Report of Major Project on

Optimization Techniques In Oil Refinery

Submitted in partial fulfillment of the requirements for

Bachelor of Technology
In
Applied Petroleum Engineering
University of Petroleum & Energy Studies
Dehradun, India

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CERTIFICATE

This is to certify that the Project Report on **"OPTIMIZATION TECHNIQUES IN OIL REFINERY"** submitted to University of Petroleum & Energy Studies, Dehradun, by **Sumit Kumar and Umang Agarwal** in partial fulfillment of the requirement for the award of Degree of **Bachelor of Technology** in **Applied Petroleum Engineering** (Academic Session 2003 – 07) is a bonafide work carried out by them under my supervision and guidance. This work has not been submitted anywhere else for any other degree or diploma.

Date: May 1, 2007.

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Acknowledgement

With great pleasure we would like to express our sincere thanks to Dr. **Deoki.N.Saraf**, College of Engineering (COE), University of Petroleum & Energy Studies, for giving us the opportunity to carry out our training and work on the project "Optimization techniques in Oil Refinery" under his guidance and support.

We are deeply indebted to our college Lab staff for their timely and generous help at every stage during the progress of our project work.

We are also thankful to ISM Dhanbad Library Department for making its library available to us to acquire valuable inputs required at various timesteps.

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INTRODUCTION

OPTIMIZATION is the use of specific methods to determine the most cost-effective and efficient solution to a problem or design for a process. This technique is one of the major quantitative tools in industrial decision making. A wide variety of problems in the design, construction, operation, and analysis of chemical plants (as well as many other industrial processes) can be resolved by optimization.

WHAT OPTIMIZATION IS ALL ABOUT

Optimization pervades the fields of science, engineering, and business. In physics many different optimal principles have been enunciated, describing natural phenomena in the fields of optics and classical mechanics. The field of statistics treats various principles termed "maximum likelihood," "minimum loss," and "least squares," and business makes use of "maximum profit," "minimum cost," "maximum use of resources," "minimum effort," in its efforts to increase profits. A typical engineering problem can be posed as follows: A process can be represented by some equations or perhaps solely by experimental data. You have a single performance criterion in mind such as minimum cost. The goal of optimization is to find the values of the variables in the process that yield the best value of the performance criterion. A trade-off usually exists between capital and operating costs. The described factors-process or model and the performance criterion-constitute the optimization "problem."

Typical problems in chemical engineering process design or plant operation have many (possibly an infinite number) solutions. Optimization is concerned with selecting the best among the entire set by efficient quantitative methods. Computers and associated software make the necessary computations feasible and cost effective.

WHY OPTIMIZE?

Engineers work to improve the initial design of equipment and strive to enhance the operation of that equipment once it is installed so as to realize the largest production, the greatest profit, the improved yields of valuable products (or reduced yields of contaminants), reduced energy consumption, higher processing rates, and longer times between shutdowns.

Optimization can also lead to reduced maintenance costs, less equipment wear, and better staff utilization. In addition, intangible benefits arise from the interactions among plant operators, engineers, and management. It is extremely helpful to systematically identify the objective, constraints, and degrees of freedom in a process or a plant, leading to such benefits as improved quality of design, faster and more reliable troubleshooting, and faster decision making.

SCOPE AND HIERARCHY OF OPTIMIZATION

Optimization can take place at many levels in a company, ranging from a complex combination of plants and distribution facilities down through individual plants, combinations of units, individual pieces of equipment, subsystems desirable to manufacture more product from an old, inefficient plant (at higher cost) than from a new, efficient one because new customers may be located very close to the old plant. On the other hand, if the old plant is operated far above its design rate, costs could become exorbitant, forcing a reallocation by other plants in spite of high transportation costs. In addition, no doubt constraints exist on production levels from each plant that also affect the product distribution plan.

THE ESSENTIAL FEATURES OF OPTIMIZATION PROBLEMS

Because the solution of optimization problems involves various features of mathematics, the formulation of an optimization problem must use mathematical expressions. Such expressions do not necessarily need to be very complex. Not all problems can be stated or analyzed quantitatively, but we will restrict our coverage to quantitative methods. From a practical viewpoint, it is important to mesh properly the problem statement with the anticipated solution technique. A wide variety of optimization problems have amazingly similar structures. Indeed, it is this similarity that has enabled the recent progress in optimization techniques.

Chemical engineers, petroleum engineers, physicists, chemists, and traffic engineers, among others, have a common interest in precisely the same mathematical problem structures, each with a different application in the real world. We can make use of this structural similarity to develop a framework or methodology within which any problem can be studied. This section describes how any process problem, complex or simple, for which one desires the optimal solution should be organized. To do so, you must (a) consider the model representing the process and(b) choose a suitable objective criterion to guide the decision making.

Every optimization problem contains three essential categories:

I. At least one **objective function** to be optimized (profit function, cost function,etc.).

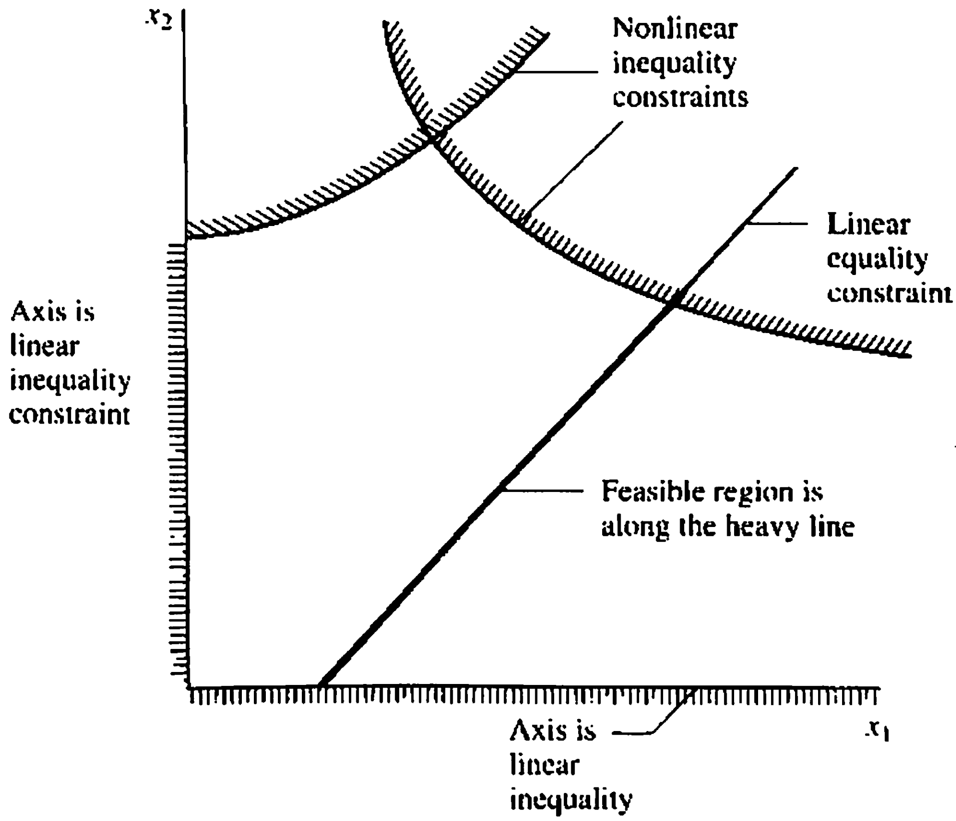
2. **Equality constraints (equations).**

3. **Inequality constraints (inequalities).**

Categories 2 and 3 constitute the model of the process or equipment; category I is sometimes called the economic model.

By a feasible solution of the optimization problem we mean a set of variables that satisfy categories 2 and 3 to the desired degree of precision. Figure illustrates the feasible region or the region of feasible solutions defined by categories 2 and 3. In this case the feasible region consists of a line bounded by two inequality constraints.

