrowed by the company from a commercial lender. An annual interest rate of 10% will be used.

1. Cash Flow on Equity.

$$(0.19925)(0.50C_{inv})$$

The capital recovery factor of 0.19925 (Grant and Ireson, 1970, p 612, Table E-18) allows for a 15% return on investment plus capital recovery at the end of 10 years.

2. Depreciation.

$$0.10C_{inv}$$

The straight-line depreciation factor of 0.10 (Grant and Ireson, 1970, pp 161-162) is based on a 10 year service life with no salvage value.

3. Profit After Taxes.

$$[(0.19925)(0.5C_{inv}) + (0.1)(0.5C_{inv}) - (0.1)C_{inv}]$$

This amount takes into consideration the cash flow on equity, the principal repayment for the loan, and the depreciation.

4. Taxable Income. Considering an effective tax rate of 50%, the taxable income becomes

$$2[(0.19925)(0.5C_{inv}) + 0.1(0.5C_{inv}) - 0.1C_{inv}]$$

5. Yearly Replacement Cost.

$$0.1C_{inv}$$

This amount assumes the money will be invested to earn a return at least as great as the rate of inflation.

6. Yearly Interest on Loan.

$$(0.06275)(0.5C_{inv})$$

The average yearly interest factor (Grant and Ireson, 1970,

p 610, Table E-16) is based on an annual interest rate of 10% for 10 years. Therefore

$$F_c = \frac{1}{C_{inv}} (\text{taxable income} + \text{replacement cost} + \text{interest cost})$$

$$F_c = 0.231$$

B. Capital Investment Cost

The capital investment cost is the total for the installed cost of all process equipment. However, in this study the pumps and drivers will not be included since these costs are easily masked by the cost of the other equipment. To determine the equipment cost one can use the data correlations compiled by Guthrie (1970). However, analytical correlations must be developed for the graphical representations reported by Guthrie. The installed cost including overhead is computed by multiplying the delivered cost by the bare module factor for that piece of equipment. The cost is up-dated from mid-1970 to January 1979 using the Marshall and Stevens index.

1. Stripping Column. The total cost of the stripping column is the sum of the cost for the vertical process vessel (Guthrie, 1970, p 151) and the column internals (Guthrie, 1970, p 152). The calculations are based on a stage (tray) efficiency of 0.70, a tray spacing of 24 in., carbon steel material, and sieve plate trays.

The stripping column cost can be expressed by the equation

$$C_{sc} = 8180.5STGS^{0.832}DS^{1.059} + 195.2STGS^{0.944}DS^{1.583}$$

where C_{sc} = the installed cost for the stripping column, dollars (1979); $STGS$ = the number of equilibrium stages in the stripping column; and DS = the diameter of the stripping column, m².

2. Absorption Column. The total cost of the absorption column is the sum of the cost of the vertical process vessel (Guthrie, 1970, p 151) and the column packing (Guthrie, 1970, p 153). The calculations are based on carbon steel material, a constant height of a transfer unit of 1 m, and 1-in. berl saddles. The absorption column cost can be expressed by the equation

$$C_{ac} = 8813.1z^{0.832}DA^{1.059} + 1027.4zDA^2$$

where C_{ac} = the installed cost for the absorption column, dollars (1979); z = the absorption column height, m; and DA = the diameter of the absorption column, m.

3. Feed Heater. The cost of the feed heater can be expressed by the following equation (Guthrie, 1970, p 138)

$$C_{fh} = 3074.5AFH^{0.646}$$

where C_{fh} = the installed cost for the feed heater, dollars (1979) and AFH = the heat transfer area of the feed heater, m².

4. Distillate Condenser. The cost of the distillate condenser can be expressed by the following equation (Guthrie, 1970, p 138)

$$C_{dc} = 3074.5ADC^{0.646}$$

where C_{dc} = the installed cost for the distillate condenser, dollars (1979) and ADC = the heat transfer area of the distillate condenser, m².

5. Absorbent Recycle Cooler. The cost of the absorbent recycle cooler can be expressed by the following equation (Guthrie, 1970, p 138)

$$C_{ac} = 3074.5AAC^{0.646}$$

where C_{ac} = the installed cost for the absorbent recycle

cooler, dollars (1979) and AAC = the heat transfer area of the absorbent recycle cooler, m².

6. Reboiler. The cost of the stripping column reboiler is based on carbon steel material and a kettle reboiler design. The cost can be expressed by the following equation (Guthrie, 1970, p 138)

$$C_{rb} = 4149.3ARB^{0.646}$$

where C_{rb} = the installed cost for the stripping column reboiler, dollars (1979) and ARB = the heat transfer area of the stripping column reboiler, m².

C. Operating Cost

The operating cost consists of the yearly cost of steam and cooling water. The yearly cost is based on 7200 operating hours per year.

