A Combined Penalty Function and Outer-Approximation Method for MINLP Optimization - Applications to Distillation Column Design

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A COMBINED PENALTY FUNCTION AND OUTER-APPROXIMATION METHOD FOR MINLP OPTIMIZATION - APPLICATIONS TO DISTILLATION COLUMN DESIGN

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ABSTRACT

An improved outer-approximation algorithm for MINLP optimization has been recently proposed which is aimed at the solution of problems where convexity conditions may not hold. This algorithm has been implemented in the computer package DICOPT++. Computational experience is presented on a set of SO test problems. Included are problems for optimum feed tray location and number of plates for distillation columns whose models are described in detail. The results show that the proposed algorithm can effectively handle these design problems.

Introduction

There has been recently an increased interest in the development and application of nonlinear optimization algorithms that can handle both continuous and integer variables, especially of the 0-1 type (see Grossmann, 1989). These problems, which are commonly referred to as mixed-integer nonlinear programming (MINLP) problems, have many applications in engineering design, planning, scheduling and marketing. Often the corresponding MINLP models exhibit special structures (e.g. graphs, networks, separable functions) that can be effectively exploited for developing specialized solution procedures. However, it is also very often the case, particularly in engineering design, that nonlinearities in the continuous variables do not exhibit any special form since they result from complex engineering models. Thus, there is clearly a strong motivation to develop MINLP algorithms that that are not overly restrictive in the assumptions of the form and properties of the functions that are involved.

Among the general purpose algorithms for MINLP, we can cite branch and bound (Beale,1977; Gupta, 1980), Generalized Benders Decomposition, GBD, (Benders, 1962; Geoffrion, 1972), the Outer-Approximation/Equality-Relaxation Method, OA/ER (Duran and Grossmann, 1986; Kocis and Grossmann, 1987), and the Feasibility Technique (Murtagh and Mawengkang, 1986; Mawengkang, 1988). The branch and bound method has the drawback that it can require the solution of a large number of NLP subproblems in the search tree, unless the NLP relaxation is very tight. GBD has the advantage that one can exploit more readily special structures in the NLP subproblems, but has the drawback that it may require a significant number of major iterations where NLP subproblems and MILP master problems must be solved successively. The OA/ER algorithm has the advantage that it typically requires only few major iterations, but has the drawback that the size of its MILP master problem is considerably larger than in GBD. Finally, the Feasibility Technique requires the least computational expense since it is based on the idea of finding a feasible integer point that has the smallest local degradation with respect to the relaxed NLP solution. However, it has the drawback that it does not guarantee optimality. Other related procedures for MINLP have been reported by Yuan et al. (1987) who extended the CA algorithm for convex nonlinear 0-1 variables, and by Floudas et al. (1988) who applied partitioning of variables in GBD to induce convex NLP subproblems.

The branch and bound, GBD and OA/ER algorithms require that some form of convexity assumption be satisfied in order to guarantee that they can find the global optimum of the MINLP. On the other hand, the OA/ER algorithm, which tends to be the most efficient method when the NLP subproblems are expensive or difficult to solve, is the most stringent in terms of convexity requirements. In particular, the OA/ER algorithm relies on assumptions of convexity of the functions f and g and also the quasi-convexity (resp. quasi-concavity) of nonlinear equality constraints, h (Kocis and Grossmann, 1987). When these conditions are met, the algorithm will determine the global optimum. Otherwise, the linearizations of the master problem can cut into the feasible region of candidate integer points which may result in sub-optimal solutions (Kocis and Grossmann, 1988).

to overcome this problem, a two-phase strategy was proposed by Kocis and Grossmann (1988) where in the first phase the OA/ER was applied. In the second phase, linearizations of nonconvex functions are identified by local and global tests so as to relax the master problem. This scheme proved successful in locating the global optimum in abou'. 80 % of a set of test problems. The implementation of the local and global tests is, however, somewhat difficult and they are not guaranteed to identify all the nonconvexities.

Motivated by observations with our experience in solving MINLP problems, it is the purpose of this paper to develop a new variant of the OA/ER algorithm which does not require the explicit identification of nonconvexities. As will be shown, this can be accomplished with a new MILP master problem that incorporates an augmented penalty function for the violation of linearizations of the nonlinear functions. Furthermore, the proposed algorithm (AP/OA/ER) has the important feature of not requiring the specification of an initial set of 0-1 variables since the algorithm starts with the solution of the relaxed NLP problem. Also, if appropriate convexity conditions hold, the AP/OA/ER algorithm has embedded the OA/ER algorithm. Numerical results are reported for a set of 20 test problems which include distillation column design problems. Although convergence to the global optimum cannot be guaranteed, the numerical results suggest that the proposed algorithm is not only computationally efficient, but also very robust for finding the global optimum solution.

Outline of the AP/OA/ER Algorithm

We consider here the MINLP (mixed-integer nonlinear program) of the form:

$$
\begin{aligned}
\text{Min}\quad & z := c^T y + f(x) \\
\text{s.t.}\quad & Ay + h(x) = 0 \\
& By + g(x) \le 0 \\
& Cy + Dx \le 0 \\
& x \in X = \{ x \in R^n : x^L \le x \le x^U \} \\
& y \in Y = \{0,1\}^m
\end{aligned}
\qquad \text{(P)}
$$

Here, x denotes the vector of continuous variables and y denotes the vector of binary variables corresponding to logical decisions (e.g. the existence of units). The functions f, g and h are defined over appropriate domains and have continuous partial derivatives. The matrices A, B, C and D have compatible dimensions. For each fixed binary vector y^K, we assume that the corresponding NLP (nonlinear program):

$$
\begin{aligned}
\text{Min}\quad & z := c^T y^K + f(x) \\
\text{s.t.}\quad & Ay^K + h(x) = 0 \\
& By^K + g(x) \le 0 \\
& Cy^K + Dx \le 0 \\
& x \in X = \{ x \in R^n : x^L \le x \le x^U \}
\end{aligned}
\qquad [P(y^K)]
$$

satisfies any of the constraint qualifications (Mangasarian, 1969) so that the solution vector is a KKT (Karush-Kuhn-Tucker) point.

The algorithm that we propose involves the following steps :

1. Solve the NLP relaxation of (P) with $y \in Y_r = \{ y \in R^m, 0 \le y \le e\}$, where e is the unity vector, to obtain the KKT point (x^0, y^0). If y^0 is integer, stop. Otherwise, go to step 2

2. Find an integer point y^1 with an MILP master problem that features an augmented penalty function to find the minimum over the convex hull determined by the half-spaces at the KKT point (x^0, y^0).

3. Solve the NLP $[P(y^1)]$ at y^1 to obtain the KKT point (x^1, y^1).

4. Find an integer point y^2 with the MILP master program that corresponds to the minimization over the intersection of the convex hulls determined by the half-spaces of the KKT points at y^0 and y^1.