An optimal solution is a set of values of the variables that satisfy the components of categories 2 and 3; this solution also provides an optimal value for the function in category I. In most cases the optimal solution is a unique one; in some it is not. If you formulate the optimization problem so that there are no residual degrees of freedom among the variables in categories 2 and 3, optimization is



Feasible region for an optimization problem involving two independent variables. The dashed lines represent the side of the inequality constraints in the plane that form part of the infeasible region. The heavy line shows the feasible region. not needed to obtain a solution for a problem. More specifically, if *me* equals the number of independent consistent equality constraints and *mi* equals the number of independent inequality constraints that are satisfied as equalities (equal to zero), and if the number of variables whose values are unknown is equal to me + mi' then at least one solution exists for the relations in components 2 and 3 regardless of the optimization criterion. (Multiple solutions may exist when models in categories 2 and 3 are composed of nonlinear relations.) If a unique solution exists, no optimization is needed to obtain a solution-one just solves a set of equations and need not worry about optimization methods because the unique feasible solution is by definition the optimal one.

On the other hand, if more process variables whose values are unknown exist in category 2 than there are independent equations, the process model is called under determined; that is, the model has an infinite number of feasible solutions so that the objective function in category I is the additional criterion used to reduce the number of solutions to just one (or a few) by specifying what is the "best" solution. Finally, if the equations in category 2 contain more independent equations than variables whose values are unknown, the process model is over determined and no solution satisfies all the constraints exactly. To resolve the difficulty, we sometimes choose to relax some or all of the constraints. A typical example of an over determined model might be the reconciliation of process measurements for a material balance. One approach to yield the desired material balance would be to resolve the set of inconsistent equations by minimizing the sum of the errors of the set of equations (usually by a procedure termed least squares).

In this text the following notation will be used for each category of the optimization problem:

Minimize: f(x) Objective function

Subject to: h(x) = 0 Equality Constraints

$g(x) \geq 0$ Inequality constraints

where x is a vector of n variables (Xl' X2' . . . , Xn)' h(x) is a vector of equations of dimension ml' and g(x) is a vector of inequalities of dimension m_2. The total number of constraints is $m = (m_1 + m_2)$

SINGLE VARAIBLE OPTIMIZATION TECHNIQUES

Some of the numerical optimization techniques used for optimizing a problem are:

- Quadratic Interpolation
- Fibonacci Search Method
- Golden Section Search Method
- Successive Quadratic Estimation Method
- Finite Difference Approximation Method

QUADRATIC INTERPOLATION

We start with three points x_1, x_2 and x_3 in increasing order that might be equally spaced, but the extreme points must bracket the minimum. we know that a quadratic function $f(x) = a + bx + cx^2$ can be passed exactly through the three points, and that the function can be differentiated and the derivative set equal to 0 to yield the minimum of the approximating function $x = - b/2c$

Suppose *that f(x)* is evaluated at x_1, x_2 and x_3 yield :

$f(x1) = f1$, $f(x2) = f2$, and $f(x3) = f3$

The coefficients band c can be evaluated from the solution of the three linear equations:

$f(x_1) = a + bx_1 + cx_1^2$

$f(x_2) = a + bx_2 + cx_2^2$

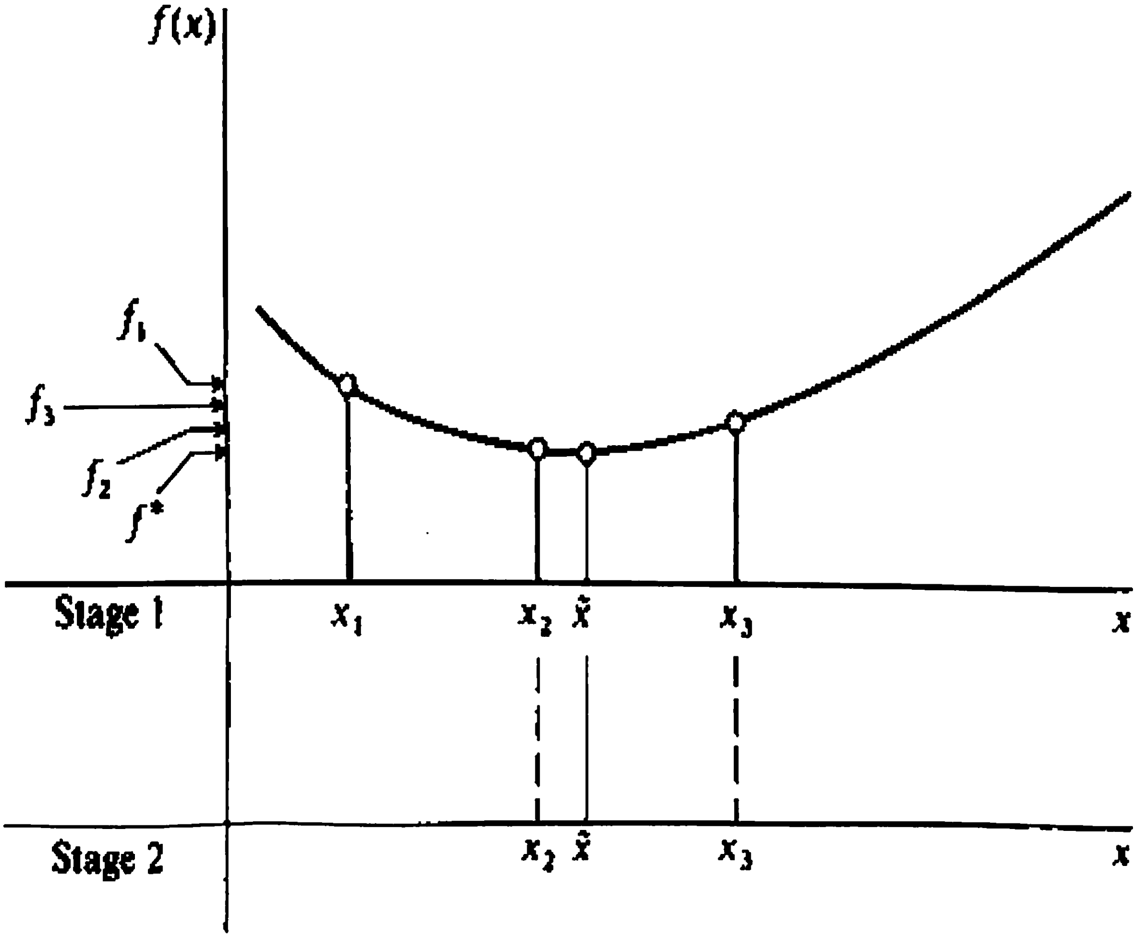
$f(x_3) = a + bx_3 + cx_3^2$

via determinants or matrix algebra. Introduction of *b* and c expressed in terms of

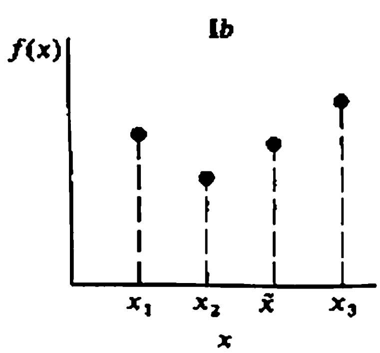
$$x^* = \frac{1}{2}\frac{[(x^2_2 - x^2_3)f1 + (x^2_3 - x^2_1)f_2 + (x^2_1 - x^2_2)f_3]}{[(x_2 - x_3)f_1 + (x_3 - x_1)f_2 + (x_1 - x_2)f_3]}$$

To illustrate the first stage in the search procedure, examine the four points in Figure for stage 1.We want to reduce the initial interval [x1 , x3] By examining

The values of f(x) [with the assumptions that f(x) is unimodal and has a minimum],We can discard the interval from x_1 to x_2 and use the region (x_2, x_3) as the new interval. The new interval contains three points, (x_2' x, x_3) that can be introduced into Equation to estimate x*, and so on. In general, we evaluate f (x*) and discard From the set { x_1' x_2' x_3} the point that corresponds to the greatest value of fix), unless



