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by

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GLOBAL OPTIMIZATION OF NONCONVEX MINLP PROBLEMS IN PROCESS SYNTHESIS '

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ABSTRACT

This paper addresses the solution of nonconvex MINLP problems for process synthesis through the Outer-Approximation/Equality-Relaxation algorithm. A two-phase strategy is proposed where in phase I nonconvexities that may cut off the global optimum are systematically identified with local and global tests. In phase II, a new master problem is proposed that attempts to locate the global optimum which may have been overlooked in phase I. The proposed procedure, which has been implemented in DICOPT, is illustrated with several examples that include the design of multiproduct batch plants and a structural flowsheet optimization problem.

INTRODUCTION

Many design and process synthesis problems can be formulated with mixed-integer optimization models that involve both continuous and discrete variables (usually 0-1). Examples of synthesis problems include heat exchanger networks (Cerda and Westerberg, 1983; Papoulias and Grossmann, 1983; Floudas et al, 1986; Saboo et al, 1986), separation sequences (Andrecovich and Westerberg, 1985; Isla and Cerda, 1985; Lin and Prokopakis, 1986; Floudas and Anastasiadis, 1987) , utility and refrigeration systems (Papoulias and Grossmann, 1983; Shelton and Grossmann, 1986), evaporation systems (Hillenbrand, 1984). Most of these problems have been formulated as mixed-integer linear programs (MILP) that rely on linear approximations and discretization of operating conditions to avoid treatment of nonlinearities.

Recent advances in mixed-integer nonlinear programming (MINLP), however, offer the possibility of explicitly accounting for the nonlinearities that are commonly encountered in process models. In particular, the outer-approximation (OA) algorithm by Duran and Grossmann (1986a) and its extension with the equality-relaxation (ER) strategy by Kocis and Grossmann (1987) have shown to provide a very efficient method for solving MINLP problems. The basic idea in the OA/ER algorithm consists of solving an alternating sequence of NLP subproblems and MILP master problems. In the NLP step, the 0-1 binary variables are temporarily fixed and the continuous variables are optimized to yield a solution which provides an upper bound for an MINLP minimization problem. The MILP master problem optimizes the discrete variables and predicts an increasing sequence of lower bounds. The master problems are obtained by successively adding linear outer-approximations that are intended* to underestimate the objective function and overestimate the feasible region of the MINLP problem. Since this master problem provides a close approximation to the original MINLP problem, relatively few iterations (typically 2 to 5) are required to converge to the optimal MINLP solution. This has been shown in the design of gas pipelines (Duran and Grossmann, 1986b), retrofit of multiproduct batch plants (Vaselenak et al, 1987), in structural flowsheet optimization (Kocis and Grossmann, 1987), and in heat integrated distillation sequences (Floudas and Paules, 1987).

However, in order to guarantee global optimal solutions with the OA/ER algorithm, sufficient conditions require quasiconvexity of the relaxed equations and active inequalities, and convexity in the objective function and inactive inequalities. Some problems exhibit this structure, or else they may be transformed to satisfy these conditions, typically through logarithmic transformations of the variables that convexity the problem (e.g. see Duran and Grossmann, 1986b).

When the MINLP problem exhibits nonconvexities that cannot be transformed to a form that satisfies the above sufficient conditions, as is commonly the case in flowsheet synthesis problems, there is the possibility that the OA/ER algorithm may produce suboptimal solutions. There are two possible reasons why the presence of nonconvexities can cause difficulties. First, the NLP subproblem may exhibit more than one local solution. Second, even if a nonconvex NLP subproblem has a unique solution, the MILP master problem may not provide rigorous lower bounds, and as a consequence may sometimes cut off the global optimum solution. This paper will address the problem on how to circumvent the second difficulty for the case when general nonlinear functions[1] are involved in the MINLP, such as is the case in structural flowsheet optimization problems.

A two-phase solution strategy is proposed in this paper that attempts to find the global optimum of nonconvex MINLP problems. In the first phase the original OA/ER algorithm is applied with local and global tests that can automatically identify nonconvexities in the objective function and constraints. When none are detected, the algorithm terminates. Otherwise, one proceeds to a second phase where the invalid outer-approximations to the nonconvex functions can be systematically relaxed to yield a modified MILP master problem that attempts to locate an improved solution from the one obtained in the first phase. This strategy has been implemented in the computer code DICOPT (Kocis and Grossmann, 1987) that can solve general purpose MINLP problems. Several numerical examples are presented which include the optimal design of multiproduct batch plants and a structural flowsheet optimization problem. The results show that in many cases the proposed scheme can identify the global MINLP optimum.

BACKGROUND

For a given superstructure that has embedded alternative designs, the associated MINLP problem is assumed to have the following form:

[1] For the particular case of concave functions of a single variable, this problem can be avoided through the use of valid linear underestimators (e.g. see Vaselenak et al, 1987).

$$z = \min_{x,y} \; c^T y + f(x)$$

$$\text{s.t.} \quad h(x) = 0$$

$$g(x) \overline{<} 0$$

$$A\,x = a \qquad \text{(MINLP)}$$

$$By + Cx \text{ £ } d$$

$$x \in X = \{x \mid x \in R^n, x^L \leq x \leq x^U\}$$

$$y \in Y = \{y \mid y \in \{0,1\}^m, E\,y \leq e\}$$

In problem (MINLP), x is the vector of continuous variables representing flows, pressures, temperatures and sizes, while the vector of 0-1 binary variables y represent the potential existence of units which are embedded in a superstructure containing alternative flowsheet designs. The equations h(x)=0 and Ax=a correspond to material and energy balances and design equations. Nonlinear process specifications are represented by g(x)≤0. Logical constraints and linear specifications that must hold for a flowsheet configuration to be selected from within the superstructure are represented by By+Cx^d and Ey^e. The variables x are specified to lie within the compact set X consisting of lower and upper bounds. The cost function involves fixed cost charges in the term $c^T y$ for the investment, while revenues, operating costs, and size dependent costs for the investment are included in the function f(x).

It should be noted that for most synthesis problems the terms f(x) in the objective function are linear in x, because it represents incomes and expenses (see Kocis and Grossmann, 1987). Also the binary variables y as shown above, are usually linear because in the objective they are used for fixed-cost charges, and in the constraints they are used to model multiple choice constraints or logical implications that can be written linearly.

For the case when the binary variables are nonlinear in a function 4>(x,y>, one can always reformulate the problem so as to have the structure that is linear in y and nonlinear in x as in problem (MINLP). This can be done simply by defining new continuous variables x* = y, so that $(x,y) can be formulated as a nonlinear function of continuous variables •(x,x^l). The additional equations x* = y are then linear in y. Also, the case when linear terms in y appear in nonlinear equations and inequalities,

$h(x)$ and $g(x)$, can be directly handled by the OA/ER algorithm.

In the OA/ER algorithm the NLP subproblems arise for a fixed choice of the binary variables $y^k \in Y$. From **(MINLP),** this leads to the problem:

$$
\begin{aligned}
z(y^k) = \min_{x} \; & c^T y^k + f(x) \\
s.t. \;\; & h(x) = 0 \\
& g(x) \le 0 \\
& Ax = a \\
& Cx \le d - By^k \\
& x \in X
\end{aligned}
\qquad \mathbf{(NLP^k)}
$$

Since this problem may not have a feasible solution for the particular choice of y^k, it is often convenient to introduce a non-negative slack variable u for constraint violations and a large scalar p. The objective function and inequality constraints in **(NLP^k)** are replaced in a modified formulation $(SNLP^k)$ as follows:

a) *Objective function:* $z(y^k) = \min_{x,u} \; c^T y^k + f(x) + p\,u$

b) Nonlinear inequalities: $g(x) \le u$

c) Linear mixed inequalities: $Cx \le d - By^k + u$

In this way, if a feasible solution to problem **(NLP^k)** exists, then the slack variable u will be zero and formulation **$(SNLP^k)$** reduces to that of (NLP^k). If a feasible solution does not exist, then the objective function in **$(SNLP^k)$** will produce continuous variables x^k that minimize the violation u of the inequality constraints.

The master problem in the OA/ER algorithm at iteration K is given by the following MILP problem:

$$
\begin{aligned}
7^{*}_{L} = \min_{x,y,\mu} \quad & c^{T}y + \mu \\
s.t. \quad & (w^{k})\, x - \mu \;\pounds\; W^{k}_{o} \\
& T^{k}R^{k}x \le T^{k}r^{k} \qquad\qquad A = i, 2 \ldots K \\
& S^{k}x \;\pounds\; s^{k} \\
& A\,x = a \qquad\qquad\qquad\qquad (M^{K}) \\
& By \bullet * \text{-} Cx \;\pounds\; d \\
& Ey \le e \\
& 7^{K''}_{L} \;\pounds\; c^{T}y + \mu \\
& \sum_{i \in B^{k}} y_{i} - \sum_{i \in N^{k}} y_{i} \le |B^{k}| - 1 \qquad k = 1, 2 \ldots /f\text{-}1 \\
& x \in X, \quad y \in \{0,1\}^{m}, \quad \mu \in R^{1}
\end{aligned}
$$

where z^{*}_{L} is the predicted lower bound at iteration K. In the above formulation, the linear approximations to nonlinear functions f(x>, h(x), and g(x) are based on a Taylor series approximations at the point x\ the optimal continuous variables in subproblem <NLP"). The linear coefficients and right hand side constants in (M") are then given by:

$$
\begin{aligned}
w^{k} &= Vf(x^{k})^{T} & w^{k}_{o} &= Vf<x^{k})^{T}\,[x^{k}] - f(x^{k}) \\
R^{k} &= Vh(x^{k})^{T} & r^{k} &= Vh(x^{k})^{T}\,[x^{k}] \\
S^{k} &= Vg(x^{k})^{T} & s^{k} &= Vg(x^{k})^{T}\,[x^{k}] - g(x^{k})
\end{aligned}
\tag{1}
$$

T^{k} is an *rXr* matrix for relaxing the linear approximations of the *r* nonlinear equations to inequalities. The diagonal elements of the matrix T^{k} are given by:

$$
t^{k}_{ii} = \begin{cases} -1 & if \;\; X^{k}_{i} < 0 \\ +1 & if \;\; X^{k}_{i} > 0 \\ 0 & // \;\; X^{k}_{i} - 0 \end{cases} \qquad\qquad i = 1.2, \ldots r \tag{2}
$$

where X^{k} are the associated optimal lagrange multipliers for the nonlinear equations h!(x)=0, i=1,2...r, in the subproblem (NLP^{k}).