5. Repeat steps 3 and 4 until there is an increase in the value of the NLP objective function. (Repeating step 4 means augmenting the set over which the minimization is performed with additional linearizations - i.e , half-spaces - at the new KKT point).

The above algorithm is in the spirit of earlier algorithms proposed by Duran and Grossmann (1986) and Kocis and Grossmann (1987), but there are some important differences.

In both the previously cited algorithms it was assumed that an initial integer point y^1 was supplied so that steps 1 and 2 were absent. Also, the termination criterion used in these algorithms, viz:

5'. Repeat steps 3 and 4 until the objective function of the MILP was greater than or equal to the lowest value of the objective function among the previously solved NLP minima at fixed values of the integer vector y.

is different from the one proposed here.

While the OA/ER algorithm has proved to be quite successful in solving a variety of problems (Kocis and Grossmann, 1989a), its major limitation has been that it relies on assumptions of convexity of the functions as discussed previously.

For the algorithm proposed here, no assumptions concerning convexity of the functions in the MINLP are made. The main idea relies on the definition of a new MILP master problem the uses a linear approximation to an exact penalty function (Zhang, Kim and Lasdon, 1985), and therefore allows violations in the linearizations of the nonlinear functions. The algorithm is also based on extensive computational experience that has confirmed the desirability of starting with the solution of the relaxed NLP and the use of termination criterion 5 instead of 5'. The algorithm embeds the OA/ER algorithm in the case the assumptions concerning convexity of the latter are fulfilled. Although the proposed method has no theoretical guarantee of finding the global optimum, it was able to locate global optima in virtually all test problems despite the presence of nonconvexities in the MINLP problem. Our experience includes solving some challenging problems in distillation column design

The following sections describe the three major items of the proposed algorithm: starting point, MILP master problem and the termination criterion. Implementation of the algorithm is discussed and numerical results are also presented.

Starting point

Both Generalized Benders Decomposition (Geoffrion, 1972) and the OA/ER algorithm (Duran and Grossmann, 1986; Kocis and Grossmann, 1987) assume that an initial integer value y^1 is supplied. On the other hand, the branch and bound method (Gupta, 1980) and the feasibility technique of Mawengkang (1988) start the calculations by solving the relaxed MINLP problem. This means that :

1. If the relaxed MINLP provides an integer solution, further calculations are not necessary.

2. The user need not provide an initial integer vector.

It is also reasonable to expect that the solution of the relaxed MINLP will provide very good estimates of the continuous variables and, hence, the linear approximation to the MINLP at this point will often be of good quality.

Thus, we begin computations by solving the relaxed MINLP:

$$
\begin{aligned}
\text{Min } \; & z := c^T y + f(x) \\
\text{s.t. } \; & Ay + h(x) = 0 \\
& By + g(x) \le 0 \\
& Cy + Dx \le 0 \\
& x \in X = \{x \in R^n : x^L \le x \le x^u\} \\
& y \in Y_r = \{y \in R^m, 0 \le y \le e\}
\end{aligned}
\qquad (1)
$$

The solution to this problem may be obtained by any NLP solver such as MINOS, SQP, etc .

Let the solution be (x^0, y^0). If y^0 is integer, we stop. Otherwise, we proceed for the search of an integer solution. Note that if problem (1) is infeasible or unbounded, the same is true of the original problem (P). As may be expected, the solution of the relaxed MINLP generally takes longer time to solve than the time required for the case of a NLP with fixed binary vector. Also, it should be noted that the NLP solution in (1) is only guaranteed to correspond to a global optimum if appropriate convexity conditions are satisfied (see Bazaraa and Shetty, 1979).

Master Problem

If y^0 is not integer, we wish to find an integer vector y^1, whose corresponding NLP solution is a likely candidate to the global optimum of the program (P). For the case where the objective function is convex and the MINLP has only inequality constraints which are also convex, the "best" integer point lies in the convex hull determined by the half-spaces at (x^0, y^0) (see Duran and Grossmann, 1986). The motivation is to find an estimate of the KKT point but with integer coordinates.

That is, given

$$\begin{aligned} \text{Min } & z^0 := c^T y^0 + \alpha \\ \text{s.t. } & f(x) - \alpha \le 0 \\ & Ay^0 + h(x) = 0 \\ & By^0 + g(x) \le 0 \\ & Cy^0 + Dx \le 0 \\ & x \in X = \{x \in R^n : x^L \le x \le x^U\} \end{aligned} \qquad (2)$$

the convex hull $C(x,\alpha,y)$ determined by the half-spaces of the KKT point of (2) at y^0 is given by

$$\begin{aligned} & f(x^0) + \nabla f(x^0)^T (x - x^0) - \alpha \le 0 \\ & T^0 [\, Ay^0 + h(x^0) + \nabla h(x^0)^T (x - x^0) \le 0 \\ & B y^0 + g(x^0) + \nabla g(x^0)^T (x - x^0) \le 0 \\ & Cy^0 + Dx \le 0 \\ & x \in X = \{ x \in R^n : x^L \le x \le x^U \} \end{aligned} \qquad (3)$$

where T^0 is the relaxation matrix of the equations $a_j^T y + h_j(x) = 0$, given by

$T^0 = \{t_{ii}^0\}$, $t_{ii}^0 = \text{sign}\{\lambda_i^0\}$, with λ_i^0 being the Lagrange multiplier of equation i.

The following proposition can then be established:

Proposition 1: If (x°, a) is a KKT point of (2) at y°, then (x°, a) is a KKT point of the problem

$$\text{Min} \quad z := c^T y° + a \qquad (4)$$

with (x°, a) satisfying (3).

Proof: The KKT conditions of (2) are given by :

$$1 - a = 0$$

$$aVf (x°) + X fciVhj(x°) + X W^9i (*°) + X v(di + p^u - \rho^L = 0$$

i i i

$$Ay^0 + h (xO) = 0$$
$$By^0 + g (x°) \leq 0$$
$$Cy° + D x° \leq 0$$
$$x^L \leq x \leq x^u$$

$$[f(x°)-a]a = 0, \qquad a \geq 0$$
$$[b_j^T y^0 + g_j(x^0)]\ \mu_j = 0, \qquad \mu_j \geq 0$$
$$[c_j^T y^0 + d_j x^0]\ v_j = 0, \qquad V J > 0$$
$$[- x_i^0 + x_i^L \ \ Jp|- = O. \qquad p| -> 0$$
$$[\ x_i^U - x_i^0\ ]\ \rho_i^U = 0, \qquad \rho_i^U \geq 0$$

These conditions are also identical for problem (4) at (x°, a) by setting

$$ajy° + hj(x^0) + Vhj(x°)^T(x - x°) \leq 0 \qquad \text{if} \quad Xj > 0$$
$$ajy° + hpfi) + Vhj(xO)^T(x - x°) \ \wedge 0 \qquad \text{if} \quad Xj < 0$$

Q.E.D.