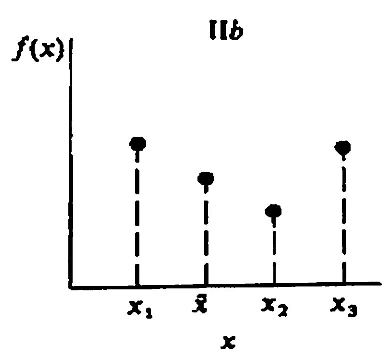
Two stages of quadratic interpolation



I. If $\tilde{x}$ lies between x_2 and x_3:

(a) $f^* < f_2$ Pick $x_2, \tilde{x}, x_3$
$f^* < f_3$

(b) $f^* > f_2$ Pick $x_1, x_2, \tilde{x}$
$f^* < f_3$



II. If $\tilde{x}$ lies between x_1 and x_2:

(a) $f^* < f_2$ Pick $x_1, \tilde{x}, x_2$
$f^* < f_1$

(b) $f^* > f_2$ Pick $\tilde{x}, x_2, x_3$
$f^* < f_1$

a bracket on the minimum of f (x) is lost by so doing, in which case you discard the x so as to maintain the bracket. The specific tests and choices of x to maintain the Bracket is illustrated in . In Figure, f* = f(x). If x* and whichever of {x_1 ,x_2 ,x_3,} corresponding to the smallest f(x) differ by less than the prescribed accuracy in x, or the prescribed accuracy in the corresponding values of f(x) is achieved, terminate the search. Note that only function evaluations are used in the search and that only one new function evaluation (for x) has to be carried out at each new iteration.

FIBONACCI SEARCH METHOD

In this method, the search interval is reduced according to Fibonacci numbers. The property of the Fibonacci numbers is that, given two consecutive numbers F_{n-2} ,F_{n-1}, and the third number is calculated as follows:

$$F_n = F_{n-1} + F_{n-2}$$

Where n = 2,3,4...

The first few Fibonacci numbers are Fo = 1, $F_1 = 1$, $F_2 = 2$, $F_3 = 3$, $F_4 = 5$, $F_5 = 8$, $F_6 = 13$, and so on. The property of the Fibonacci numbers can be used to create a search algorithm that requires only one function evaluation at each iteration. The principle of Fibonacci search is that out of two points required for the use of the region-elimination rule, one is always the previous point and the other point is new. Thus, only one function evaluation is required at each iteration. At iteration *k*, two intermediate points, each L^*_k away from either end of the search space*(L =b - a)* are chosen. When the region-elimination rule eliminates a portion of the search space depending on the function values at these two points, the remaining search space is L_k

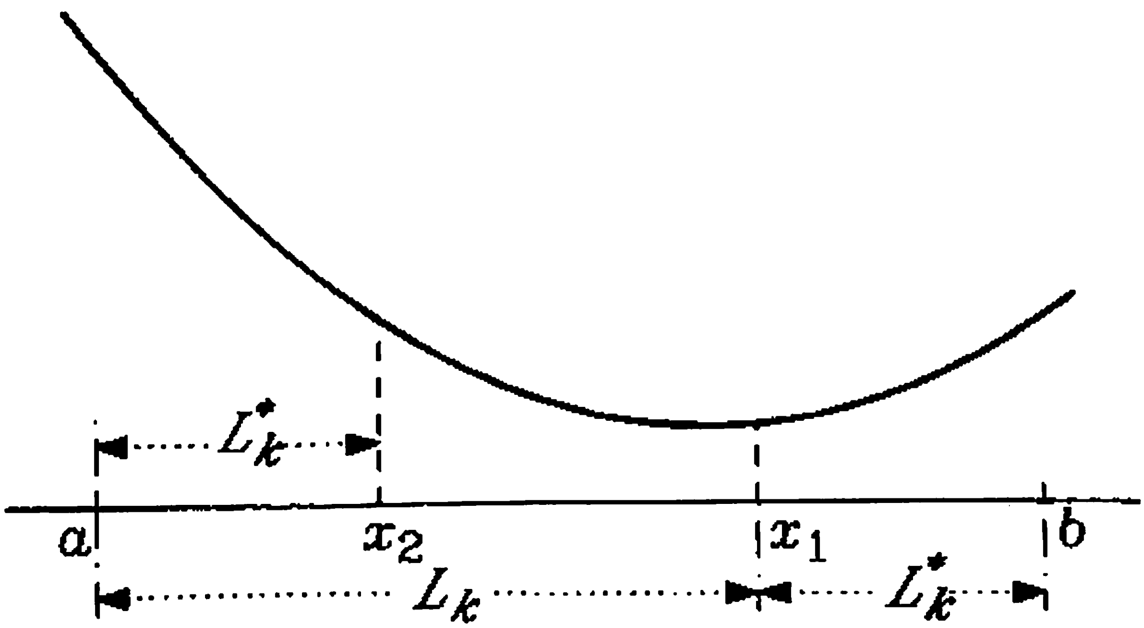
By defining

$$L^*_k = (F_{n-k+1} / F_{n+1}) \quad \text{and}$$

$$L_k = (F_{n-k+2} / F_{n+1}), \quad \text{it can be shown that}$$

$$L_k - L^*_k = L^*_{k+1}$$

which means that one of the two points used in iteration *k* remains as one point in iteration (k + 1). This can be seen from Figure. If the region *(a,x2)* is eliminated in the k-th iteration, the point X_1 is at a distance (L_k - L^*_k) or L^*_{k+1} from the point X_2 in the (k + 1)-th iteration. Since, the first two Fibonacci numbers are the same, the algorithm usually starts with k = 2.



Algorithm

Step 1 : Choose a lower bound *a* and an upper bound *b*. Set *L* =*b*- *a*. Assume the desired number of function evaluations to be *n*. Set *k* = 2.

Step 2 : Compute $L^*_k = (F_{n-k+1}/ F_{n+1})L$. Set $X_1 = a + L^*_k$ and $X_2 = b - L^*_k$

Step 3 : Compute one of $f(X_1)$ or $f(X_2)$, which was not evaluated earlier. Use the fundamental region elimination rule to eliminate a region. Set new a and b.

Step 4 : Is k = n? If no, set k = k + 1 and go to Step 2;

Else Terminate.

In this algorithm, the interval reduces to $(2/F_{n+1})L$ after *n* function evaluations. Thus, for a desired accuracy €, the number of required function evaluations *n* can be calculated using the following equation:

$$\frac{2(b-a)}{F_{n+1}} = €.$$

As is clear from the algorithm, only one function evaluation is required at each iteration. At iteration k, a proportion of F_{n-k}/F_{n-k+2} of the search space at the previous iteration is eliminated. However, one difficulty with this algorithm is that the Fibonacci numbers must be calculated in each iteration.

GOLDEN SECTION SEARCH METHOD

One difficulty of the Fibonacci search method is that the Fibonacci numbers have to be calculated and stored. Another problem is that at every iteration the proportion of the eliminated region is not the same. In order to overcome these two problems and yet calculate one new function evaluation per iteration, the golden section search method is used. In this algorithm, the search space (a, b) is first linearly mapped to a unit interval search space (0,1). Thereafter, two points at Γ from either end of the search space are chosen so that at every iteration the eliminated region is (1 - Γ) to that in the previous iteration. This can be achieved by equating 1 - Γ with (Γ X Γ). This yields the golden number: $\Gamma = 0.618$. The figure can be used to verify that in each iteration one of the two points X_1 and X_2 is always a point considered in the previous iteration.