The lower bound $z\pounds^{-1}$ of the constraint on $c^{T}y+//$ is introduced to expedite the solution of the MILP. The next set of inequalities are integer cuts that eliminate the assignments of binary variables analyzed at the previous K-1 iterations (see Duran and Grossmann, 1986a). For any integer combination y^k, the index sets are such that $B^k=\{j: y_j=1\}$ and $N^k=\{j: y_j^k=0\}$.

It should be noted that the above master problem is a slightly modified version of the one presented in Kocis and Grossmann (1987) in that the constraint $c^T y + p < z_U$ has been removed, where z_u represents the best current upper bound predicted by the NLP subproblems. In this way the stopping criterion is given not when the master problem (M^K) is infeasible, but rather when the predicted lower bound z_L^K exceeds the current best estimate z^

The OA/ER algorithm requires an initial guess of the binary variables y^1 at iteration K=1 and then alternates between the NLP subproblems in **(NLP^K)** and the master problems in (M^K). In order for the master problems to provide rigorous lower bounds, sufficient conditions require quasiconvexity of the relaxed equations $T^k h(x) \leq 0$ and active inequalities $g_A(x) \leq 0$, and convexity of objective function term f(x) and inactive inequalities $g_I(x)<0$ (see Kocis and Grossmann, 1987). When these conditions are not met, the master problem may cut off the global optimum. On the other hand, the global optimum solution might still be obtained since the above conditions are only sufficient. The following section illustrates these two points.

MOTIVATING EXAMPLES

Example 1.

The following small example illustrates how the MILP master problem can sometimes cut off the global optimum solution in nonconvex problems. The problem is given by,

$$
\begin{aligned}
& z = \min_{x,y}\ 2x + y \\
s.t.\quad & -x^2 - y \leq -1.25 \\
& x + y \leq 1.6 \qquad\qquad \textbf{(EX-1)} \\
& x \geq 0 \\
& y \in \{0,1\}
\end{aligned}
$$

where the nonlinear inequality contains a nonconvex term for the continuous variable x. The feasible region and the objective function contours are shown in Figure 1.a.

The global optimum of problem **(EX-1)** is located at (x,y)=(0.5,1) where 2=2.000, since at (x,y)=(1.118,0) 2=2.236. Note that at each of the two integer values the solution of the corresponding NLP subproblem is unique.

In applying the OA/ER algorithm to this small nonconvex MINLP problem, assume that y=0 is selected as the initial point. This yields an NLP subproblem with the solution (x,y)=(1.118,0) and objective function value 2=2.236. To set up the MILP master problem at iteration 1, the nonlinear constraint in **(EX-1)** is linearized at (x,y)=(1.118,0) and the integer cut y £ 1 is introduced. The master problem formulation is given below and its feasible region is shown in Figure 1.b.

$$
\begin{aligned}
& 2 = \min_{x,y} \; 2x + y \\
s.t.\quad & -2.236\,x - y \leq -2.5 \\
& x + y \; £ \; 1.6 \qquad\qquad (M^1) \\
& y \; Z \; 1 \;,\; y \in \{0,1\} \;,\; x \; Z \; 0
\end{aligned}
$$

Note in Figure 1.b that the linearization of the nonconvex function cuts into its feasible region. Since the integer cut forces y=1, the feasible region defined by the two linear inequalities is empty. Thus the master problem (M^1) is infeasible. Therefore, due to the nonconvexity of the nonlinear inequality the global optimum has been cut off. In the procedure that will be presented later in the paper this difficulty will be overcome and the global optimum will be found.

Example 2.

This example will illustrate the use of nonlinear 0-1 variables and the fact that the global optimum can still be identified despite nonconvexities that may be present. The problem is a pure 0-1 problem corresponding to a nonconvex quadratic capital budgeting problem (see Kettani and Oral, 1987) of the form:

$$
\begin{aligned}
& 2 = \min_{y} \; \lessdot K_1 + 2/_2 + 3y_3 - yj\,(2y_1 + 5/_2 + 3/_3 - 6y] \\
s.t.\quad & y_i + 2y_2 + y_3 + 3y_A \; Z \; 4 \qquad\qquad \textbf{(EX-2)} \\
& y \in \{0,1\}^4
\end{aligned}
$$

The global optimum of this problem is z=-6.0 at y=(0,0,1,1). There are 16 possible combinations of the 4 binary variables, of which 8 are feasible as determined by the linear inequality constraint. Applying the OA/ER algorithm from each of the 8 feasible starting points yields the optimal solution as seen in Table I, where the progress of the lower and upper bounds at each iteration is presented. Since **(EX-2)** is a pure 0-1 problem, the NLP subproblems for fixed y^k require only an objective function evaluation rather than an optimization. Note, however, that in the starting point $y^{l}=[0,1,0,1]$, the lower bound at iteration 1 (-4.0) does not underestimate the objective function of the next NLP subproblem (-6.0). This example then shows that global solutions can often be obtained despite the presence of nonconvexities.

OUTLINE OF TWO-PHASE STRATEGY

As was shown in the previous section, when sufficient conditions for the OA/ER algorithm are not satisfied, one may or may not obtain the global optimum solution. However, problem **(EX-2)** and computational experience by the authors has shown that in a good number of cases the OA/ER algorithm will find the global optimum solution for nonconvex MINLP problems. This would then suggest that a suitable strategy to tackle these problems is to solve them in two phases. In the first phase the OA/ER algorithm will be applied in its original form, but with special provisions for the identification of nonconvex functions that may cut off the global solution. If none are detected the search is terminated. Otherwise, one proceeds to a second phase where linearizations are systematically modified in a new master problem so as to try to yield valid outer-approximations. Here the search is terminated at the point when no further improvements are found in the NLP subproblems. The main steps in the two-phase strategy for handling nonconvex MINLP problems are shown in Figure 2.

Phase I consists of the OA/ER algorithm by Kocis and Grossmann (1987), and an identification procedure for nonconvex functions. Given an MINLP problem, the OA/ER algorithm involves the solution of a series of alternating NLP subproblems and MILP master problems. The NLP subproblem **(NLP^K)** corresponds to the continuous optimization for fixed values of the binary variables y\ Its solution $z(y^K)$ yields a valid upper bound z_U to the MINLP solution, and it is used to derive linearizations for the nonlinear functions that are to be included in the master problem.

The MILP master problem <M^K) is an approximation to the MINLP that is based on cumulative linearizations up to iteration K, and its role is to predict new values of the binary variables y^{K+1} and provide a lower bound, z_L^*, to the MINLP. If the lower

bound lies below the current best upper bound z_{yf} a new NLP subproblem is solved. Otherwise, phase I is terminated, and at that point the global optimum is assumed to correspond to the current upper bound, z_y. Convexity tests are then applied to challenge this assumption.

The proposed identification procedure is based on two types of tests: local tests and global tests. Both tests are used to determine which linearizations are cutting into the feasible region of the original MINLP problem. The local tests consist of checking convexity conditions of the functions by perturbing the NLP subproblems. The global tests consist of checking whether solutions that are generated from the NLP subproblems in phase I are feasible for the linearizations of the master problem. When all the functions in the MINLP are convex, these tests will not record any violations, and the search would then be terminated. On the other hand, when nonconvex functions are present in the MINLP, these tests may detect those linearizations that violate the convexity assumptions for phase I. One must then proceed to phase II where an attempt is made to correct invalid linearizations.

Once the violating linearizations are identified, a new MILP master problem is defined for phase II that will attempt to expand the feasible region by modifying the linear approximations in order to include the space of the original MINLP. This task is handled through a shifting of linearizations which failed the global test via new right hand side coefficients. Also, nonnegative slack variables are added to linearizations which failed either the local or global test and to the objective function with a large positive coefficient. Finally, a constraint which forces the lower bound to be no greater than the current upper bound is included in the phase II master problem. Qualitatively, this master will attempt to produce valid outer-approximations to the nonconvex region. In this way it will yield a new set of binary variables whose lower bound lies below the current best solution, $z_{(j/}$ while minimizing the sum of infeasibilities introduced by the slack variables.

The solution corresponding to the new binary variables y^K is then optimized through its NLP subproblem to yield the objective function value $z(y^K)$ at x^K. If $z(y^K)$ is greater or equal than z_y, the search in phase II is terminated and z_u is assumed to be the global optimum solution. Otherwise, the current upper bound is updated to $z_u^s z(y^K)$, and the new linearizations are derived. These are then checked with the local test and the global tests. All previous linearizations are checked through the global test at the new point x^K. The MILP master problem is then derived accounting for the new linearizations and violations recorded in the two tests. Iterations in phase II are then repeated up to the point where no further improvement is obtained in the upper bound z_y. Note that in phase II, no use is made of the lower bounds of the master problem since in general these will exhibit a gap due to the relaxation of the linearizations.