If f and g are convex and tjjhj is quasiconvex (see Bazaraa and Shetty, 1979), then the integer vector y^1 that has the "best" potential for yielding the lowest value for the objective function is given by the solution of the following MILP (see inequalities (3)) :

$$z[= \text{Min} \quad c^T y + a \qquad (5)$$

$$\text{s.t} \quad (x,a,y) \in C(x,a,y) \cap \{0,1\}^m$$

Furthermore, z_L^1 provides a valid lower bound to the solution of problem (P) (see Duran and Grossmann, 1986).

In the general case, where the assumptions concerning the convexity of f, g and h are not met, we cannot assert that problem (5) will provide a valid lower bound nor that it has a feasible integer solution even when problem (P) has. To circumvent this problem, we consider the following MILP with an augmented penalty function :

$$z_A^0 := \text{Min} \quad c^T y + \alpha + w^0 s^0 + \sum_i w_i^p p_i + \sum_j w_j^q q_j$$

$$\begin{aligned} \text{s.t.} \quad & f(x^0) + \nabla f(x^0)^T (x - x^0) - \alpha \le s^0 \\ & T^0 [\, Ay + h(x^0) + \nabla h(x^0)^T (x - x^0) \le p \\ & By + g(x^0) + \nabla g(x^0)^T (x - x^0) \le q \\ & Cy + Dx \le 0 \\ & x \in X = \{ x \in R^n : x^L \le x \le x^U \} \\ & y \in \{0,1\}^m, \; s^0 \ge 0, \; p \ge 0, \; q \ge 0 \end{aligned} \tag{6}$$

where $w^0 > |\sigma|$, $w_i^p > |\lambda_i|$, $w_j^q > |\mu_j|$ are the weights on the slack variables.

Using a similar argument as before, the following proposition can then be easily proved:

<u>Proposition 2:</u> If (x^0, α) is a KKT point of (2), then it is also a KKT point of (6) at y^0.

Thus, problem (6) can be used to formulate a master problem which has the flexibilty of violating inequalities should this prove necessary when searching for a new integer vector y^1. We also note that in case the convexity assumptions are met and the weights are sufficiently large, problem (6) reduces to problem (5) Qualitatively, the convex hull described by (6) is an expansion of the convex hull determined by (3).

Assuming that the integer vector y^1 has been found and its corresponding NLP solved, we need to find a new integer vector y^2 where there is a further decrease in the objective function. Since an improved representation of the MILP master problem is required, we will consider the intersection of half-spaces at x^0 and x^1 following a similar reasoning as in the OA/ER algorithm, but the master problem will be defined with an augmented penalty function as in (6). More generally, if x^k, $k = 0,1,...K$, with x^0 the solution of the relaxed

MINLP and x^k, k= 1,...K, are the NLP solutions found at the previously determined integer vectors, the MILP for determining the integer vector y^{K+1} is :

$$z_A^K := \text{Min } c^T y + \alpha + \sum_k w_k^0 s_k^0 + \sum_{ik} w_{ik}^p p_{ik} + \sum_{ik} w_{ik}^q q_{ik}$$

subject to :

$$\left.\begin{aligned} f(x^k) + \nabla f(x^k)^T(x - x^k) - \alpha &\le s_k^0 \\ T_k^0 [\, Ay + h(x^k) + \nabla h(x^k)^T(x - x^k) \,] &\le p_k \\ By + g(x^k) + \nabla g(x^k)^T (x - x^k) &\le q_k \end{aligned}\right\} \quad k = 0,1,..K \qquad (7)$$

$$Cy + Dx \le 0$$

$$\sum_{i \in B_k} y_{i,k} - \sum_{i \in N_k} y_{i,k} \le |B_k| - 1 \qquad k = 1,\dots K$$

$$x \in X = \{ x \in R^n : x^L \le x \le x^U \}, \quad y \in \{0,1\}^m$$

$$s_k^0, p_{i,k}, q_{i,k} \ge 0 , \quad k = 0,1,\dots K$$

In the MILP (7) above, integer cuts have been introduced to eliminate the previously determined integer vectors $y^1, y^2, \dots, y^K$ from further consideration. Note also that if convexity conditions hold, then for sufficiently large weights the above MILP reduces to the master problem of the OA/ER algorithm by Kocis and Grossmann (1987).

Infeasible NLP Subproblems

In the proposed algorithm it is possible that the MILP master problem in (7) may predict an integer vector y^{K+1} for which there is no feasible solution in the corresponding NLP subproblem. In this case there are two possible schemes to handle this problem. One is to simply disregard the associated infeasible continuous point x^{K+1} for the linearization, and just introduce an integer cut for y^{K+1} for the next master problem. The other option is to also add to the master problem the linearization at the infeasible continuous point. However, since in this case information on the Lagrange multipliers is required to relax the equations, it is desirable that the equations be satisfied at the infeasible NLP subproblem. This can be accomplished by reformulating the MINLP problem (P) as (Kocis and Grossmann, 1987):

$$
\begin{aligned}
\text{Min} \quad & z := c^T y + f(x) + r|u \\
\text{s.t.} \quad & Ay + h(x) = 0 \\
& By + g(x) \leq u \\
& Cy + Dx \leq u \\
& x \in X = \{x \in R^n : x^L \leq x \leq x^u\} \\
& u \geq 0, u \in R^1 \\
& y \in \{0,1\}^m
\end{aligned} \qquad (8)
$$

where u is a scalar variable and ^ is a large positive constant. In this way the idea in (8) is that if the NLP subproblem has a feasible solution, the variable u is driven to a zero value. If it is infeasible for the given integer vector, it will determine a continuous point that satisfies the equations and minimizes the violation of the inequalities. It is clear that care must be excercised in this reformulation to ensure that these properties in fact hold.

Termination Criterion

The MILP in (7) will not, in general, produce valid lower bounds for the objective function of problem (P) unlike the convex case (Duran and Grossmann, 1986; Kocis and Grossmann, 1987). Therefore, we resort to termination based on the progress of the objective function of the NLP sub-problems. For the case when no integer solution is found in the NLP relaxation problem, the search is stopped when at iteration $k \geq 2$, we have $z(y^k) \geq z(y^{k-1})$ assuming the corresponding NLP subproblems are feasible. When this is not the case, the termination criterion is applied between two successive feasible NLP subproblems. Interestingly, for the convex case, we have observed that if we use this criterion for all the test problems we have examined, the global solution is correctly found in all cases. Hence, this criterion has been adopted in this work. Note that if an integer solution y^0 is not obtained in the relaxed NLP, the proposed algorithm would examine at least two additional NLP sub-problems with fixed 0-1 variables.

Finally, it should also be noted that for the implementation it would always be possible to use a termination criterion based on the lower bound of the MILP master problem for those cases when it is known a-priori that the convexity conditions are satisfied.