1. Steam Cost. Steam is available at 100 psig. This steam, therefore, has a specific heat of condensation of 488 kcal/kg. Cost data was obtained from Peters and Timmerhaus (1968, p 772). Cost for 1967 was reported as 1.10–2.20 dollars/1000 kg. Using a mean value and escalating to January, 1979, dollars yields a cost of 3.65 dollars/1000 kg.

The yearly cost for steam is expressed by the following equation

$$C_s = 0.0539Q_r$$

where C_s = the yearly cost for steam, dollars/year.

2. Cooling Water Cost. The total cooling water cost is the sum of the cost for the cooling water required by the distillate condenser and that required by the absorbent recycle cooler. The inlet temperature is 20 °C and the outlet temperature is 25 °C. Therefore, the maximum heat load that can be absorbed by the cooling water is 4990 kcal/1000 kg. Cost data was obtained from Peters and Timmerhaus (1968, p 772). Cost for 1967 was reported as 0.044–0.176 dollars/1000 kg. Using a mean value and escalating to January, 1979, dollars yields a cost of 0.24 dollars/1000 kg.

The yearly cost for distillate condenser cooling water is expressed by the equation

$$CW_{dc} = 0.003514MW_3Q_r$$

where CW_{dc} = the yearly cost for the cooling water used by the distillate cooler, dollars/year.

The cooling water cost for the absorbent recycle cooler can be expressed by the equation

$$CW_{ac} = 70.2857AAC\Delta T_{lmac}$$

where CW_{ac} = the yearly cost of cooling water used by the absorbent recycle cooler, dollars/year.

D. Product Revenue

The product revenue is based on a density of 800 kg/m³ (50 lb_m/ft³), and a unit price of 52.5 dollars/m³ (0.20 dollars/gallon).

The product revenue can be expressed by the equation

$$R_p = 27750.08D$$

where R_p = the yearly revenue for the product stream, dollars/year.

Substitution of the individual terms into the general cost function (C.1) yields the objective function.

$$\begin{aligned} \text{COST} = & 1889.7DS^{1.059}STGS^{0.832} + \\ & 45.091DS^{1.583}STGS^{0.944} + \\ & 2035.8DA^{1.059}z^{0.832} + 237.33DA^2z + \\ & 710.21AFH^{0.646} + 710.21ADC^{0.646} + 710.21AAC^{0.646} + \\ & 958.49ARB^{0.646} + 0.2592Q_r + \\ & 70.285714AAC\Delta T_{lmac} - 27750.08D \end{aligned}$$

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Data Inputs and Interchange in Integrated Solution/Design Tower Packages

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Generalized equations are derived allowing fast calculation of the degrees of freedom of single or multiple interconnected tower systems. Moreover, the external data requirements for the stage design correlations are identified and their significance on the overall column design is evaluated. In the process of analysis the phase property requirements for the stage-to-stage and stage design correlations are identified and the column operation and stage performance data to be interchanged are listed.

Introduction

A staged operations problem is completely defined when a unique solution of its stage-to-stage and stage design correlations exists. Such solution requires a number of process variables and design parameters to be externally fixed, phase property correlations to be provided, and finally, column operation and stage performance data to be interchanged (Economopoulos, 1978a).

Enumeration methods for calculating the degrees of freedom have been described by Dunstan (1938), Gilliland and Reed (1942), Kwauk (1956), and Howard (1967) and appear in textbooks, as in Smith (1963). The enumeration procedure, however, is cumbersome and for this reason is rarely used in practice. Moreover, the analysis has been limited to the stage-to-stage calculations, with the stage pressure drops and holdups reported as degrees of freedom and the stage efficiencies ignored.

In the present study, generalized equations are developed allowing direct calculation of the degrees of freedom of individual towers with any number of material and heat leaks, as well as multiple interconnected tower systems. In the process of analysis the internal system relationships (equations of the mathematical model), as well as the required physical properties and stage performance characteristics, are identified and listed.

The parameters to be externally fixed for the stage design correlations are identified and their significance to the overall column design evaluated. The required column operation and physical property data are also listed.

Through the above process, the required external specifications for and data interchanges among the stage-to-stage and stage design correlations are established.

Process Variables and Relationships

A staged operations problem is completely defined when the total number of variables in the process is equal to the total number of independent relationships which can be written for the process. The latter is the sum of the internal system relationships (equations of the mathematical model) and the externally imposed specifications. Thus

$$Nv = Ni + Nf \quad (1)$$

The total number of variables involved in a process composed of U units is given by equation

$$(Nv)_p = (Nr)_p + \sum_{u=1}^U (Nv)_u \quad (2)$$

where $(Nr)_p$ accounts for the decisions to be made regarding the number of units in the process and the location of the incoming and outgoing material and heat leaks.

The number of internal relationships which can be written for the above process is

$$(Ni)_p = (Ni)_{com} + \sum_{u=1}^U (Ni)_u \quad (3)$$

where $(Ni)_{com}$ is the number of independent relationships, which are generated when the U units are combined to form the process: (i) one temperature, $(M - 1)$ component