It should be noted that the main advantage of the two-phase algorithm is that it can automatically identify nonconvexities in the MINLP problem that could prevent the OA/ER algorithm from finding the global optimum solution. However, no rigorous guarantee on global optimality can be given if phase II is activated. This follows from the fact that no special structure on the functions has been assumed to guarantee validity of the modified outer-approximations and uniqueness of the solutions of the NLP subproblems. Despite these unavoidable limitations, the strategy represents a systematic procedure by which one can intelligently use all the information generated in phase I to try to locate the global solution, in fact, as will be shown in the examples, this strategy is able to find the global optimum in many of the nonconvex MINLP problems that have been tested so far. Finally, it is interesting to note that when nonconvexities are not involved in the MINLP, the strategy will be able to automatically identify this situation and terminate at phase I with the global optimum. The following sections describe the local and global tests, as well as the master problem used in phase II.

LOCAL TEST

The purpose of the local test is to provide information required to analyze locally convexity conditions of a nonlinear constraint through its corresponding linearization. First consider the nonlinear equations **h(x)=0** and let $h^{\wedge IN}$ denote the linearization of equation h_i. x^k, the optimal solution to subproblem (NLP^k), is selected as the point at which the linearization are derived.

$$h_i^{LIN}(x) \ll /?_i(x'') + Vh_i(x^k)^T \; [x - x^k] \tag{3}$$

Since the point x^k *must satisfy* $/?_i(x^k)=0$

$$h_i^{LIN}(x) = Vh_i(x^k)^T \; [x - x^k] \tag{4}$$

As discussed in Kocis and Grossmann (1987), the condition for quasiconvexity of $h_i(x)$ requires satisfying the following relation:

$$\textit{if } Mx) \; £ \; 0 \textit{ then } Vh(x^k)^T \; [x-x^k] \; £ \; 0 \tag{5}$$

Then for a function $h_i(x)$ to be quasiconvex, the above statement must hold for alt x. In the local test, we attempt to find a point >T^k near x^k which violates this condition. But since there are an infinite number of candidate points to consider, a logical choice is a point $\bar{x}^k$ which produces a decrease in the objective function. Such a point can be found by solving a relaxed NLP subproblem **<LNLP^k)** which is identical to (NLP^k), except that the lower and upper bounds for nonzero x_i^k, y_i^k are given by:

$$x_i^k(1-\epsilon) \leq x_i \leq x_i^k(1+\epsilon) \tag{6a}$$

$$y_i^k(1-\epsilon) \leq y_i \leq y_i^k(1+\epsilon)$$

and for zero x_i^*, y_i^* by:

$$-(\leq x_i \leq (\tag{6b}$$

$$-« \wedge y._i * \epsilon$$

where £ is a small number (i.e. 0.05). These bounds insure that the solution point $\bar{x}^k$ will remain near x^k. Also, since the solution to **(NLP^k)** has already been determined, a very good starting point is provided for this NLP so the solution point $\bar{x}^k$ should be found quickly.

It is clear that at the solution of **(LNLP^k),** h_iÜ^k)«0. Referring back to the quasiconvexity condition in (5), the local test reduces to verifying if $\nabla h_i(x^k)^T$ $[\bar{x}^k - x^k]$ ^ 0, which is equivalent to testing the feasibility of the linearization at $\bar{x}^k$. In terms of the master problem linearizations in (M^k), the local test for quasiconvexity in the nonlinear equations **h(x)*0** and active inequalities g_A<x)^{s}0 reduces then to checking if

$$T^k R^k \bar{x}^k \text{ £ } T^k r^k, \quad S_A^k \bar{x}^k \text{ £ } s\wedge \tag{7}$$

If the above inequalities are satisfied for each row i, then the local test for quasiconvexity is passed for the corresponding linearizations.

Next, consider the inactive inequality constraints **g_I(x)<0** and the nonlinear objective function term f(x). In order to guarantee that the OA/ER algorithm will converge to the global solution, the inactive inequality constraints and the objective function term are required to be convex. From Mangasarian (1969), for a differentiable convex function, $g_I(x)$:

$$g_,(x) \;;> g_f(x^k)+ \nabla g\wedge x V \; [x-x^k] \tag{8}$$

The right hand side of the above condition is precisely the linearization of $g_l(x)$ at the point x^k so the convexity condition can be restated as:

$$g_l(x) \le g_t^{u,N}(x) \tag{9}$$

The local test for the linearizations in (M⁻) of the inactive nonlinear inequalities $g_l(x)<0$ and objective function f(x) then reduces from (9) to checking the following inequalities at the local test points $\bar{x}^k$:

$$g_l(\bar{x}^k) \le S_l^k \bar{x}^k - s_l^k \ , \qquad f(\bar{x}^k) \ge (w^k)^T \bar{x}^k - w_o^k \tag{10}$$

GLOBAL TEST

The local test provides a means of checking convexity and quasiconvexity conditions near the point at which the linear approximation is derived. However, this procedure does not determine whether the linearization provides a valid outer-approximation at other points in the feasible space of the MINLP. The proposed global test provides this information in addition to a simple mechanism for modifying linearizations which do not provide valid outer-approximations.

At completion of the OA/ER algorithm, the solution of K NLP subproblems are available with the corresponding values of x^k for k=1,2,..K. If the master problem is truly underestimating the objective function and overestimating the feasible region of the MINLP problem, then each of these points should be feasible in the final master problem. This provides a simple method for identifying linearizations which may be excluding the global MINLP solution by cutting into its feasible region.

The global tests are similar to the local tests, except that they are applied to the linearizations of iteration t for the points x^k, k=1,2,..K, k # l. That is, from (7) the conditions that must be verified for each row i of the equations and active inequalities are:

$$T^l R^l x^k \le jt\text{-}r^1 \ , \qquad S_A^l x^k \le s_A^l \qquad l,k=1,2,\ldots K, \quad l \ne k \tag{11}$$

while from (10), for the inactive nonlinear inequalities and objective function, the conditions to be tested are:

$$g_l(x^k) \le S_l^l x^k - s_l^l \ , \qquad f(x^k) \ge (w^l)^T x^k - w_o^l \qquad l,k = 1,2,\ldots K \ , \quad l \ne k \tag{12}$$

Note that since the linearizations of iteration l must be tested at a point x^k corresponding to a different iteration (i.e. $l \ne k$). the global test can only be applied if two or more iterations take place for the OA/ER algorithm. Also, note that this test is very easy to apply as (11) only requires matrix multiplication, while (12) requires matrix multiplication and function evaluation of the inactive constraints and nonlinear objective function term.

Finally, those linearizations found to fail the global test conditions in (11) and (12) are modified so as to satisfy these conditions at all the points x\ This can be accomplished by simply determining for each linearization, the maximum violation at a point x^m and setting

r -R x . S A - S A x M3)

i f - sf x^m - g(<x^k> . ŵ f = $(v/)^T x^m$ - $l(x^m)$

L f - f l

where f , & , &~, and v^ are new coefficient values that provide valid outer-
A I o
approximatipns for the points $\mathbf{x^k}$, k=1,2,...K.

MASTER PROBLEM FOR PHASE II

The phase II master problem formulation is similar to the phase I formulation except for the addition of an upper bound to the original objective function and the treatment of linearizations which failed either the local or global test through slack variables and modified right hand side coefficients. The master problem linearizations for each iteration k will be partitioned into the three sets P^k, FG^k, and FL^k, denoting linearizations that passed all tests, failed a global test, and failed only a local test, respectively. Note that if a linearization fails both a global and a local test it is included in the set FG^k.

The candidate test points, $\bar{x}^k$ for k=1,2,..K, for the local test are generated by perturbing the NLP subproblem solution points x\ Based on the form of the linearizations in master problem (M^K), a given linearization fails the local test if the conditions in (7) **and** (10) are not satisfied. A nonnegative slack variable C_i is introduced to each linearization i of iteration k which failed only a local test to allow this constraint to be violated when the slack becomes positive. The coefficient of the slack variable is chosen so that the corresponding violation is relative to the magnitude of the right hand sides. Hence, the modified linearizations in FL^k are given by:

$$\left.\begin{array}{l} (w_i^k)^T x - u_i^k - |w_{io}^k|\, \zeta_i^k \le w_{io}^k \\ T_i^k R_i^k x - |T_i^k r_i^k|\, \zeta_i^k \le T_i^k r_i^k \\ S_i^k x - |s_i^k|\, \zeta_i^k \le s_i^k \end{array}\right\} \quad i \in FL^k \;, \; k=1,2,...K \qquad (14)$$

where the index i is used to denote the i^{th} element of the vectors and matrices corresponding to the linearizations that failed the local test. Note that if $\zeta_i^k = 0$ the original linearization is kept, whereas if $\zeta_i^k > 0$ the linearization is relaxed in proportion to the right hand side coefficient. For numerical convenience, we define the absolute value function for $|.| < \epsilon$ as $|.| = \epsilon$ where ϵ is a small positive tolerance.