Summary of Algorithm

The main steps in the proposed AP/OA/ER algorithm are as follows:

Step 1. Solve the relaxed NLP problem in (1) to determine a KKT point (x°, y°). If y° is integer, the solution is found, stop. Otherwise, set K=0, z^{OLD} « +©^ and go to step 2.

Step 2. Set up the MILP master problem in (7), and solve to find the integer vector y^{K+1}.

Step 3. Solve the NLP subproblem $[P(y^{K+1})]$ to determine the KKT point (x^{K+1}, y^{K+1}) with objective value z^{K+1}. If the NLP is infeasible set FLAG-0. If the NLP is feasible, set $z^{NEW} = z^{K+1}$, FLAG=1.

Step 4. (a)If FLAG-1, determine if $z^{NEW} > z^{OLD}$; if satisfied, stop. The optimal solution is z^{OLD}. Otherwise, set $z^{OLD} \leftarrow z^{NEW}$, set K-K+1 and return to step 2.

(b) If FLAG-0, set K-K+1 and return to step 2.

It should be noted that the above algorithm will terminate in one iteration if an integer solution is found in step 1, or else it will terminate after 3 or more iterations when the termination condition in step 4 (a) is satisfied. Note that in the latter case, N iterations implies the solution of N NLP subproblems, and N-1 MILP subproblems. Also, as was mentioned previously, if convexity of the MINLP can be established a-priori, the termination criterion in step 4 can be replaced by the use of the lower bound predicted by the MILP master problem as in the OA/ER algorithm.

Computer Implementation

The proposed AP/OA/ER algorithm has been implemented as the program DICOPT++ in the GAMS system (Brooke et al, 1988) for both IBM/CMS and VAX/VMS systems. The NLP solver used is MINOS (Murtagh and Saunders, 1985). On IBM, the MILP step is executed by MPSX/370 (IBM, 1979), and on VAX by ZOOM (Marsten, 1986) or SCICONIC (SCICONIC, 1986). The authors may be contacted about the availability of DICOPT++.

As for some of the implementation details, the weights in the penalty function for the master problem in (7) have been set to 1,000 times the absolute magnitude of the Karush-Kuhn-Tucker multipliers. Also, as indicated previously, for the case of infeasible NLP subproblems, only the corresponding integer cut to that NLP is added to the master problem in step 2. Addition of linearizations of infeasible NLP problems are only added to the master problem if the original MINLP is reformulated with a slack variable for inequalities with a large penalty as in (8). Finally, for the case when there is a very small difference between two successive NLP solutions, no new linearizations are added to the master problem for the second NLP since they are commonly almost identical. The default value of $1x10^{-4}$ for the relative tolerance between successive NLP's has shown to yield satisfactory results.

Computational Results

The AP/OA/ER algorithm in DICOPT++ has been tested on the set of 20 MINLP problems that are shown in Table 1. Note that in terms of size, these problems involve up to 60 0-1 variables, 709 continuous variables and 719 constraints.

Following is a brief description of the test problems. LAZIMY is a bilinear MINLP reported by Lazimy (1982). HW74 is a small convex planning problem for the selection of 3 processes by Kocis and Grossmann (1987). NONCON is a small nonconvex MINLP and CAPITAL is a quadratic capital budgeting problem reported in Kocis and Grossmann (1988). YUAN is a convex MINLP problem by Yuan et al (1987). Since the problems LAZIMY, CAPITAL and YUAN exhibit nonlinearities in the 0-1 variables, these problems were reformulated with additional continuous variables in order to have linear 0-1 variables, (see Kocis and Grossmann, 1989a).

Problem FLEX is the MINLP formulation for the flexibility analysis of a heat exchanger network with uncertain flowrate by Grossmann and Floudas (1987). REL1 is a nonconvex reliability design problem considered by Kocis and Grossmann (1989a). Problems EX3 and EX4 are taken from the work of Duran and Grossmann (1986). The former corresponds to a small synthesis problem, and the latter to an optimal product positioning problem. EX4 was in fact the only problem that was reformulated as in (8) since it has the tendency of producing many feasible solutions. The three BATCH problems correspond to convexified formulations for the design of multiproduct batch plants described in Kocis and Grossmann (1988), while TABATCH corresponds to a batch design with tasks assignments to be determined.

The last set of 7 MINLP problems correspond to various types of process applications. Problem UTILRED corresponds to the retrofit of a utility plant where the replacement of turbines by electric motors is considered (Kocis and Grossmann, 1989a). TFYHEN corresponds to the retrofit of a small heat exchanger network that involves the aftercooler of a compressor and the reboiler of a column (Yee and Grossmann, 1988). EX5FEED, UNI5FEED, EX5T11 and EX5T12 are distillation column design problems for optimal feed tray location and number of trays. The formulation of these problems is described in detail in the next section. Finally, HDASS corresponds to the MINLP model for the synthesis of the hydro-dealkylation of toluene process developed by Kocis and Grossmann (1989b).

The results in Table 1 were obtained on the IBM-3090 computer at the Cornell Theory Center. MINOS 5.2 was used as the NLP solver and MPSX 1.7 as the MILP solver. As can be seen in Table 1, the computational requirements with the AP/OA/ER are quite modest. Note that the solution of 4 problems, NONCON, LAZIMY, EX5FEED and UNI5FEED was achieved in one single major iteration since the integer solution was found in the relaxed NLP. All the other problems required only between 3 and 5 major iterations, which implied solving between 3NLP/2MILP and 5NLP/4MILP problems, respectively.

Table 2 shows the integrality gap between the relaxed NLP and the optimal integer NLP solution. As can be seen, this gap is quite significant in a number of problems (FLEX, CAPITAL, HW74, EX3, EX4, TFYHEN). Also shown in this table is the objective value of the MILP master problem at the last iteration. For the case of convex problems these correspond to rigorous lower bounds for integer solutions other than the ones examined previously in the iterations. Note that in the convex problems HW74, YUAN, EX3, EX4, rigorous termination is achieved with the lower bound since it exceeds the optimal integer NLP solution. On the other hand, in the three BATCH problems which are convex, the lower bound lies below the integer NLP solution (in the case of BATCH the difference is very small). Nevertheless, in the three cases the global optimum was identified . As for the rest of the problems which are nonconvex, the MILP solution at the last iteration exceeded the optimal integer NLP, except for the case of problem REL1.

Perhaps, one of the more significant facts from the results shown in Tables 1 and 2 is that the global optimum was found in all cases despite the fact that 11 out of the 20 problems are in fact nonconvex . Thus, although the proposed algorithm has no guarantee of finding the global solution, it is clear that the AP/OA/ER algorithm has shown a remarkable degree of robustness. We feel that this is mainly due to a combination of two factors. First the initialization with the relaxed NLP which seems to provide very good linearization points. Secondly, the new MILP master problem which allows if needed the violation of any function linearization.

Distillation Column Design Problems

In this section the detailed description of the MINLP models EX5FEED, UNI5FEED, EX5T11 and EX5T12 will be presented. These problems deal with the optimization of feed tray location and number of trays using rigorous plate by plate models.