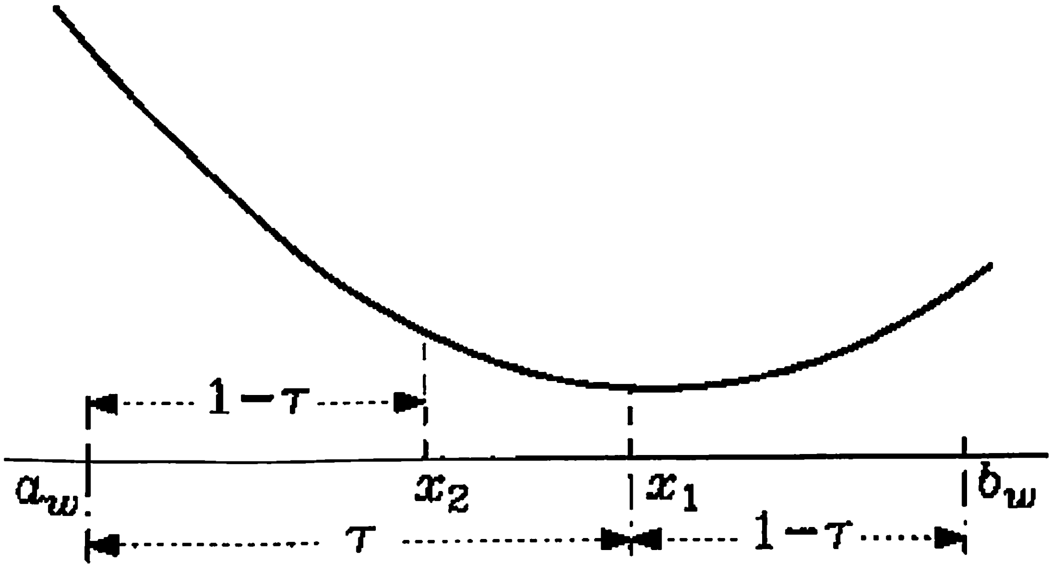
Algorithm:

Step 1: Choose a lower bound a and an upper bound b. Also choose a small number €. Normalize the variable X by using the equation:

$W = (x - a)/(b - a)$. Thus, $a_w = 0$, $b_w = 1$, and $L_w = 1$. Set $k = 1$.

Step 2: Set $W_1 = a_w + (0.618)L_w$ and $W_2 = b_w - (0.618)L_w$.

Compute $f(W_1)$ or $f(W_2)$, depending on whichever of the two was not evaluated earlier. Use the fundamental region-elimination rule to eliminate a region. Set new a_w and b_w.



Step 3: Is |Lw| < € small? If no, set k = k + 1, go to Step 2;

Else Terminate.

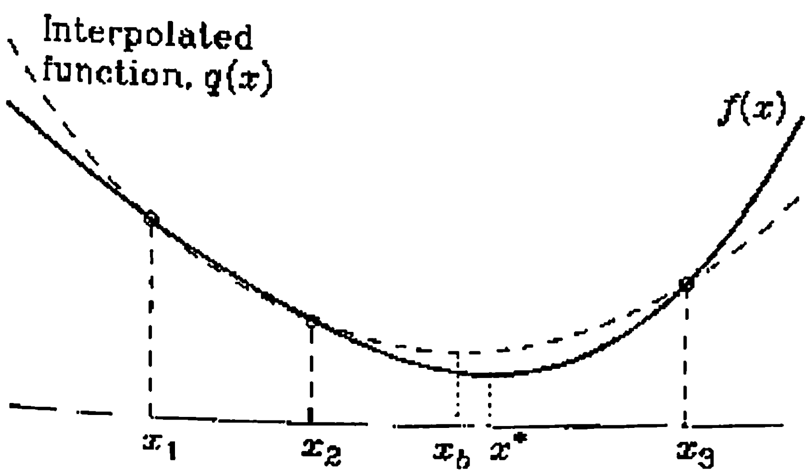
In this algorithm, the interval reduces to $(0.618)^{n-1}$ after *n* function evaluations. Thus, the number of function evaluations *n* required to achieve a desired accuracy € is calculated by solving the following equation:

$$(0.618)^{n-1}(b - a) = €.$$

Like the Fibonacci method, only one function evaluation is required at each iteration. This quantity is the same as that in the fibonacci search for large n. In fact, for a large n, the fibonacci search is equivalent to the golden section search.

SUCCESSIVE QUADRATIC ESTIMATION METHOD

In, this algorithm, the fitted curve is a quadratic polynomial function. Since any quadratic function can be defined with three points, the algorithm begins with three initial points. This figure shows the



original function and three initial points X_1, X_2, and X_3. The fitted quadratic curve through these three points is also plotted with a dashed line. The minimum (x*) of this curve is used as one of the candidate points for the next iteration. For non quadratic functions, a number of iterations of this algorithm is necessary, whereas for quadratic objective functions the exact minimum can be found in iteration only.

A general quadratic function passing through two points X_1 and X_2 can be written as:

$$Q(x)=a_0 + a_1(x-x_1) + a_2(x-x_1) + a_2(x-x_1)(x-x_2)$$

If (x_1, fi), (x_1, f_2), and (x_3, f_3), are three points on this function, The following relationships can be obtained:

$a_0 = fi$

$a_1 = (f_2 - f_1)/(x_2 - x_1)$

$a_1 = [(f_3 - f_1)/(x_3 - x_1) - a_1]$

in differentiating q(x) with respect to X and setting it to zero, it can be shown that the minimum of the above function is

$$X^* = [(x_1 + x_2)/2] - [a_1/2]$$

The above point is an estimate of the minimum point provided $q''(x) > 0$ or $a_2 > 0$, which depends only on the choice of the three basic points. Among the four points (X_1, X_2, X_3,) and X^*), the best three points are kept and a new interpolated function q(x) is found again. This procedure continues until two consecutive estimates are close to each other. Based on these results, Powell's algorithm (Powell, 1964) is presented

Algorithm:

Step 1:

Let X_1 be an initial point and Δ be the step size. Compute $X_2 = X_1 + \Delta$

Step 2:

Evaluate $f(X_1)$ and $f(X_2)$

Step 3

If $f(X_1)) > f(X_2)$, let $X_3 = X_1 + 2\Delta$

Else let $X_3 = X_1 - \Delta$ Evaluate $f(X_3)$

Step 4

Determine Fmin = min (f_1, f_2, f_3)and X min is the point Xi that corresponds to Fmin.

Step 5

Use points X_1, X_2, and X_3 to calculate X* using the above equation.

Step 6

Are l Fmin - f(x*)l and l Xmin- xl small? If not, go to

Step 7;

Else the optimum is the best of current four points and terminate. Save the best point and two bracketing it, if possible; Otherwise, save the best three points. Re label them according to $X_1 < X_2 < X_3$ and go to Step 4. In the above algorithm, no check is made to satisfy $a_2 > O$. The same can be incorporated in Step 5. If a_2 is found to be negative, one of the three points may be replaced by a random point. This process is continued until the quantity a_2 becomes nonnegative.

FINITE DIFFERENCE APPROXIMATION METHOD

If f(x) is not given by a formula, or the formula is so complicated that analytical derivatives cannot be formulated, we can use a finite difference approximation

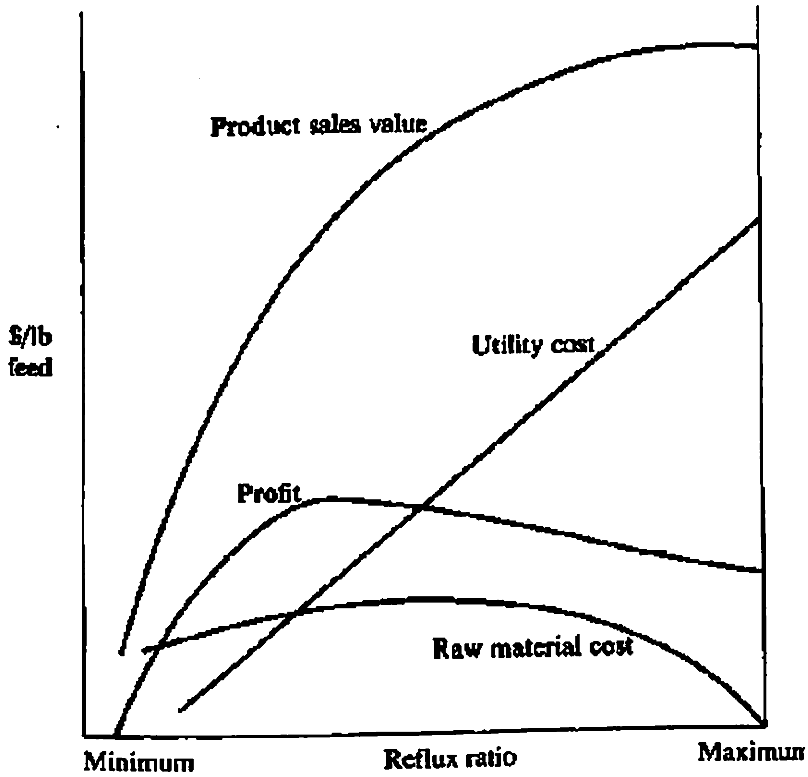
$$x^{k+1} = x^{k} - \frac{[f(x+h)-f(x-h)]/2h}{[f(x+h) - 2f(x) + f(x-h)]/h2}.$$

Central differences were used in Equation (5.8), but forward differences or any other difference scheme would suffice as long as the step size *h* is selected to match the difference formula and the computer (machine) precision with which the calculations are to be executed. The main disadvantage is the error introduced by the finite differencing.