As mentioned earlier, it is the global test that provides information required to modify an invalid linearization to yield valid outer-approximations at the NLP solution points x^k, k=1,2,...K. By substituting the new coefficients in (13) into (11) and (12) for linearizations which failed to satisfy these inequalities, and introducing slack variables as in (14) the linearizations in FG^k are given by:

$$\left.\begin{array}{l} (w_i^k)^T x - u_i^k - |\hat{w}_{io}^k|\, \zeta_i^k \le \hat{w}_{io}^k \\ T_i^k R_i^k x - |T_i^k \hat{r}_i^k|\, \zeta_i^k \le T_i^k \hat{r}_i^k \\ S_i^k x - |\hat{s}_i^k|\, \zeta_i^k \le \hat{s}_i^k \end{array}\right\} \quad i \in FG^k \;, \; k=1,2,...K \qquad (15)$$

The nonnegative slack variables, ζ_i^k in (14) and (15), are included in the objective function with a large positive coefficient ρ so that the sum of violations for the modified linearizations is minimized.

Lastly, an upper bound given by the best solution from the phase I NLP subproblems (z_U) is placed on the objective function, $c^T y + \rho$, to ensure that the predicted lower bound in the modified master problem does not exceed its value. The lower bound from the previous master problem however is excluded. The phase II master problem is then given by:

$$z_L^K = \min_{x,y,\mu} \; c^T y + \mu + \rho \sum_{k=1}^{K} \sum_{i \in FL^k,\, i \in FG^k} \zeta_i^k$$

$$
\begin{aligned}
\text{s.t.}\quad & \left.\begin{aligned}
& (w_i^k)^T x - \mu \le w_{io}^k \\
& T^k R_i^k x \le T^k r_i^k \\
& S_i^k x \le s_i^k
\end{aligned}\right\} \; i \in P^k \,,\; k = 1,2,\ldots K \\
& \left.\begin{aligned}
& (w_i^k)^T x - \mu - |w_{io}^k| \, \zeta_i^k \le w_{io}^k \\
& T^k R_i^k x - |T^k r_i^k| \, \zeta_i^k \le T^k r_i^k \\
& S_i^k x - |s_i^k| \, \zeta_i^k \le s_i^k
\end{aligned}\right\} \; i \in FL^k \,,\; k = 1,2,\ldots K \\
& \left.\begin{aligned}
& (\hat{w}_i^k)^T x - \mu - |\hat{w}_{io}^k| \, \zeta_i^k \le \hat{w}_{io}^k \\
& T^k R_i^k x - |T^k \hat{r}_i^k| \, \zeta_i^k \le T^k \hat{r}_i^k \\
& S_i^k x - |\hat{s}_i^k| \, \zeta_i^k \le \hat{s}_i^k
\end{aligned}\right\} \; i \in FG^k \,,\; k = 1,2,\ldots K \\
& Ax = a \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (RM^K) \\
& By + Cx \le d \\
& Ey \le e \\
& c^T y + \mu \le z_U \\
& \sum_{i \in B^k} y_i - \sum_{i \in N^k} y_i \le |B^k| - 1 \qquad k = 1,2,\ldots K-1 \\
& x \in X \,,\; y \in \{0,1\}^m \,,\; \mu \in R^1
\end{aligned}
$$

The application of the master problem shown above will be demonstrated using the small nonconvex MINLP example problem (EX-1). Since this problem has only one continuous and one binary variable, details can be illustrated graphically in order to provide a geometrical interpretation of the local test procedure and the phase II master problem. Recall that the global optimum of problem (EX-1) is located at (x,y)=(0.5,1) where z=2.000, and if y=0 is selected as the initial point for the OA/ER algorithm, it yields the suboptimal solution (x,y)=(1.118,0) with objective function value z=2.236. Since the master problem (M^1) was infeasible, phase I was terminated with z_u=2.236. Because only one iteration has been completed, no candidate points exist for the global test (i.e. the linearization derived at x^1 will be satisfied at x^1 by definition). However, the local test can be performed through the NLP problem **(LNLP^1)** with the bounds as in (6). For the value of €=0.05 this yields:

$$z = \min_{x,y}\ 2x + y$$

$$\text{s.t.}\quad -x^2 - y \leq -1.25$$

$$x + y <> 1.6 \qquad \textbf{(LNLP}^1\textbf{)}$$

$$1.118\,(1-c) * 1.062\ £\ x \leq 1.174 = 1.118(1+*)$$

$$-* = -0.05\ £\ y <> 0.05 = e$$

The. solution to this problem is $(\bar{x}\backslash\bar{y}^1$Hi. 140,-0.05) with z=2.230. Checking if the linearization in (M^1) is satisfied at this point,

$$-2.236\,\bar{x}"^1 - \hat{}^1 = -2.236(1.140) + 0.05 = -2.4992 \leq -2.500 \qquad (16)$$

Since -2.4992 > -2.5, the linearization fails the local test and phase II is activated. A slack variable is added to the invalid linearization and to the objective function to yield the following phase II master problem (RM^2).

$$z = \min_{x,y}\ 2x + y + 100\,C$$

$$\text{s.t.}\quad -2.236\,x - / - 2.5\,C* \ -2.5$$

$$x + / \leq 1.6 \qquad (\text{RM}^2)$$

$$2\,x + /\ £\ 2.236$$

$$y\ £\ 1\ ,\ yE\ \{0,1\}\ ,\ x\ £\ 0$$

The solution to (RM^2) is (x,y,{)=(0.6,1.0,0.063) with 2x+y=2.200 which is less than the current upper bound of $z_u{}^s$2.236. The local test identified the nonconvexity and relaxed the linearization through the slack { as shown in Figure 3. y^2 is fixed at 1 and the next **NLP** is solved to yield z(y^2)=2.000 at X^2=1.118 which is the global minimum of (EX-1). Technically, one would continue in phase II since z(y^2)=2.000 < z_y=2.236. But it is clear that the search at this point would terminate since there are only two possible values for the binary variable y in (EX-1). Larger and more interesting test problems will be presented later, but this small example clearly shows the role of the local test and the form of the relaxed phase II master problem.

ALGORITHM FOR TWO-PHASE STRATEGY

Having presented the local and global tests, and the modified master problem, the steps in the proposed two-phase strategy for solving nonconvex MINLP problems are as follows (see Figure 2):

Step 1 Select initial binary assignment y\ set K=1.
Initialize lower and upper bounds, z_L^o=-oo z^oo.

Step 2 Solve **(NLP^K)** for fixed y^K yielding $z(y^K)$, x\ and X''.
If $z(y^K)<z_{ur}$ then set $y^{\#}$=y\ $x^{\#}=x^K$, and $z_u=z(y^K)$.
Define the matrix T^K as in (2).

Step 3 Determine at x^K the coefficients in (1) for the linear approximations of f(x), h(x), and g(x), and set up with T^K the master problem (M^K).

Step 4 Solve the MILP master problem (M^K):

[a] If a feasible solution y^{K+1} exists with lower bound $z_L^* < z_y$,
set K=K+1, go to **Step** 2.

[b] If no such solution exists, phase I solution is z_u at y\ x\
Go to Step 5.

Step 5 [a] Determine local test points $\bar{x}^k$ for k=1,2,..K by solving the problems **(LNLP^k)** which are given by **(NLP^k)** with the bounds in (6) Check the local test conditions in (7) and (10) to determine those linearizations which fail the test.

[b] Check the global test conditions in (11) and (12) and update the right hand sides of those linearizations which fail the test as in (13).

[c] Add slack variables to the linearizations which failed the local and global test as in **(14)** and (15).

Step 6 If no linearizations failed any of the tests, the global optimum is assumed to be z_{U} at x\y$^{\#}$; stop.
Otherwise set K=K+1 and go to **Step 7.**

Step 7 Set up and solve the phase **II** MILP master problem (RM^K) to obtain y^K

[a] If a feasible solution y^K exists, go to **Step** 8.

[b] If no feasible solution exists, then stop
The global optimal solution is assumed to be z_u at y\x\

Step 8 Solve **(NLP^K)** for fixed y^K yielding $z(y^K)$, x^K, and X\
[a] If $z(y^K)<z_u$, set $y^{\#}=y^K$, $x^{\#}=x^K$, and $z_u=z(y^K)$.
Define the matrix T^K as in (2).
[b] If $z(y^K)>z_{uf}$ stop.
The global optimal solution is assumed to be z_u at $y^{\#}$,x\

Step 9 Derive at x^K the linear approximations for f(x), h(x), and g(x) as in Step 3.

Step 10 Perform local and global tests for the current linearizations as in Step 5. Set K=K+1 and go to Step 7.

The steps given above define the two-phase strategy in its entirety. Note that in phase I at each iteration K, the NLP subproblem is solved first followed by the MILP master problem. In phase II the MILP is solved first and then the NLP at each iteration K.

It should be also noted that different variations of this algorithm are possible. For instance, one may wish to perform only the global test for identifying nonconvexities since the points for this test are readily available at the end of phase I. The local test, however, requires the solution of the NLP problems **($LNLP^k$),** k=1,2,..K, to generate the test points $\bar{x}^k$. In addition, initial experience with the convexity tests has indicated that in many cases the slack variables for the linearizations which failed the tests take the value of zero. Resetting the right hand side coefficients as in (13) has been found to usually yield a feasible phase II master problem with an objective function value less than the upper bound (z_u> from phase I.

The proposed two-phase strategy has been implemented in the computer code DICOPT (Discrete Continuous OPTimizer) for solving general purpose MINLP problems with the OA/ER algorithm (see Kocis and Grossmann, 1987). DICOPT was used to solve the problems in this paper on the IBM 3090-600 supercomputer at the Cornell Theory Center. This code has as an interface the modelling system GAMS (General Algebraic Modelling System, Kendrick and Meeraus, 1985), allowing the user to supply the MINLP problem formulation in algebraic form with indexed equations and without the need for MPS files nor gradient information. MINOS (Murtagh and Saunders, 1985) was used to solve NLP subproblems and MPSX (IBM, 1979) was used to solve the MILP master problems. Note that an initial point is required only for the first NLP subproblem since the solution from the MILP master problems (M^k), k=1,2,...K-1 provide the starting point for subproblems (NLP^k), k=2,3,..K. With the newly developed strategy for handling nonconvexities, a larger class of MINLP problems can be handled in DICOPT.