Optimum Feed Plate Location

Consider a distillation column (see Fig.1) with N stages including the condenser and the reboiler (We consider the total condenser case; the other cases are dealt with similarly). Let the trays be numbered bottom upwards so that the reboiler is the first tray and the condenser is the last (N th) tray.

Let I = { 1,2,...N } denote the set of trays and let R - {1} , C « { N }$_f$ COL - { 2,3, ...N-1 } denote the subsets corresponding to the trays in the reboiler, the condenser and those within the column respectively.

Let c be the number of components in the feed and let F, T_{fy} Pf_y z/, h_{fy} denote respectively, the molar flowrate,temperature,pressure, the vector of mole-fractions(with components z/y, j = 1,2,...c) and the molar specific enthalpy of the feed.

The pressure prevailing on tray i is denoted by *Pi.* Let *Preb* = Pi , *Phot* = P2, *Ptop* = PAM, *Peon* = *PN* be given. We have *Pi^Pi^* ••^ *PNI* ^ *PN* $_t$ and for simplicity we assume *Pf^* p_{bot} .

Let *Li M* ,/zf , and ft;ˆdenote the molar flowrate, the vector of mole-fractions, the molar specific enthalpy and the fugacity of component j, respectively of the liquid leaving tray i . Similarly, let V,- ,y* A^V and ***fij*** denote the corresponding quantities of the vapor leaving tray i. Denoting the temperature of tray i by 7,; $_f$ we have

$$f^L_{ij}(T_i\ ,\ p_i, x_{i1}, x_{i2}, \ldots x_{ic})$$

$$f^V_{ij} = f^V_{ij}(T_i\ ,\ p_i, y_{i1}, y_{i2}, \ldots y_{ic}) \qquad (9)$$

$$p_i, x_{i1}, x_{i2}, \ldots x_{ic})$$

hj = hfiTi, Pi₉yn₉yi2,...yi$_C$)

where the functions on the right hand sides depend on the thermodynamic model used.

Pi and/>2 will denote the top and bottom product rates, respectively.

The subset of (contiguous) candidate tray locations for the feed are specified by the index set LOC, where LOC **c** COL<= I. Let z; , i € LOC , denote the binary variable associated with the selection of i as the feed tray; i,e., z_i = 1 iff i is the feed tray. Let F_{it} i e LOC denote the amount of feed entering tray i.

The modelling equations are then as follows:

(a) phase equilibrium : $f_{ij}^{L} = f_{ij}^{V}$ j = l.—c , i e / (^ 0)

(b) phase equilibrium error : 2, *(l - 2* yi/ = 0 / € / (11)

(c) component material balances :

$V_{i-1} y_{i-1,j} - (L_i + P_i) x_{ij} = 0$ j = l,...c, / € C

$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} = 0$ j = l,...c , /€ COL-LOC

$L_i x_{ij} + V_i y_{ij} - L_{i+1} x_{i+1,j} - V_{i-1} y_{i-1,j} - F_i z_{fj} = 0$ j = L - C , i6 LOC (12)

$V_i y_{ij} + P_i x_{ij} - L_{i+1} x_{i+1,j} = 0$;˙ = l,...c,/€ R

(d) enthalpy balances :

$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V - F_i h_f = 0$ /€ LOC

$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h_{i-1}^V = 0$ i6 COL - LOC (13)

(e) constraints on feed location :

$$\sum_{i \in LOC} z_i = 1$$

(14)

i s LOC

$F_i - F z_i \leq 0$, / € LOC

.The last constraint expresses the fact that if / e LOC is selected as the feed tray, then the amount of feed entering other candidate locations is zero. In addition, there may be constraints on purity, recovery, reflux ratio.etc. The MINLP problem, then, is to minimize (or maximize) a given objective function subject to the equality and inequality constraints (9) to (14).

The data for the test problem EX5FEED, which involves 10 candidate trays for the separation of benzene and toluene, are given in Table 3. The optimal solution is given by:

Obj. function	«	20.823
r	=	0.9324
Pi	-	67.44
Pi	=	32.56
feed plate	-	tray no. 10

The solution was found in the first step (relaxed NLP) . The CPU time required was 5.56 seconds (IBM 3090) .

The data for problem UNI5FEED are given in Table 4. This problem has been adapted from Naka et al. (1979). The form of the objective function is due to Kumar and Lucia (1988). As pointed out in Vasantharajan et al. (1989), the GAMS modelling system allows the problem to be solved in a completely equation-based manner.

The optimal solution for this problem is given by:

Objective function	-	-79.90
Px	=	9.11
Pi	=	90.89
reflux ratio	=	16.59
feed plate	**=**	**tray no. 9**
purity of acetone in top vapor product	=	0.913

The solution was found in the first step (relaxed NLP). The CPU time required was 66.8 seconds (IBM 3090).

Optimization of number of trays

It is assumed that reasonable upper bounds are known on the number of trays required in the rectification and stripping sections. (Rough estimates may be obtained, for example, using the Gilliland correlation). If lower bounds on the number of trays are also known, they may be used to speedup the solution as will be seen below.

We consider the case of a column with a single feed and a total condenser(see Fig. 2). Modifications required for other cases are straightforward.

As before, let I = { 1,2,...N } denote the set of all possible trays and let R = **(1},C** = {N} and COL = {2,...,N-1 }. Let FLOC - {//} denote the set consisting of the feed tray location and let

AF = { *i: if<i<N* } = the set of trays above the feed tray (excluding the condenser)

BF = { *i*: 1 < / < *if* } = the set of trays below the feed tray (excluding the reboiler)

Note that COL = $F\,LOC \cup AF \cup BF$. The location i_f is to be fixed based on the estimates of the number of trays in the stripping and rectifying sections.

The amount of reflux entering tray i will be denoted by ref_i, $i \in AF$ and let bu_i , $i \in BF$ denote the amount of reboiled vapor (boil-up) entering tray i .

Let z_i , $i \in COL$ denote the binary variable indicating whether or not tray i is required to achieve the desired objective. For ease and uniformity in writing many equations and inequalities, we will introduce two additional binary variables z_1 and z_N , but will fix them at zero, i.e, $z_1 = z_N = 0$. For the same reason, the continuous variables L_N and V_1 are set to zero.

The idea is to 'disable' all trays above the tray on which the reflux enters and all trays below the tray on which the reboiled vapour enters. That is, if L is the tray on which the reflux enters , we ensure that no heat or mass transfer takes place on trays L+1,... N-1. We do this by ensuring that: (a) no liquid leaves the trays L+1,...N-1; (b) the temperatures and pressures of the vapour leaving trays L+1,...N-1 are the same as that leaving tray L. Analogous reasoning applies for the stripping section.

In practical terms, item (a) takes effect as follows. Nonlinear optimization programs require that bounds on variables be specified. One sets the lower bound on all flowrates at zero and any reasonable value for the upper bound .