DETERMINATION OF THE OPTIMAL REFLUX RATIO FOR A STAGED-DISTILLATION COLUMN

Once a distillation column is in operation, the number of trays is fixed and very few degrees of freedom can be manipulated to minimize operating costs. The reflux ratio frequently is used to control the steady-state operating point. Figure E12.4a shows typical variable cost patterns as a function of the reflux ratio. The optimization of reflux ratio is particularly attractive for columns that operate with

1. High reflux ratio
2. High differential product values (between overhead and bottoms)
3. High utility costs
4. Low relative volatility
5. Feed light key far from 50 percent



Variable cost trade offs for a distillation column

The lighter component (propylene) is more valuable than propane.

For example, propylene and propane in the overhead product were both valued at $O.20/lb (a small amount of propane was allowable in the overhead), but propane in the bottoms was worth $O.12/lb and propylene $O.09Ilb. The overhead stream had to be at least 95 percent propylene. Based on the data in Table

we will determine the optimum reflux ratio for this column

The Eduljee correlation involves two parameters: Rm. The minimum reflux ratio, and Nm, the equivalent number of stages to accomplish the separation at total reflux. His operating equations relate N, α , X_F, X_D, and X_B (seeTable for notation) all of which have known values except XB as listed in Table. Once R is specified, you can find XB by sequential solution of the three following equations:

Rm is calculated by:

$$R_m = 1/(\alpha-1)\ [X_D/X_F - \alpha(1-X_D)/(1-X_F)] \quad \text{.......................(a)}$$

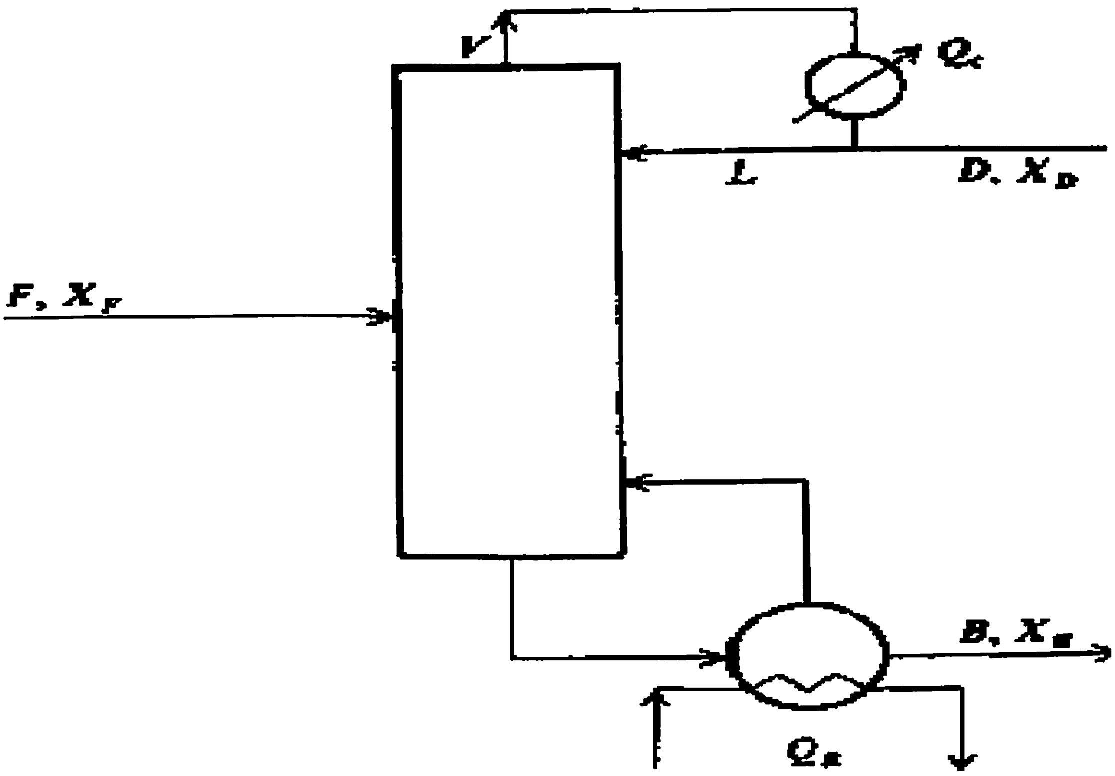
After calculating Rm, Nm can be calculated by:

$$[(N-N_M)/N+1] = 0.75\ [1-\{R-R_m/R+1\}^{0.5668}] \quad \text{...................(b)}$$

Lastly compute XB by:

$$N_M = \ln\{[X_D/(1-X_D)].[(1-X_B)/X_B]\}/\ln\alpha \quad \text{...................(c)}$$

Equations (a) – (c) comprise equality constraints relating XB and R



Distillation Column Flow Chart

Once XB is calculated, the overall material balance for the column shown in Figure can be computed. The pertinent equations are (the-units are moles)

$F = D + B$

$X_F F = X_D D + X_B B$

In addition, if the assumption of constant molal overflow is made, then the liquid *L* and vapor flows *V* are

$L = RD$

$V = (R + 1)D$

Objective function. Next we develop expressions for the income and operating costs. The operating profit *f* is given by

f = Propylene sales + Propane sales - Utility costs - Raw material costs

$$\mathbf{f = (C_D X_D D + C_B X_B B) + [C'_D(1 - X_D)D + C'_B(1 - X_B)B] - [C_1 Q_R + C_2 Q_C] - [C_F X_F F + C'_F(1 - X_F)F]}$$

The brackets [ ] indicate the correspondence between the words in Equation (h) and the symbols in above Equation. Q_R is the reboiler heat requirement and Qc is the cooling load. Equation can be rearranged by substituting for *DxD* in the propylene sales and for *BxB* in the propane sales using above Equation and defining - $W = C_B - C_D$ and - $U = C_D - C_{B'}$ follows

DATAS

For given staged distillation column

TABLE

Notation and values for the propane-propylene splitter

SYMBOL	DESCRIPTION	VALUE
B	Bottoms flow rate	3.27×10^5 Lb/day
C_1	Reboiler heat cost	$3.00 x 10^6Btu
C_2	Condenser cooling cost	$0.00 x 10^6 Btu
C_B	Value of propylene in bottoms\	
C_F	Cost per pound of propylene	
C'_F	Cost per pound of propane	
C_D	Value of propylene in overhead	
C'_D	Value of propane in overhead	
D	Distillate flow rate	8.72×10^5 Lb/day
F	Feed rate	1,200,000 Lb/day
L	Liquid flow rate	function of R (mol/day)
N	Number of equilibrium stages	94
N_M	Minimum equilibrium stages	function of reflux ratio, *R*
Q_C	Condenser load requirement	$Q_C = \lambda V$
Q_R	Reboiler heat requirement	$QR = \lambda V$
R	Reflux ratio	(To be optimized)
R_M	Minimum reflux ratio	11.17