EXAMPLE PROBLEMS

Three types of examples will be presented to illustrate the application of the two-phase strategy. The first one is a small MINLP problem that will serve to illustrate in detail the steps of the algorithm. The second example is an MINLP for the optimal design of a multiproduct batch plant. This example will serve to compare the direct solution of a nonconvex MINLP with the use of transformations that can convexify the problem. The third example is a structural flowsheet optimization problem that involves nonconvexities and where no special structure is present in the MINLP model.

<u>**Example**</u> <u>3</u> The following MINLP problem has the characteristic that although nonconvexities are present, the NLP subproblems have unique solutions. However, the effect of the nonconvex terms will be seen in the master problem where the linear approximations fail to overestimate the feasible region of the original MINLP formulation.

Example problem **(EX-3)** has three binary variables and two nonnegative continuous variables. The objective function is linear and the only nonlinear terms appear in the two equality constraints, h_i and h_2.

$$z = min 2x_1 + 3x_2 + 1.5/_1 + 2/_2 - 0.5/_3$$

$$s.t. \quad h\hat{}x.y) = (x\hat{}^2 + K_I = 1.25$$

$$/7_2(x,y) = (x_2)^{15} + 1.5\,y_2 = 3.00$$

$$x_} + y_y <> 1.60 \qquad \textbf{(EX-3)}$$

$$1.333\,x_2 + y_2 \pounds 3.00$$

$$- y, - y_2 + y_3 * o$$

$$x * 0 , y€ \{0,1\}^3$$

There are 2^3 different combinations of the binary variables, meaning 8 NLP subproblems exist. Of these, only 1 combination, y=[0,0,1] is infeasible because it violates the pure integer constraint. The global solution of **(EX-3)** is y'=[0,1,1], x'=[1.118,1.310] with $z^{\#}$=7.667.

Each of the 8 different starting points were tested with DICOPT and the results of phase I are given in Table II. Included in this table are the initial point y^1, the progress of the iterations, and the phase I solutions. Note that 4 of the 8 starting points lead to the global optimal solution in phase I (see Table Ha) while the remaining 4 terminated at the second best solution, y=[1,1,1] with z=7.931 (see Table lib). The two-phase strategy was applied to these 4 starting points. As shown in Table lib, for 3 of these points the global optimum (z=7.667) was identified. Only the starting point $y^{1=}$[1,0,0] failed to yield the global optimum. Interestingly, the value of each binary variable in this starting point is different from the values in the global solution $y^{\#s}$[0,1,1].

To illustrate in some detail the two-phase algorithm, consider the starting point V^1»[1.0,1]. Continuing to **Step** 2, **NLP^1** yields z(y^1)=8.240, x^1=[0.500,2.080], and X^1=[-2.000,-1.387]. z(y^1) < z^oo so z_u is set to 8.240, $y^{\#}$=[1,0,1], and $x^{\#}$={0.500,2.080]. The direction matrix T^1 has diagonal elements t_1 ,$^=t_{22}$=-1. In Step 3, the relaxed linearizations at x^1 for h_l and h_2 are derived:

$$/?^{!;INn)}(x,y)=-x_i - K_l \leq -1.50 \qquad (17)$$

$$/_{?2}^{JNn)}(x,y)=-2.163x_2 - 1\text{-}50/_2 < -4.50$$

With these linear approximations, the master problem (M^1) is formulated and solved in **Step** 4 yielding y^2=[1,1,1] with z^=8.160. Set K=2 and return to **Step** 2 where **(NLP^2)** is solved to give z(y^2)=7.931, x^2=[0.500,1.310], and X^2=[-2.000,-1.747]. z_y is then set to 7.931. Since both of the multipliers remained negative, T^2=T^1. Also, note that (x_1^y^Mx^y^^{2} meaning that in **Step** 3 the linearization of h_i at iteration 2 is identical to that at iteration 1. The master problem at iteration 2 then involves the following linearizations:

$$h_1^{LIN(1)}(x,y) = -x_1 - y_1 \;£\; -1.50 \qquad (18)$$

$$h_2^{LIN(1)}(x,y) = -2.163\,x_2 - 1.50/_2 \leq -4.50$$

$$h_2^{LIN(2)}(x,y) = -1.717\,x_2 - 1.50y_2 \;£\; -3.750$$

From the above linearizations the master problem (M^2) is formulated and solved in Step 4. The lower bound provided by the solution to (M^2) is z_L^2=9.052 which is greater than z_U«7.931; so according to Step 4 b we proceed to Step 5.

In Step 5[a], the local test is performed which first requires that $(\bar{x},\bar{y})^1$ and $(\bar{x},7)^2$ be determined through **(LNLP^1)** and **(LNLP^2)** by setting *=0.05 in (6). By solving these NLP problems, $(\bar{x}$^$\bar{y})^1$ and $(\bar{x},\bar{y})^2$ were found to be [0.475,2.045,1.024,0.050,1.050] and [0.475,1.266,1.024,1.050,1.050], respectively.

The local tests at these two points are as follows:

$h_1^{LIN(1)}(\bar{x}\backslash\bar{y}')$ « -0.475 - 1.024 = -1.499 ≤ -1.500 -> *fails*

$h_2^{LIN(1)}(\bar{x}^1,\bar{y}^1)$ = -2.163*2.045 - 1.500*0.050 = -4.498 ≤ -4.500 → *fails*

$h_1^{LIN(2)}(\bar{x}^2,\bar{y}^2)$ = "0.475 - 1.024 = -1.499 ≤ -1.500 -» *fails*

/ £$^{N(2)}$($\bar{x}^2$,$\bar{y}^2$) = -1.717* 1.266 - 1.500*1.050 = -3.749 <> -3.750 -> *fails*

It can be seen that all 4 linearizations failed the local test.

Step 5[b] is the global test where the linearizations derived at tay)^1 will be checked using the point $(x,y)^2$ and the linearization derived at $(x,y)^2$ will be checked using the point (x,y)\ The global test for the 4 linearizations are shown below.

/?^{l};$^{IN(1>}$(x^2,y^2)=-0.500 - 1.000 = -1.500 £ -1.500 -» *passes*

/7$^L{}_2{}^{im)}$(x^2,y^2)= -2.163* 1.310 - 1.500*1.000 = -4.334 £ -4.500 -» *fails*

/?^{l}J$^{IN(2>}$(x^1/y^1)=-0.500 - 1.000 = -1.500 £ -1.500 -> *passes*

/£$^{N<2)}$(x^1,yV-1.717* 2.080 - 1.500*0.000 = -3.571 £ -3.750 → *fails*

It is the linearization of h_2 which was* found to fail the global test at both test points. Thus, following a similar treatment as in (13), the right hand side coefficients of these two linearization are replaced by the value of the left hand side expressions, -4.334 and -3.571 respectively. In **Step** 5[c] the slack fJ is added to h*;$^{IN(1>}$ according to (14), while the slacks *C* and C_2^2 are added to h^$^{Nn)}$ and h^$^{IN(2)}$ according to (15). Using the information from the above tests, the phase II relaxed master problem is now formulated in **Step 7.**

$$z^2_L = \min_{x,y} 2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 + 100[C_1^+ + C_2^+ + C_3^2]$$

s.t. $-x_1 - y_1 - 1.50\,C_1 \le -1.50$

$-2.163\,x_2 - 1.50\,y_2 - 4.334\,C_2^1 \le -4.334$

$-1.717\,x_2 - 1.50\,y_2 - 3.571\,C_2^2 \le -3.571$

$x_1 + y_1 \le 1.60$ (RM[3])

$1.333\,x_2 + y_2 \le 3.00$

$-y_1 - y_2 + y_3 \le 0$

$2x_1 + 3x_2 + 1.5y_1 + 2y_2 - 0.5y_3 \le 7.931$

$y_1 - y_2 + y_3 \le 1$

$y_1 + y_2 + y_3 \ge 2$

$x \ge 0,\ C \ge 0,\ y \in \{0,1\}^3$

The solution to the relaxed phase II master problem is z^3_L=7.931 at y^3=[0,1,1], with x=[1.500,1.144], and {=[0.000,0.083,0.030]. Proceeding with Step 8, (NLP[3]) is solved to give $z(y^3)$=7.667 at x^3=[1.118,1.310], which corresponds to the global solution of **(EX-3K** Since $z(y^3)<z_u$=7.931, $y^\#$ is set to (0,1,1) and z_y to 7.667.

The linearizations are then derived at x^3 and the local test point $(\bar{x},\bar{y})^3$ is determined through **(LNLP[3]).** These new linearizations are subjected to the local test at $(\bar{x},\bar{y})^3$ and the global test is applied at $(x,y)^1$ and $(x,y)^2$. Finally, the previous linearizations are checked via the global test at $(x,y)^3$. Using the results of these tests, the next phase II master problem is formulated and solved to provide y^4=[0,1,0]. The solution to **(NLP[4])** is $z(y^4)$=8.167 which exceeds the current upper bound of z_u=7.667. At this point, phase II terminates having found the global solution to this nonconvex MINLP problem.