The notation is as in the previous section. We assume that the values of p_{reb} ,p_{bot} ,p_{top} , and p_{con} are given, although one may treat them as quantities to be determined, if desired. (One may, of course, simplify matters by assuming that they are all equal to the same value --- this may be quite adequate in most cases). As before, for simplicity, we assume that $p_f \geq p_{bot}$.

The modelling equations are as follows:

(a) phase equilibrium : $f_{ij}^L = f_{ij}^V \qquad j = 1,...c \;, i \in I$ (15)

(b) phase equilbrium error : $\sum_j x_{ij} - \sum_j y_{ij} = 0 \qquad i \in I$ (16)

(c) reflux ratio : $\sum_{i \in AF} ref_i - r\, P_1 = 0$ (17)

(d) elimination of variables introduced for simplification :

$$L_N = V_1 = 0$$

$$z_1 = z_N = 0 \qquad (18)$$

(e) component material balances : (for j = 1,... c)

$$(\sum_i refi + Pi)\, Xij - Vi._{xyi\cdot X}j = 0 \qquad / \in C$$

$$L_i xij + VMJ - L_{i+1}x_{MJ} - Vi.iyi.ij - refi\, x_{Nj} = 0 \qquad i \in AF$$

$$L_i x_{ij} + Vyj - L^{\wedge}iX^{\wedge}u - Vuyuj - Fzjj = 0 \qquad i \in FLOC \qquad (19)$$

$$LiKij + Vjyij - L_M x_{i+}ij - Vi.tfi.ij - bui\, y\backslash j = 0 \qquad i \in BF$$

$$U Xij + (\sum_i fcu,)\, y;y - L_M\, x_{M\%j} = 0 \qquad i \in R$$

(f) enthalpy balances :

$$L_i t + V f - L^{\wedge}hlx - V^{\wedge}hl, - ref^{\wedge\wedge}O \quad i \in AF$$

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-1} h^V_M - Fh_f = 0 \qquad /e\ FLOC \qquad (2Q)$$

$$L_i h_i^L + V_i h_i^V - L_{i+1} h_{i+1}^L - V_{i-x} h^V_{iA} - bu\}i\backslash = 0 \qquad i \in BF$$

(g) configurational constraints :

$$Z_i - Z_{i;i} \leq 0 \qquad i \in AF \qquad (21.a)$$

$$z_i - z_{i+1} \leq 0 \qquad i \in BF \qquad (21.b)$$

(h) monotonicity of temperatures :

$$U - t_{-i} \leq 0 \qquad i \in AF\ vC$$

$$t_i - t_{i+1} \geq 0 \qquad i \in BF \cup R \qquad (22)$$

(i) Let $S = (p^{\wedge}_o l - Ptop)/(N - 2)$. The constraints on pressure may be expressed as

$$PN = Peon$$

$$Pi-\backslash\ 'Pi \wedge Ptop - Peon \qquad i \in C$$

$$PM - PI \geq Szi \qquad i \in AF$$

$$Pi - PM \geq Szi \qquad i \in BF$$

$$Pi - p_{i+}i \leq /v^*fc - phot \qquad i \in /?$$

$$P. = Preb$$

$$\sum_{i \in AF} (P«-l\ ''\ P^*) + \sum_{i \in BF} (P^*\ ''\ P«+l) \leq Pbot\ '\ Ptop \qquad (M)$$

(j) constraints on reflux and boil-up : Let f_{max} *be* an estimate on the upper bounds of *refi* and *bui*. Then

$$refi\ Zfmac\ (zi - z»i) \qquad i \in AF \qquad (24.a)$$
$$bui \leq f_{max}\ \{it - z_{tt}) \qquad i \in 5F \qquad (24.b)$$

We comment briefly on the constraints (21) and (24). (21 .a) says that if tray i is required (i.e. exists), then so is tray (i-1). (Recall that trays are numbered bottom upwards). A similar argument applies for (21 .b). (24.a) ensures that all reflux enters exactly on one tray. (24.b) ensures that a similar situation obtains for the reboiled vapor.

If it is known that a certain minimum no. of trays are always required in the stripping and rectifying sections , then we can form the s6t FIX (including, of course, the feed tray) and introduce the following additional constraint :

(k) fixed locations : $z_i = 1$, $i \in FIX$ (25)

In addition to the constraints above, there may be constraints on purity, recovery, reflux ratio,etc.

The MINLP problem, then, is the minimization (or maximization) of an objective function subject to the equality and inequality constraints (15) to (25).

The data for problem EX5T11 are given in Table 5. It is interesting to see the path of the binary variables for this problem during the solution process of the proposed algorithm in Table 6. In the solution of the relaxed NLP, the binary variables *z-j,* zg, *zixan,* and Z23 have fractional values, $z_i = 1$, $i = 9,\ldots,20$, and $z_i = 0$, $i = 2,\ldots,6$ and $z_i = 0$, $i = 24,\ldots,29$. . The first MILP determines $z_i = 1$, $i = 6,\ldots,20$ (and zero for other binary variables),but this is found to be infeasible . The second MILP determines $z_i = 1$, $i = 7,\ldots,21$, but this is also found to be infeasible. The third MILP determines $z_i = 1$, $i = 6,\ldots,21$ and the fourth determines $z_i = 1$, $i = 7,\ldots,22$.

The configuration $z_i = 1$, $i = 6,\ldots,21$ (16 trays, feed at 5th tray) is selected as it entails a smaller value of the reflux ratio, 1.086, as against $z_i = 1$, $i = 7,\ldots,22$ (also 16 trays, but feed at 4th tray) which requires a reflux ratio of 1.094. Thus, the optimal configuration is :

No. of trays in the stripping section	4
No. of trays in the rectifying section	11
Feed tray	1
Total no. of trays required	16

Problem EX5T12 is identical to EX5T11 except that the upper bound on the reflux ratio was increased to 1.2 . The results are shown in Table 7. The optimal configuration corresponds $z_i = 1$, $i = 7,\ldots,20$ (14 trays, feed at 4th tray) and the optimal value of the reflux ratio is 1.191.

The differences between the results between the two cases are striking. The advantages of the MINLP approach are clearly illustrated even on the simple, ideal system considered here .

Conclusions

This paper has presented an augmented penalty version of the outer-approximation/equality-relaxation algorithm. The proposed'algorithm has as main features that it starts with the solution of the NLP relaxation problem, and that it features an MILP master problem with an augmented penalty function that allows violations of linearizations of the nonlinear functions. This scheme provides a direct way of handling nonconvexities which are often present in engineering design problems. The proposed algorithm has been implemented in DICOPT++ as part of the modeling system GAMS. The numerical performance, which has been tested on a variety of applications, has shown that the computational requirements of this method are quite reasonable while providing a high degree of reliability for finding global optimum solutions. Finally, MINLP models have been presented for the optimization of feed tray location and number of trays to illustrate the capability of the proposed algorithm for handling complex nonlinear problems.