U	Heavy key differential value	$0.08/Lb
V	Vapor flow rate	function of R (mol/day)
W	Light key differential value	$O.ll/Lb
X_B	Bottom light key mole fraction	(To be optimized)
X_D	Overhead light key mole fraction	0.95
X_F	Feed light key mole fraction	0.70
α	Relative volatility	1.105
λ	Latent heat	130 Btu/Lb (avg. mixture)

$$\mathbf{f = C_D X_F F + C'_B(1 - X_F)F - C_F X_F F - C'_F(1 - X_F)F - C_1 Q_R - C_2 Q_C - W X_B B - U(1 - X_D)D}$$

Note that the first four terms *off* are fixed values, hence these terms can be deleted from the expression for *f* in the optimization. In addition, it is reasonable to assume $QR = Qc = \lambda V$. Lastly, the right-hand side of Equation *(j)* can be multiplied by −1 to give the final form of the objective function (to be minimized):

$$\mathbf{f_1 = (C_1 + C_2)\lambda V + W X_B B + U(1 - X_D)D}$$

Note: λ must be converted to Btu/mol, and the costs to $/mol.

QUADRATIC INTERPOLATIONAL SEARCH METHOD

The final form of objective function to be minimized:

$$f_1 = (c_1 + c_2)\lambda V + WX_B B + U(1-X_D)D$$

Where, C1= Reboiler heat cost = $3.00 x 10^6 Btu

C2=condenser cooling cost = $0.00 x 10^6 Btu

λ = Latent heat =130 Btu/Lb (avg. mixture)

V= Vapor flow rate function of R (mol/day)

W= Light key differential value = $ O.11/Lb

XB=Bottom light key mole fraction

B= Bottoms flow rate

U= Heavy key differential value =$0.08/Lb

XD= Overhead light key mole fraction =0.95

D = Distillate flow rate

The above equation takes the form as

$$f_1 = (c_1 + c_2)\lambda(R+1)D + WX_B B + U(1-X_D)D$$

Based on the data, we minimize f_1, with respect to R using a

Quadratic interpolation one-dimensional search

The value of R_m from Equation was 11.17. The initial bracket was (12<= R <= 20), and R =16, 18, and 20 were selected for the initial three points.

At, **R=16, Minimum Reflux Ratio** is calculated from formula

$$\mathbf{R_m = 1/(\alpha\text{-}1)\ [X_D/X_F - \alpha(1-X_D)/(1-X_F)]}$$

$$= 1/.105\ [.95/.70 - 1.105\ (0.05/0.36]$$

$$= 1/.105\ [1.357 - 0.184]$$

$$= 11.17$$

N_M, Minimum equilibrium stages

$$\mathbf{[(94 - N_M)/95] = 0.75\ [1 - \{R - R_m/R+1\}^{0.5668}]}$$

$$[(94 - N_M)/95] = 0.75\ [1 - \{16 - 11.17/16+1\}^{0.5668}]$$

$$N_M = 57.66$$

XB=Bottom light key mole fraction is calculated as

$$\mathbf{N_M = \ln\{[X_D/(1-X_D)].[(1-X_B)/X_B]\}/\ln\alpha}$$

$$= \ln\{[.95/.05].[(1-X_B)/X_B]\}/\ln 1.105$$

$$\mathbf{X_B = 0.056}$$

B, Bottoms flow rate is calculated as

$$\mathbf{X_F F = X_D D + X_B B}$$

$$0.70\times1.2\times10^6 = 0.95D + 0.056\ B$$

$$0.70\times1.2\times10^6 = 0.95(1.2\times10^6 - B) + 0.056\ B$$

$$B = 3.35\times10^5$$

$$D = 8.64\times10^5$$

Therefore,

$$f_1 = (c_1 + c_2)\lambda(R+1)D + WX_B B + U(1-X_D)D$$

$$= (3\times10^6 \times130\times17\times 8.64\times10^5) + 0.11\times0.056\times3.35\times10^5 - 0.04(1-0.95)\times8.64\times10^5$$

= $ 4491.26

Interpolated value of χ is calculated by the formula

$$\chi^* = \frac{1}{2} \frac{\{(\chi_2^2-\chi_3^2) f_1 + (\chi_3^2-\chi_1^2) f_2 + (\chi_1^2-\chi_2^2) f_3\}}{(\chi_2-\chi_3) f_1 + (\chi_3-\chi_1) f_2 + (\chi_1-\chi_2) f_3}$$

Similarly, At various values of R iterations is done and optimum range of optimum reflux ratio is calculated

	Left bracket		Centre bracket		Right bracket		Interpolated values	
	χ	f	χ	f	χ	f	χ^*	f
1	16.00	4491.26	18.00	4243.87	20.00	4582.14	17.85	4232.59
2	18.00	4243.87	17.85	4232.59	16.00	4491.26	17.57	4216.75
3	17.85	4232.59	17.57	4216.75	16.00	4491.26	17.48	4216.72
4	17.57	4216.75	17.48	4216.72	16.00	4491.26	17.52	4327.93

Optimum range for reflux ratio lies in the range (17.57 to 17.48)

FIBONACCI SEARCH METHOD

In this method, the search interval is reduced according to Fibonacci numbers. The property of the Fibonacci numbers is that, given two consecutive numbers F_{n-2} ,F_{n-1}, and the third number is calculated as follows:

$$F_n = F_{n-1} + F_{n-2}$$

Where n = 2,3,4...

The first few Fibonacci numbers are Fo = 1, F_1 = 1, F_2 = 2, F_3 = 3, F_4= 5, F_5 = 8, F_6= 13, and so on

We calculate the optimum interval of optimum reflux ratio in the interval between R=16 and R= 18

Algorithm

Step 1 :

a= 16 and b= 18 so, L = b- a= 2

Let n=3 and **k=2**

Step 2 :

Lk* = (Fn-k+1/ Fn+1) L.

L2* = (F3-2+1/ F3+1) L. = (F2 / F4).L =(2/5).2 = 0.8

Xl = a + Lk^* = 16 + 0.8 = 16.80

X2= b - Lk^* = 18-0.8 = 17.20

At **R=16.8**

N_M, Minimum equilibrium stages

$$[(94- N_M) / 95] = 0.75 [1-\{R- R_m/R+1\}^{0.5668}]$$

$$N_M = 56.89$$

XB=Bottom light key mole fraction is calculated as

$$N_M = \ln \{ [X_D/(1- X_D)].[(1- X_B)/ X_B] \} / \ln \alpha$$

$$X_B = 0.060$$

B, Bottoms flow rate is calculated as

$$\mathbf{X_F F = X_D D + X_B B}$$

$$B = 3.37 \times 10^5$$

$$D = 8.62 \times 10^5$$

$$f = (c_1 + c_2)\lambda(R+1)D + WX_B B + U(1-X_D)D$$

$$= \$\ 4796.5569$$

At **R=17.20**

$$N_M = 60.84$$

$$X_B = 0.041$$

$$B = 3.3 \times 10^5$$

$$D = 8.69 \times 10^5$$

$$f = (c_1 + c_2)\lambda(R+1)D + WX_B B + U(1-X_D)D$$

$$= \$\ 4216.317$$

Step 3 :

Since, $f(16.8) > f(17.20)$

So, we eliminate the region (16, 16.8).

We set a= 16.8 and b= 18 so, $L = b - a = 1.2$

Step 4 :

$Xl = a + Lk^* = 17.20 + 0.32 = 17.52$

$X2 = b - Lk^* = 18 - 0.32 = 17.68$

At **x_1= R=17.52**

$N_M = 61.9518$

$X_B = 0.038$

$B = 3.29\times10^5$

$D = 8.70\times10^5$

$f = (c_1 + c_2)\lambda(R+1)D + WX_BB + U(1-X_D)D$

$= \$\ 4210.23$

. At **x_2= R=17.68**

$N_M = 61.9518$

$X_B = 0.0376$

$B = 3.28\times10^5$

$D = 8.71\times10^5$

$f = (c_1 + c_2)\lambda(R+1)D + WX_BB + U(1-X_D)D$

$= \$\ 422095$

Step 2 :

Set **k = 3** and go to Step 2;

Lk* = (Fn-k+1/ Fn+1) L.