In order to provide further geometrical insight into phase II, refer to Figure 4 where the nonlinear equation h_2 is plotted along with the phase I linearizations and the phase II relaxed linearizations. It is clear that the feasible region defined by the linear inequalities in phase I has cut into the feasible region of h_2. Note also, the global test points $(x,y)^1$ and $(x,y)^2$, and the expansion of the master problem feasible region that results from the modified linearizations of phase II.

Example 4 This example problem addresses the optimal design of muitiproduct batch plants (see Grossmann and Sargent, 1979). It is assumed that the plant consists of M processing stages where fixed amounts Q_i of N products must be manufactured. The design problem consists of determining for each stage j the number of parallel units N_j and their sizes V_j, and for each product i the batch sizes B_i and cycle times T_{Li}. Data for the problem are the horizon time H, cost coefficients α_j, β_j, for the units, and size factors S_{ij} and processing times t_{ij} for each product i at stage j.

The optimal design of muitiproduct batch plants can be formulated as the following MINLP problem **(MIPB1):**

$$z = \min \sum_{j=1}^{M} \alpha_j N_j V_j^{\beta_j} \qquad \textit{(Investment cost)}$$

$$\text{s.t.} \quad V_j \geq S_{ij} B_i \qquad i = 1,N,\ j = 1,M \qquad \textit{(Volume for stage j)}$$

$$N_j T_{Li} \geq t_{ij} \qquad i = 1,N,\ j = 1,M \qquad \textit{(Cycle time for product i)}$$

$$\sum_{i=1}^{N} \frac{Q_i T_{Li}}{B_i} \leq H \qquad \textit{(Horizon constraint)}$$

$$N_j = 1 + \sum_{k=1}^{\bar{K}} 2^{k-1} Y_{kj} \qquad j = 1,M \qquad \textit{(Number parallel units)}$$

$$1 \leq N_j \leq N_j^U \qquad j = 1,M \qquad \textit{(Bounds)}$$

$$V_j^L \leq V_j \leq V_j^U \qquad j = 1,M$$

$$T_{Li}^L \leq T_{Li} \leq T_{Li}^U \qquad i = 1,N$$

$$B_i^L \leq B_i \leq B_i^U \qquad i = 1,N$$

$$Y_{kj} = 0,1 \qquad k = 1,\bar{K},\ j = 1,M$$

where N_j^U, V_j^L and V_j^U are specified bounds, while valid bounds for T_{Li} and B_i can be determined as follows:

$$T_{Li}^L = \max_j \left\{ \frac{t_{ij}}{N_j^U} \right\}, \quad T_{Li}^U = \max_j \{ t_{ij} \} \tag{19}$$

$$B_i^L = \frac{Q_i}{H} \max_j \left\{ \frac{t_{ij}}{N_j^U} \right\}, \quad B_i^U = \min \left\{ Q_i,\ \min_j \frac{V_j^U}{S_{ij}} \right\}$$

The above formulation is similar to the one in Grossmann and Sargent (1979), except that the number of parallel units N_j is expressed in terms of 0-1 variables Y_{kj} through a binary expansion (see Garfinkel and Nemhauser, 1972). As an example, if a maximum number of 4 units is considered for stage j, then $N_j = 1 \cdot Y_{1j} + 2Y_{2j}$ (R=2). In this way, by assigning the different combinations of 0-1 values for Y_{1j} and Y_{2j}, the values $N_j = 1,2,3,4$ can be obtained.

Note that the inequality constraints for volumes and the equations for the number of parallel units are linear, but the rest on the model involves nonlinear functions. The nonlinear inequalities for the cycle times are quasiconvex meaning that the corresponding linearizations will provide valid outer-approximations when the point of linearization satisfies these inequalities as equations. The remainder of the model, the horizon time constraint and the objective function are nonconvex and these functions can cause the OA/ER algorithm to terminate with suboptimal solutions.

Through logarithmic transformations, the above formulation can be modelled as a convex MINLP problem. This requires the definitions of the transformed variables $v_j=\ln[V_j]$, $n_j=\ln[N_j]$, $b_i=\ln[B_i]$, and $t_{Li}=\ln[T_{Li}]$. Also, in this formulation the variables n_j must be expressed in terms of 0-1 variables y_{kj} for each choice of k parallel units, $k=1,..N_j^u$. Using these transformation for the variables V_j, N_j, B_i, and T_{Li} yields the following MINLP problem **(MIPB2):**

$$z = \min \sum_{j=1}^{M} \alpha_j \exp[n_j + \beta_j v_j] \qquad \textit{(investment cost)}$$

$$\text{s.t.} \quad v_j \geq \ln[S_{ij}] + b_i \qquad i = 1, N, \; j = 1, M \qquad \textit{(Volume for stage j)}$$

$$n_j + t_{Li} \geq \ln[t_{ij}] \qquad i = 1, N \; j = 1, M \qquad \textit{(Cycle time for product i)}$$

$$\sum_{i=1}^{N} Q_i \exp[t_{Li} - b_i] \leq H \qquad \textit{(Horizon constraint)}$$

$$n_j = \sum_{k=1}^{N_j^U} \ln[k] \, y_{kj} \qquad j = 1, M \qquad \textit{(Number parallel units)}$$

$$\sum_{k=1}^{N_j^U} y_{kj} = 1 \qquad j = 1, M \qquad \textit{(Only one choice of } n_j\textit{)}$$

$$0 \leq n_j \leq \ln[N_j^U] \qquad j = 1, M \qquad \textit{(Bounds)}$$

$$\ln[V_j^L] \leq v_j \leq \ln[V_j^U] \qquad j = 1, M$$

$$\ln[T_{Li}^L] \leq t_{Li} \leq \ln[T_{Li}^U] \qquad i = 1, N$$

$$\ln[B_i^L] \leq b_i \leq \ln[B_i^U] \qquad i = 1, N$$

$$y_{kj} = 0, 1 \qquad k = 1, N_j^U, \; j = 1, M$$

Note that in this formulation, all nonconvexities have been eliminated. The nonlinearities in this model appear only in the objective function and in the horizon time constraint, and in both cases the exponential terms are convex. Hence, by solving problem **(MIPB2),** one is guaranteed to obtain the global optimum with the OA/ER algorithm.

Table III contains the data for a plant consisting of 6 stages and 5 products and a maximum of 4 parallel units per stage. In **(MIPB1)** only two 0-1 variables are needed per stage due to the use of binary expansions for the number of units in parallel. Hence, the MINLP formulation **(MIPB1)** contains 12 binary variables and 22 continuous variables. The objective function and 31 of the 67 constraints in the model are nonlinear. With formulation **(MIPB2),** there are 24 binary variables and 22 continuous variables. Only the objective function and 1 of the 73 constraints are nonlinear. The global optimum for the 2 equivalent formulations has an investment cost of $285,506 and details of the optimal solution are shown in Table IV.

The two-phase strategy was applied with DICOPT on an IBM 3090-600 to both formulations so as to determine the optimal design and the results from various starting points are given in Table V[2]. As expected, the global optimum is found in phase I with the convex formulation **(MIPB2),** and no violations were detected in the local and global test. Note however, that formulation **(MIPB2)** tends to typically require one or two more iterations and an average of 6% more CPU-time than the original nonconvex formulation **(MIPB1).** The drawback of the nonconvex formulation is that phase I predicts suboptimal solutions in 5 of the 10 starting points which were investigated. Phase **II** was then applied in attempt to improve upon the phase I solution. In this problem, only the global test was activated in phase **II.** In almost all cases, the objective function and horizon constraint failed the global tests, and in some instances a few of the cycle time constraints failed the global tests.

The phase **II** results for the 5 starting points which lead to suboptimal solutions in phase I with formulation **(MIPB1)** are shown in Table VI. 3 out of the 5 cases improved upon the phase I solution, locating the global optimum twice. Note that on the average, the phase **II** procedure increased the CPU-time requirement by 87% with respect to phase I. Taking into account the 5 starting points which lead to the global optimum in phase I, the optimal solution of z=$285506.5 was found in 7 of the 10 cases studied. The suboptimal solutions of z=$304,660. and $328,260. were found twice and once respectively.

Example 5,

The final example will demonstrate the use of the proposed two-phase strategy on a nonconvex MINLP problem which arises in the synthesis of chemical processes. The goal is to determine both the optimal structure and operation of a chemical process flowsheet. First, a superstructure is proposed which contains several alternative flowsheets candidates. The problem is then modelled as an MINLP involving the maximization **of** profit subject to material and energy balances, equilibrium relations, and design specifications. The resulting formulation contains a wide variety of **nonlinear functions, many** of which introduce nonconvexities, making this MINLP problem a very **good** candidate for the two-phase procedure.

The superstructure selected for this example is shown in Figure 5. Feedstock F1 contains only component A whereas feedstocks F2 and F3 are mixtures of components A, B, and inert D with different compositions and purchase costs. These

[2] **For convenience starting points are given in terms of number of parallel units instead of 0-1 variables.**

3 streams enter at 300 K and 1.0 MPa and will require compression since the reactor must operate above 2.5 MPa. A choice between single-stage compression or two-stage compression with intermediate cooling exists. The reactor feed stream can then be either heated or cooled before entering one of the three available reaction units. Reactor R1 has the highest conversion per pass and is the most expensive reactor, followed by R2 and R3. The reaction is 2A+B-»C and component D is inert. The reactor effluent stream is then expanded and cooled before entering a flash separation tank where the heavy product C is separated from unreacted raw materials A and B and inert D. The bottom stream can then be sold (P1), or purified further in a second flash separator and sold at a higher price (P2). The vapor streams from the flash units can be recycled and mixed with the reactor feed stream or sent to a membrane separator. The permeate stream leaving the membrane separator is rich in component A and can reduce the requirement of feedstocks F1, F2, and F3.