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TABLE 1. Computational Results with DICOPT++

Problem	0-1 Var.	Cont. Var.	Constr.	Nonzeroes (nonlinear)	Iterations[1]	Time[2] (sec)	% NLPrMILP
LAZIMY	2	8	5	22(5)	1	0.06	100:00
HW74	3	9	9	28(2)	4	0.33	45:55
NONCON	3	3	6	17(2)	1	0.03	100:00
YUAN	4	4	10	32(9)	3	0.35	66:34
CAPITAL	10	3	7	46(2)	4	0.35	48:52
FLEX	4	12	16	47(4)	3	0.37	67:33
REL1	16	21	18	69(36)	3	3.77	52:48
EX3	8	26	32	101(5)	5	0.82	51:49
EX4	25	7	31	227(127)	5	12.33	12:88
BATCH	24	23	74	191(22)	3	1.67	92:08
BATCH8	40	33	142	353(32)	4	5.06	76:24
BATCH12	60	41	218	545(40)	4	9.96	52:48
TABATCH	24	71	129	462(124)	3	4.23	68:32
UTILRED	28	118	168	467(10)	3	8.2	19:81
TFYHEN	30	74	144	465(18)	3	22.7	20:80
EX5FEED	10	238	239	1103(826)	1	5.4	100:00
UN15FEED	12	587	586	3318(2336)	1	66.8	100.00
EX5T11	30	338	467	1943(1278)	4	114.1	43:57
EX5T12	30	338	467	1943 (1278)	3	53.48	79.21
HDASS	13	709	719	2204(462)	4	123.9	77:23

[1]N iterations require N NLP subproblems and N-l MILP master problems.
[2]Total CPU time, NLP:MINOS 5.2/MILP: MPSX 1.7, IBM-3090.

TABLE 2. Integer Gap in Test Problems

Problem	Relaxed Optimum	Integer Optimum	% Gap[1]	MILP Master Last Iteration
LAZMY	333.89	333.89	0	--
HW74	-6.299	-1.923	227	-1.433
NONCON	7.931	7.931	0	—
YUAN	4.488	4.579	2	4.672
CAPITAL	-3.5	1.5	333	10.25
FLEX	-4339	-7.077	61200	-5
REL1	178.9	216.5	17	179.4
EX3	15.08	68.01	77	72.56
EX4	-16.42	-8.064	104	-7.832
BATCH	259.2	285.5	9	284.9
BATCH8	361.9	412.6	12	380.4
BATCH12	2537	2687	6	2669
TABATCH	256.7	262.8	0	273.1
UTILRED	999.5	999.6	lxl(H	999.6
TFYHEN	3777.2	24066	84	29094
EX5FEED	20.79	20.79	0	20.79
UN15FEED	-79.9	-79.9	0	--
EX5T11	14.46	17.086	15	17.13
EX5T12	14.05	15.19	8	15.98
HDASS	-5746	-5459	5	-1831

[1] Gap = 100x | (Integer optimum-relaxed optimum)/Integer optimum)|

Table 3. Data for EX5FEED

System	Benzene-Toluene
Thermodynamic model	liquid - ideal vapor - ideal
Source of thermodynamic data	Reid et al. (1987)
Condenser type	Total
No. of trays (N)	25
LOC	{ 3,4,... 12 }

$F = 100$, $p_f = 1.12$ *bar* , $T_f = 359.6$ *K* , $z_f = (0.70, 0.30)$

$p_{reb} = 1.20$, $p_{bot} = 1.12$, $p_{top} = 1.08$, $p_{con} = 1.01$ *bar*

Constraints : r = reflux ratio ≤ 1

$x_{N,1} \geq 0.99$

Objective function : $P_1 - 50 * r$

Table 4. Data for UNIFEED5

System	Acetone-Acetonitrile-Water
Thermodynamic model	liquid -UNIQUAC vapor - virial
Source of thermodynamic data	Prausnitz et al (1980)
Condenser type	Partial
No. of trays (N)	17
LOC	{ 4,... 14 }

F = 100,/?f= 1.055 *bar* , 7>= 348.67 *K* , Zf= (0.10 , 0.75 , 0.15)

$p_{r}eb$ = 1.10 j)bot = L055 ,p_{top} = 1.035 ,p_{con} = 1.015 *bar*

Constraints : r = reflux ratio ^ 20

Obj. function = 3.3e-07 * $(q_{reb} - q_{con})$ - $(vikc + kkr)$

where q_{reb} = reboiler duty

q_{con} = condenser duty

v_{lkc} = flowrate of light key (acetone) in top vapor product

l_{hkr} = flowrate of heavy key (acetonitrile) in bottom liquid product

Table 5. Data for EX5T11

System	Benzene-Toluene
Thermodynamic model	Liquid - ideal Vapor- ideal
Source of thermodynamic data	Reid et al. (1987)
Condenser type	Total
Estimated max . no. of trays	30
Feed tray location	10

$F = 100$, $p_f = 1.12$ bar, $T_f = 359.6$ K, $z_f = (0.70, 0.30)$

$p_{reb} = 1.20$, $p_{bot} = 1.12$, $p_{top} = 1.08$, $p_{con} = 1.01$ bar

Constraints : $x_{\#,i} \geq 0.992$

r = reflux ratio ≤ 1.1

Objective function : $\sum_{i \in COL} z_i + r$

TABLE 6. Progress of Iterations in EX5T11

Step	Iteration Number	Obj. Function	CPU Time
NLP	1	14.436	24.04
MILP	1	16.000	6.60
NLP	2	∞^*	9.48
MILP	2	16.042	5.40
NLP	3	∞	7.70
MILP	3	16.945	7.80
NLP	4	17.086	8.15
MILP	4	17.134	54.00
NLP	5	17.094	6.28

TABLE 7. Progress of Iterations in EX5T12

Step	Iteration Number	Obj. Function	CPU Time
NLP	1	14.045	28.81
MILP	1	15.045	4.80
MLP	2	15.191	6.72
MILP	2	15.976	6.60
NLP	3	16.137	6.55