L2* = (F3-3+1/ F3+1) L. = (F1 / F4).L =(1/5).2 = 0.4

$Xl = a + Lk^* = 16 + 0.4 = 16.40$

$X2 = b - Lk^* = 18\text{-}0..4 = 17.60$

Step 3 :

At **x_1= R=16.40**

$$N_M = 58.7985$$

$$X_B = 0.050$$

$$B = 3.33 \times 10^5$$

$$D = 8.66 \times 10^5$$

$$f = (c_1 + c_2)\lambda(R+1)D + WX_BB + U(1-X_D)D$$

$$= \$\ 4278.01$$

. At **x_2= R=17.60**

$$N_M = 61.7128$$

$$X_B = 0.038$$

$$B = 3.29 \times 10^5$$

$$D = 8.70 \times 10^5$$

$$f = (c_1 + c_2)\lambda(R+1)D + WX_BB + U(1-X_D)D$$

$$= \$\ 4224.43$$

Optimum range for reflux ratio lies in the range (17.52 to 17.60)

GOLDEN SECTION SEARCH MEHOD

Step 1:

The transformation equation for this method is: $W = (x - a)/(b - a)$.

Taking a=16, b=18

Transformation equation becomes: $W = (x-16)/2$

Thus, aw = 0, bw = 1, and Lw = 1

Step 2:

Since, w1= aw + (0.618) Lw 1

= 0 + (0.618) x 1

= 0.618 &

w2 = bw – (0.618) Lw 2

=1 – (0.618) x 1

= 0.382

Now $f(w) = (C_1 + C_2)\lambda V + WX_B B + U(1-X_D)D$......................................3

Also, $R_1 = 2w_1 + 16$

=2 x 0.618 + 16

= 17.236 &

$R2 = 2w_2 + 16$

=2 x 0.382 + 16

=16.764

Calculating f(R1) and f(R2) via eqn (3)

$f(R_1) = 4214.9738$ & $f(R_2) = 4226.0368$

Since, $f(R_1) < f(R_2)$

Using fundamental region-elimination rule

New $a_w = 0.382$, $b_w = 1$, So $L_w = 0.618$

Step 3:

$€.=(0.618)^{n-1}(b - a)$..4

$€ = 0.5$

and $|L_w| > €$

So $k = 1+1$

$= 2$

Again calculating w_1 and w_2 via eqn (1) and (2)

$w1=0.382 + (0.618) \times 0.618$

$=0.764$

$w_2 = 1 - (0.618) \times 0.618$

$=0.618$

At w1 = 0.764, R1 = 17.528 &

At w2 = 0.618, R2 = 17.236

Again Calculating f(R1) and f(R2) via eqn (3)

$f(R_1) = 4217.9382$ & $f(R_2) = 4214.9846$

Here, $f(R_1) > f(R_2)$

Again by using fundamental region-elimination rule

New $a_w = 0.382$, $b_w = 0.764$, So $L_w = 0.382$

and from eqn (4), $\epsilon = 0.381$

Since $|l_w| = 0.382$

So Again $|L_w| > \epsilon$

Again repeating same procedure , $k = 3$

Calculating w_1 and w_2 via eqn (1) and (2)

$$w1 = 0.382 + (0.618) \times 0.382$$
$$= 0.618$$

$$w2 = 0.764 - (0.618) \times 0.382$$
$$= 0.582$$

At $w1 = 0.618$, $R1 = 17.236$ &

At $w2 = 0.528$, $R2 = 17.056$

Again Calculating $f(R1)$ and $f(R2)$ via eqn (3)

$f(R_1) = 4214.9846$ & $f(R_2) = 4219.0224$

Here, $f(R_1) < f(R_2)$

Again by using fundamental region-elimination rule

New $a_w = 0.528$, $b_w = 0.764$, So $L_w = 0.236$

and from eqn (4), € = 0.236

Since $|L_w| = 0.236$

Here $|L_w| =$ €

So iterating one more time to get optimum solution , k = 4

Calculating w_1 and w_2 via eqn (1) and (2)

$$w1 = 0.582 + (0.618) \times 0.236$$
$$= 0.6738$$

$$w2 = 0.764 - (0.618) \times 0.236$$
$$= 0.618$$

At w1 = 0.673, R1 = 17.34 &

At w2 = 0.618, R2 = 17.236

Again Calculating f(R1) and f(R2) via eqn (3)

$f(R_1) = 4210.88$ & $f(R_2) = 4214.9846$

Iteration	Calculated Ropt	Minimum Total cost, F
1	17.236	$ 4214.9738
2	17.34	$ 4210.88
3	17.528	$ 4217.1029

Optimum range for reflux ratio lies in the range (17.52 to 17.23)

FINITE DIFFERENCE APPROXIMATION METHOD

The formula used for calculating optimum reflux ratio via this method is:

$$x_{k+1} = xk - \frac{[f(x+h)-f(x-h)]/2h}{[f(x+h) - 2f(x) + f(x-h)]/h2}$$

Or

$$R_{k+1} = Rk - \frac{[f(R+h)-f(R-h)]/2h}{[f(R+h) - 2f(R) + f(R-h)]/h2} \text{ (in terms of reflux ratio)}$$

Taking interval , **h = - 0.19.**

Reflux ratio, **R = 18**

$$Rk+1 = 16 - \frac{[f(18 - 0.19)-f(18 + 0.19)]/2x(-0.19)}{[f(18+0.19) - 2f(18) + f(18 + 0.19)]/(-0.19)^2}$$

$$=16 - \frac{[f(17.81)-f(18.19)]/2x0.19}{[f(17.81) - 2f(18) + f(18.19)]/(0.19)^2} \quad ....1$$

At, **R=18, Total cost** calculated as in previous case is:

f = \$ 4243.87 2

At, **R=17.81, Minimum Reflux Ratio** is calculated from formula:

$$\mathbf{R_m = 1/(\alpha-1)\ [X_D/X_F - \alpha(1-X_D)/(1-X_F)]}$$

$$=1/.105\ [.95/.70 - 1.105\ (0.05/0.36]$$

$$=1/.105\ [1.357-0.184]$$

$$= 11.17$$

N_M, Minimum equilibrium stages

$$\mathbf{[(94-N_M)/95] = 0.75\ [1-\{R-R_m/R+1\}^{0.5668}]}$$

$$[(94-N_M)/95] = 0.75\ [1-\{17.81-11.17/17.81+1\}^{0.5668}]$$

$$N_M = 62.23$$

XB=Bottom light key mole fraction is calculated as

$$\mathbf{N_M = \ln\{[X_D/(1-X_D)].[(1-X_B)/X_B]\}/\ln\alpha}$$

$$=\ln\{[.95/.05].[(1-X_B)/X_B]\}/\ln 1.105$$

$$\mathbf{X_B = 0.0366}$$

B, Bottoms flow rate is calculated as

$$\mathbf{X_F F = X_D D + X_B B}$$

$$0.70\times1.2\times10^6 = 0.95D - X_B B$$

$$0.70\times1.2\times10^6 = 0.95(1.2\times10^6 - B) + 0.0366B$$

$$B=3.2844\times10^5$$

$$D=8.7155\times10^5$$

Therefore,

$$f(17.81) = (c_1 + c_2)\lambda(R+1)D + WX_B B + U(1-X_D)D$$

$$= (3\times10^6\times130\times18.81\times8.7155\times10^5) + 0.11\times0.0366\times3.2844\times10^5 - 0.08(1-0.95)\times8.7155\times10^5)$$

$$= \$\ 4229.7030 \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 3$$

Similarly

At, **R=18.91**, **Minimum Reflux Ratio** is calculated from formula:

$$R_m = 1/(\alpha-1)\ [X_D/X_F - \alpha(1-X_D)/(1-X_F)]$$

$$= 1/.105\ [.95/.70 - 1.105\ (0.05/0.36]$$

$$= 1/.105\ [1.357-0.184]$$

$$= 11.17$$

N_M, Minimum equilibrium stages

$$[(94-N_M)/95] = 0.75\ [1-\{R-R_m/R+1\}^{0.5668}]$$

$$[(94-N_M)/95] = 0.75\ [1-\{18.91-11.17/18.91+1\}^{0.5668}]$$

$$N_M = 63.04$$

XB=Bottom light key mole fraction is calculated as

$$N_M = \ln\{[X_D/(1-X_D)].[(1-X_B)/X_B]\}/\ln\alpha$$

$$= \ln\{[.95/.05].[(1-X_B)/X_B]\}/\ln 1.105$$

$$X_B = 0.0339$$

B, Bottoms flow rate is calculated as

$$X_F F = X_D D + X_B B$$

$$0.70\times1.2\times10^6 = 0.95D - X_B B$$

$$0.70\times1.2\times10^6 = 0.95(1.2\times10^6 - B) + 0.0339B$$

$$B = 3.2747\times10^5$$

$$D = 8.7252\times10^5$$

Therefore,

$$f(15.85) = (c_1 + c_2)\lambda(R+1)D + WX_BB + U(1-X_D)D$$

$$= (3\times10^6\times130\times19.91\times8.7252\times10^5) + 0.11\times0.0339\times3.2747\times10^5 - 0.08(1-0.95)\times8.7252\times10^5)$$

= $ 4261.08 .... **4**

Substituting all values of 2,3 and 4 in eqn 1,we get:

$$R^{k+1} = 18 - \frac{[4229.7030 - 4261.08]/2x(-0.19)}{[4229.7030 - 2x4243.87 + 4261.08]/(-0.19)^2}$$

= 17.02

Again, by same calculations at R = 17.02, our minimum total cost comes out to be **$ 4220.412**

Similarly. At various values of R iterations is done and optimum range of optimum reflux ratio is calculated:

Iteration	Calculated Ropt	Minimum Total cost, F
1	18	$ 4243.87
2	17.02	$ 4220.412
3	17.26	$ 4211.6173
4	17.58	$ 4210.5645

Optimum range for reflux ratio lies in the range (17.26 to 17.58)

SUCCESSIVE QUADRATIC ESTIMATION METHOD

We take the interval for optimum reflux ratio between 17 and 18.

Step 1:

Let x_1=17 and Δ=1. Thus, x_2=18

Calculating equilibrium stages, bottom fraction, bottom and top flow rate from the formulas

Minimum Reflux Ratio is calculated from formula:

$$R_m = 1/(\alpha-1)\ [X_D/X_F - \alpha(1-X_D)/(1-X_F)]$$

N_M, Minimum equilibrium stages

$$[(94-N_M)/95] = 0.75\ [1-\{R-R_m/R+1\}^{0.5668}]$$

XB=Bottom light key mole fraction is calculated as

$$N_M = \ln\{[X_D/(1-X_D)].[(1-X_B)/X_B]\}/\ln\alpha$$

B, Bottoms flow rate is calculated as

$$X_F F = X_D D + X_B B$$

R	N_m	x_B	B	D	f
17	60.3577	0.043855	331073.1489	868926.8511	$ 4221.2932
18	0.035	0.03521	327944.5871	872055.4129	$ 4243.87

Since, f(17) < f(18), therefore

$X_3 = X_1 - \Delta$ =17-1 = 16

f(16)= $ 4491.26

Step 4:

F_{min}=minimum ($4221.2932, $4243.87, $4491.26)

=$4221.2932

Corresponding X_{min}=17

Step 5:

We calculate the following parameters from the formula:

$$a_0 = f_1$$

$$a_1=(f_2- f_1)/(x_2-x_1)$$

$$a_2=[(f_3- f_1)/(x_3-x_1)- a_1]/(x_3-x_2)$$

therefore,

$$a_0 = 17$$

$$a_1=(4243.87-4221.2932)/(18-17)$$

$$= 22.5768$$

$$a_2=[(4491.26-4221.2932)/(16-17)- 17]/(16-18)$$

$$= 146.2718$$

Since, $a_2 > 0$,the estimated minimum is

$$X* = (X_1+X_2)/2 - a_1/2a_2$$

$$= (17+18)/2 – 22.5768/2*146.2718$$

$$= 17.42282$$

Calculating equilibrium stages, bottom fraction, bottom and top flow rate

At R= 17.42282

R	N_m	X_B	B	D	f
17.42282	61.36855	0.03981	329602.72	870397.275	$ 4215.61282

Step 6 :

Let us assume that |$ 4491.26 - $ 4215.61 | and |17.42282 - 16..00| are not small enough to terminate. Thus, we proceed to step 7.

Step 7:

We compare the values obtained at various values of reflux ratio

Reflux Ratio,R	Minimum Total cost,f
17	$ 4221.2932
17.42	$ 4215.6128
18	$ 4243.87

F_{min}=minimum ($4221.2932, $4215.6128, $ 4243.87)

=$ 4215.6128

Corresponding

X_{min}=17.42

We calculate the following parameters from the formula:

$$a_0 = f_1$$

$$a_1 = (f_2 - f_1)/(x_2 - x_1)$$

$$a_2 = [(f_3 - f_1)/(x_3 - x_1) - a_1]/(x_3 - x_2)$$

therefore,

$$a_0 = 17$$

$$a_1 = -13.5247$$

$$a_2 = 62.24$$

Since, $a_2 > 0$,the estimated minimum is

$$X* = (X_1 + X_2)/2 - a_1/2a_2$$

$$= 17.6086$$

Calculating equilibrium stages, bottom fraction, bottom and top flow rate

At R= 17.6086

R	N_m	X_B	B	D	f
17.6086	61.7921	0.03822	329029.9416	870970.5522	$ 4220.6368

Let us assume that |$ 4220.6368 - $ 4215.61 | and |17.6086-17.42| are not small enough to terminate. Thus, we proceed to next step.

Compare the values obtained at various values of reflux ratio

Reflux Ratio,R	Minimum Total cost,f
17	$ 4221.2932
17.42	$ 4215.6128
17.60	$ 4220.6368

F_{min} = minimum ($4221.2932, $4215.6128, $ 4220.6368)

= $ 4215.6128

Corresponding

X_{min} = 17.42

We calculate the following parameters from the formula:

$$a_0 = f_1$$

$$a_1 = (f_2 - f_1)/(x_2 - x_1)$$

$$a_2 = [(f_3 - f_1)/(x_3 - x_1) - a_1]/(x_3 - x_2)$$

therefore,

$$a_0 = 17$$

$$a_1 = -13.5247$$

$$a_2 = 69.09583$$

Since, $a_2 > 0$,the estimated minimum is

$$X* = (X_1+X_2)/2 - a_1/2a_2$$
$$= 17.5979$$

Calculating equilibrium stages, bottom fraction, bottom and top flow rate

At R= 17.6086

R	N_m	X_B	B	D	f
17.5979	61.7681	0.03831	329061.2712	870938.7288	$ 4220.4149

Optimum range for reflux ratio lies in the range (17.42 to 17.60)

ANALYSIS OF OPTIMIZATION TECHNIQUES

Optimization Technique	Calculated Ropt interval
Quadratic Interpolation	17.57 to 17.48
Fibonacci Search Method	17.52 to 17.60
Golden Section Method	17.52 to 17.23
Finite Difference Approximation Method	17.26 to 17.58
Successive Quadratic Estimation Method	17.42 to 17.60

These are the calculated values Of Optimum Reflux Ratio via different optimization techniques for a single variable distillation problem. On evaluating these results the optimum range of reflux ratio comes out to be between **17.23 to 17.60.**

So, Distillation Column operated at this optimum reflux ratio interval would require minimum operating cost.

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