This superstructure was modelled as an optimization problem having the structure of problem **(MINLP).** The formulation contains 9 binary variables (see Figure 5) and 416 continuous variables. There are 420 constraints, of which 130 are nonlinear equations. Important problem data is given in Table VII and a summary of the unit models are given in Table VIII (see Kocis, 1988, for detailed models). This nonconvex MINLP problem was solved using the OA/ER algorithm with the phase **II** procedure for handling nonconvexities. The results presented were obtained on an IBM 3090-600 using DICOPT.

The results obtained using two different starting points are given in Table IX. Since in this problem the objective function (profit) is being maximized, the NLP subproblems provide the lower bound and the MILP master problems supply the upper bound. In both cases the global solution with a profit of 10.173 (10^6\$/yr) was identified. The optimal assignment of binary variables is $y^{\#}$=[001111000] which corresponds to the flowsheet structure shown in Figure 6. Feedstock F3 with single stage feed compression, reactor R1, and both flash separators were present in the optimal flowsheet. Most of the vapor stream from the first flash was recycled and mixed with the reactor feed stream, and the rest was sent to the membrane separator where the permeate stream was recycled. The membrane raffinate stream BP3 was sold as a byproduct. All of the bottom stream from the first flash was sent to the second flash. The vapor phase was recycled and mixed with the reactor feed while the liquid phase was sold as the high purity product P2. Table X summarizes the optimal operating conditions in this flowsheet.

As seen in Table IX, the first starting point considered was y^1=[110101000]. This flowsheet, which is shown in Figure 7a, uses feedstock F1 and F2, single-stage compression, reactor R1, both flash separators but no membrane separator. The objective function value for this NLP subproblem is 4.050 (10^6\$/yr). Phase I terminates at the second iteration with z*=7.925 since the upper bound predicted by the second master problem (1.010) is less than the current lower bound. Nonconvexities in the MINLP model have caused the OA/ER algorithm to terminate at a suboptimal solution.

In phase II only the global test was used to identify nonconvexities. Linearizations which failed the global test were shifted through relaxation of right hand side coefficients. The first phase II master problem provided a valid upper bound (26.600) and identified the global solution y=[001111000]. The binary variables were fixed at the master problem solution and the resulting NLP subproblem was solved to yield z=10.173 (10^6\$/yr). Since this is an improvement upon the previous lower bound of 7.925, another iteration of phase II is performed. The next master problem predicted a new set of binary variables and a valid upper bound on the global optimum. However, the NLP subproblem for the value of binary variables from this master problem had a solution of 4.584 and phase II terminated since no improvement was made upon the current best solution of 10.173. From this starting point, the two-phase strategy required the solution of only 4 NLP subproblems in locating the global solution of this nonconvex MINLP problem. With this starting point, the total CPU time required with DICOPT for the NLP and MILP problems was 106.8 seconds.

y^t 101011000] was selected as the second starting point. As shown in Figure 7b, this corresponds to a flowsheet with feedstocks F1 and F3, single-stage compression, reactor R1, one flash separator and the membrane separator. The NLP subproblem was solved yielding a profit for this flowsheet of 7.926 (10^6\$/yr). Phase I terminated in just 3 iterations, this time with the global solution of 10.173 (10^6\$/yr). The global tests and relaxation of right hand side coefficients were performed to yield the phase II master problem. The solution to this MILP lead to an NLP subproblem with z=8.926, which is not an improvement over the phase I solution of 10.173, and therefore phase II terminates. As in the previous starting point, the two-phase procedure required a total of just 4 iterations to converge to the global optimum. The solution of NLP and MILP problems in DICOPT required a total 147.0 CPU seconds for this starting point.

The MINLP formulation of this problem involved 9 binary variables meaning that approximately 500 different flowsheet configurations were embedded within the selected superstructure. The two-phase strategy was quite efficient in identifying the global solution since it had to examine and optimize less than 1% of the different configurations.

CONCLUSIONS

It has been shown in this paper that the master problem in the outer-approximation algorithm for solving MINLP problems can sometimes cut off the global optimum solution when nonconvexities are present. This case arises in synthesis problems that involve complex nonlinear models. To remedy this problem, a two-phase strategy has been proposed that relies on local and global convexity tests in phase I, and a modified relaxed master problem in phase II. Although the proposed scheme is not mathematically guaranteed to always find the global optimum, it represents a strategy where all the numerical information is fully exploited in attempt to find the global solution.

Numerical experience with the two-phase strategy has been encouraging as was shown in the example problems. In examples 3 and 4, the global solutions were found in 7 of 8, and 7 of 10 initial points, respectively, and in example 5 in both of the starting points. The results of example 4, the design of multiproduct batch plants, illustrates the importance of convexifying a problem through transformations when this is possible in order to guarantee the global optimum. The experience with a structural flowsheet optimization problem, example 5, showed that nonconvexities in these problems can lead to suboptimal solutions with the OA/ER algorithm. Since in this case, convexification is virtually impossible due to the complexity of the models, there is a clear need for global optimization strategies such as the one presented in this paper.

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Table I. Results for Capital Budgeting Problem with OA/ER algorithm

INITIAL POINT	ITERATION	1	2	3	4
y^{1}=[0.0,1,1]	NLP	- 6.0			
	MILP	- 5.0			
y'-M.o.i.n	NLP	- 3.0	0.0	- 6.0	
	MILP	- 9.0	- 8.0	1.0	
y^{1}=[O,1,O,1]	NLP	- 1.0	- 6.0		
	MILP	- 4.0	- 3.0		
y^{1}=[1.0,0,1]	NLP	0.0	6.0	- 3.0	- 6.0
	MILP	-24.0	-12.0	- 8.0	1.0
y^{1}=[1,1,0,1]	NLP	2.0	0.0	- 6.0	
	MILP	-10.0	- 6.0	- 1.0	
y'=[0,1,1,1]	NLP	8.0	0.0	- 6.0	
	MILP	-10.0	-6.0	- 1.0	
y^{1s}[1.1.1,1]	NLP	20.0	0.0	- 3.0	- 6.0
	MILP	-40.0	-12.0	- 8.0	1.0
y^{1}=[1.1.1.0]	NLP	60.0	0.0	- 3.0	- 6.0
	MILP	-84.0	-12.0	- 8.0	1.0

Table II. Results for Problem (EX-3)

a. Starting Points Which Found Optimal Solution in Phase I

INITIAL POINT	ITERATION	1	2
$y^{1=}$[0,1,1]	NLP	7.667	
	MILP	8.167	
y^{1s}[0,1,0]	NLP	8.167	7.667
	MILP	7.667	8.788
y^EO.O.O]	NLP	8.476	7.667
	MILP	7.896	8.396
yMO.0.1]	NLP	infeasible	7.667
	MILP	7.896	8.788

b. Starting Points Which Found Sub-Optimal Solution in Phase I

INITIAL POINT	ITERATION	1	2	3	4
yM 1.1.1]	NLP	7.931	7.667	8.167	
	MILP Phase I	8.431			
	MILP Phase II		7.931	7.667	
yMi.0.1]	NLP	8.240	7.931	7.667	8.167
	MILP Phase I	8.160	9.052		
	MILP Phase II			7.931	7.667
y'-E 1.1.0]	NLP	8.431	7.931	7.667	8.167
	MILP Phase I	7.931	8.431		
	MILP Phase II			7.931	7.667
y'»[1.0,0]	NLP	8.740	7.931	8.240	
	MILP Phase I	8.160	8.552		
	MILP Phase II			7.931	

Table III. Problem (EX-4) Data

	Stages M=6	Products N=5	
Cost Coefficients:	a_j = \$250	V = 0.6	i-i ,6
Bounds on Volumes:	V_j^L = 300 l	V_j^U = 3000 l	i»i ,6
Maximum Number of Parallel Units:		N_j^u = 4	i-i ,6

Horizon Time: H = 6000 hrs

Q_i: Production Rate of Product i (kg)

A	B	C	D	E
250000.	150000.	180000.	160000.	120000.

S_{ij}: Size Factor for Product i in Stage j (l/kg)

	1	2	3	4	5	6
A	7.9	2.0	5.2	4.9	6.1	4.2
B	0.7	0.8	0.9	3.4	2.1	2.5
C	0.7	2.6	1.6	3.6	3.2	2.9
D	4.7	2.3	1.6	2.7	1.2	2.5
E	1.2	3.6	2.4	4.5	1.6	2.1

t_{ij}: Procesing Time for Product i in Stage j (hr)

	1	2	3	4	5	6
A	6.4	4.7	8.3	3.9	2.1	1.2
B	6.8	6.4	6.5	4.4	2.3	3.2
C	1.0	6.3	5.4	11.9	5.7	6.2
D	3.2	3.0	3.5	3.3	2.8	3.4
E	2.1	2.5	4.2	3.6	3.7	2.2

Table IV. Optimal **Solution** for **Problem (EX-4)**

Investment Cost $285,506.

Product	**A**	**B**	**C**	**D**	**E**
T_{Lj} **(hr)**	**3.2**	**3.4**	**6.2**	**3.4**	**3.7**
B_i **(kg)**	380.	770.	730.	638.	525.

Stage	**1**	**2**	**3**	**4**	**5**	**6**
N_i	2	2	3	2	1	1
V_i *(l)*	3000.	1892.	1975.	2619.	2328.	2110.