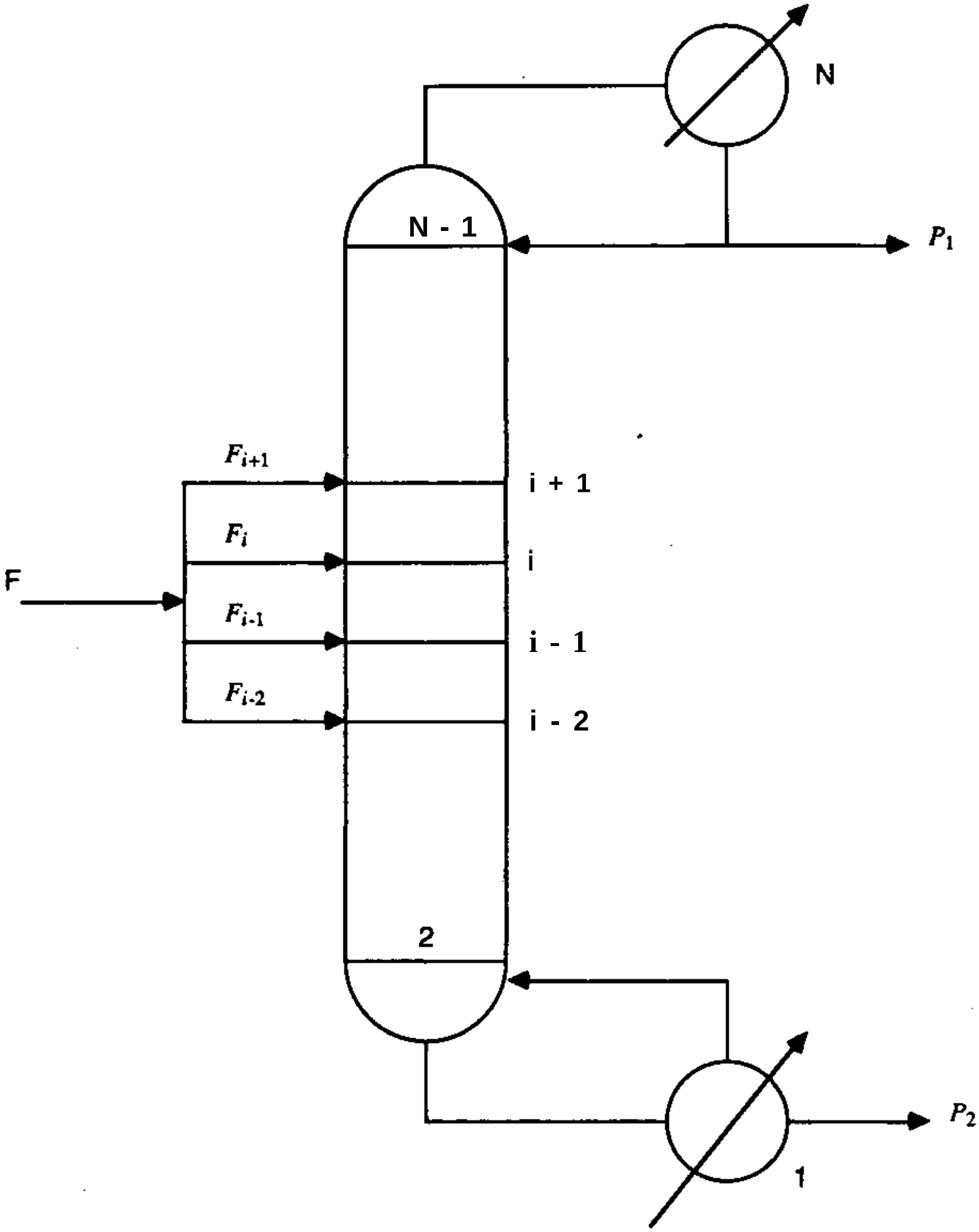

Figure 1. Optimum Feed Plate Location

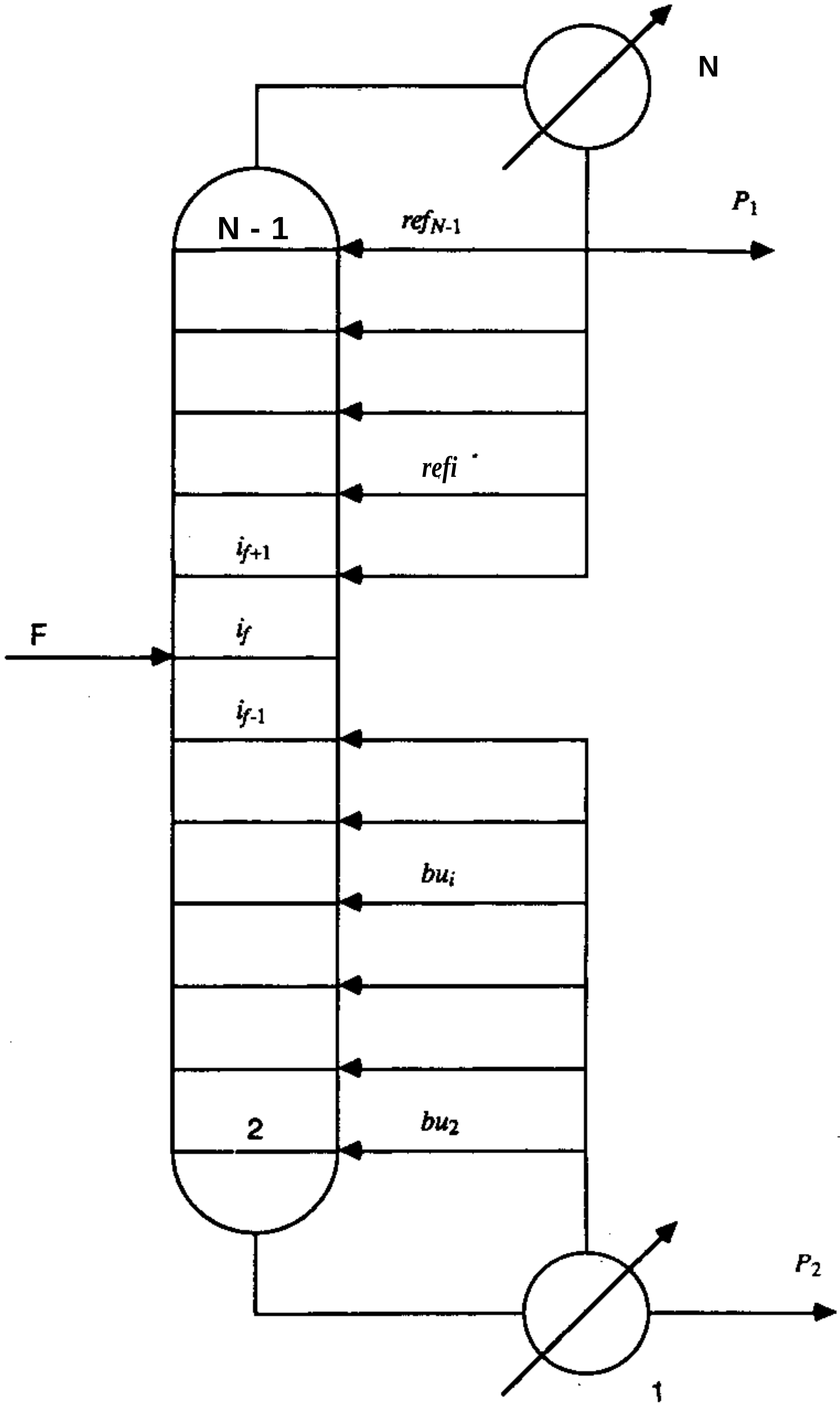

Figure 2 . Determination of number of trays to achieve a specified objective of separation