Binary Variables in Formulation **(MIPB1):** Y_{k_j}

1	1	1	0	1	0	0
2	0	0	1	0	0	0

Binary Variables in Formulation **(MIPB2):** y_{k_j}

1	0	0	0	0	1	1
2	1	1	0	1	0	0
3	0	0	1	0	0	0
4	0	0	0	0	0	0

Table V. Phase I Results in Problem (EX-4)

INITIAL POINT	FORMULATION (MIPB1)		FORMULATION (MIPB2)	
NO. UNITS N_j	SOLUTION	ITERATIONS	SOLUTION	ITERATIONS
(4,4,4.4,4.4)	304,660.	3	285,506.5	4
(1,1,1.1,1,1)	304.660.	2	285,506.5	5
(3,3,3,3,3,3)	313.575.	3	285.506.5	4
(2.2,2.2,2,2)	285,506.5	3	285,506.5	**2**
(3,3,4,4,3,3)	304,660.	3	285.506.5	4
(2,2,3,2,2.2)	285,506.5	3	285,506.5	3
(2.1,2.2,1.1)	285,506.5	3	285,506.5	**5**
(1.1,2.1,1,1)	285,506.5	3	285,506.5	4
(2,1,1,1,1,1)	**285,506.5**	2	285.506.5	**4**
(3,3,4,3,3,3)	**349,864.6**	2	285,506.5	3

Average Total CPU-time	5.26 seconds	**5.55 seconds**
Average Total NLP CPU-time	0.97 seconds	**1.52 seconds**
Average Total MILP CPU-time	4.29 seconds	**4.03 seconds**

Table VI. Phase **II** Results in Problem **(EX-4)** for **(MIPB1)**

INITIAL POINT NO. UNITS N_j	PHASE I SOLUTION	PHASE II SOLUTION	PHASE II ITERATIONS	TOTAL ITERATIONS
(4,4,4,4,4.4)	304,660.	329,222.	1	4
(1,1,1,1,1,1)	304,660.	285,506.5	2	4
(3,3,3,3,3,3)	313,575.	285,506.5	3	6
(3,3,4,4,3,3)	304,660.	322,166.	1	4
(3,3,4,3,3,3)	349,864.6	328,260.	2	4
Average Total CPU-time			3.78 seconds	9.85 seconds

Table VII. Problem Data for Problem (EX-5)

Feedstock or Product/Byproduct	Composition	Costs/Price <$/kg-mole)
F1	100% A	0.163
F2	40% A 50% B 10% D	0.065
F3	35% A 50% B 15% D	0.049
Product PI	≥ 97.5% C ≤ 172,800 kg-mol/day	0.441
Product P2	£ 99% C £ 172,800 kg-mol/day	0.490
Byproduct BP1		0.039
Byproduct BP2		0.039
Byproduct BP3		0.082
Byproduct BP4		0.098

Utilities	Costs
Electricity	\$0.03/kW-hr
Heating (steam)	$\$8.0/10^6$ kJ
Cooling (water)	$\$0.7/10^6$ kJ

<u>Design Specifications</u>

Reactor

Pressure, MPa	$2.5 \leq P \leq 15.$
Temperature, K	$423 \leq T^{IN} \leq 623.$ $523 \leq T^{OUT} \leq 673.$

Flash Separators

Pressure, MPa	$1. \leq P \leq 10.$
Temperature, K	300. £ T^{IN} £ 500.

Table **VIII. Model Types** Used in Problem **(EX-5)**

COMPRESSION:		
Power Requirement -	Isentropic - ideal gas	nonlinear
EXPANSION VALVE:		
Heat Balance -	Adiabatic - ideal gas	nonlinear
FLASH SEPARATION:		
Equilibrium Relation -	Raoult's Law	nonlinear
Vapor Pressures -	Antoine relation	nonlinear
Mass Balance -		linear
HEAT EXCHANGER:		
Heat Balance -	Constant heat capacity	nonlinear
MEMBRANE SEPARATION:		
Recovery Relation -	Constant split fraction	linear
Mass Balance -		linear
MIXER:		
Heat Balance -	Constant heat capacity	nonlinear
Mass Balance -		linear
SPLITTER:		
Mass Balance -	Through split fractions	nonlinear
REACTOR:		
Equilibrium Conversion -	Correlation	nonlinear
Heat Balance -	Adiabatic exothermic	nonlinear
Mass Balance -		nonlinear
OBJECTIVE FUNCTION		
Revenue from sales , raw material and utility costs		linear
Investment costs		linear with fixed charges

Table **IX.** Two-Phase Strategy Results for **(EX-5)**

INITIAL POINT y^1	ITERATION	1	2	3	4
			(10*$/yr>		
[110101000]	NLP	4.050	7.925	10.173	4.584
MILP	Phase I	12.350	1.010		
MILP	Phase II			**26.600**	24.185

Total NLP CPU-time = 96.1 seconds
Total MILP CPU-time = 10.7 seconds
Total CPU-time = 106.8 seconds .

INITIAL POINT y^1	ITERATION	1	2	3	4
			do^5$/yr>		
[101011000]	NLP	7.926	9.173	10.173	8.926
MILP	Phase I	12.532	9.290	7.667	
MILP	Phase II				10.910

Total NLP CPU-time = 135.6 seconds
Total MILP CPU-time * 11.4 seconds
Total CPU-time « 147.0 seconds

Table X. Optimal Solution for Problem (EX-5)

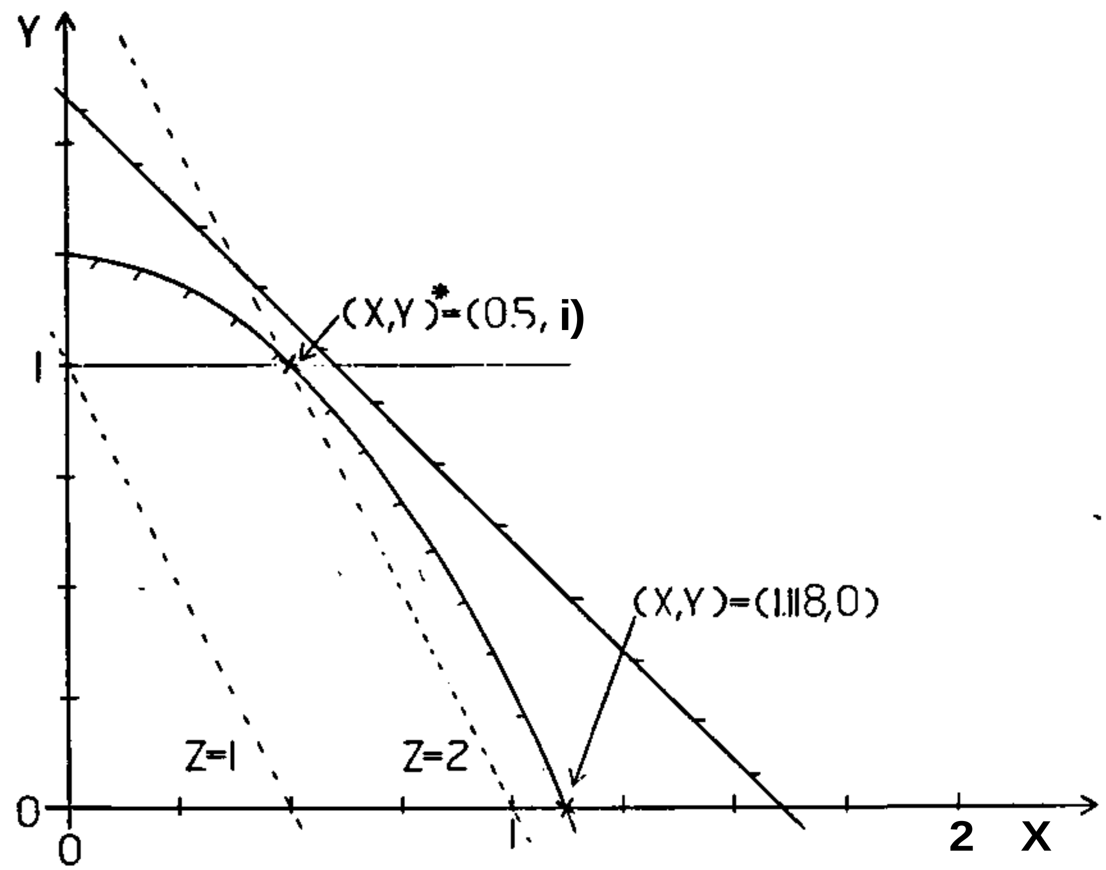
Feedstock or Product/Byproduct	Flowrate (kg-mol/day)	
F3	760,130	
P2	172,800	
BP3	511,090	

Utilities		Requirement
Electricity (kW)	compressor #1	3490.
	compressor #4	1443.
Heating (steam, kW)	heat exchanger #2	8.265
Cooling (water, kW)	heat exchanger #3	106.84

Reactor		
Pressure, MPa	2.5	
Temperature, K	347. (inlet)	**449. (outlet)**
Conversion per Pass of A	25.28 %	
Flash Separators	**F-1**	**F-2**
Pressure, MPa	**2.04**	**2.04**
Temperature, K	**300.**	**422.**
Recycle Flowrates		
RC1 (kg-mol/day)	**1.629.115**	
RC2 (kg-mol/day)	**274,717**	
Overall Conversion of A	**92.34 %**	

Figure 1. Feasible Region **and** Objective Function **in (EX-1)**

(a) Objective Function Contours and Nonlinear Feasible Region



(b) Feasible Region in Phase I Master Problem

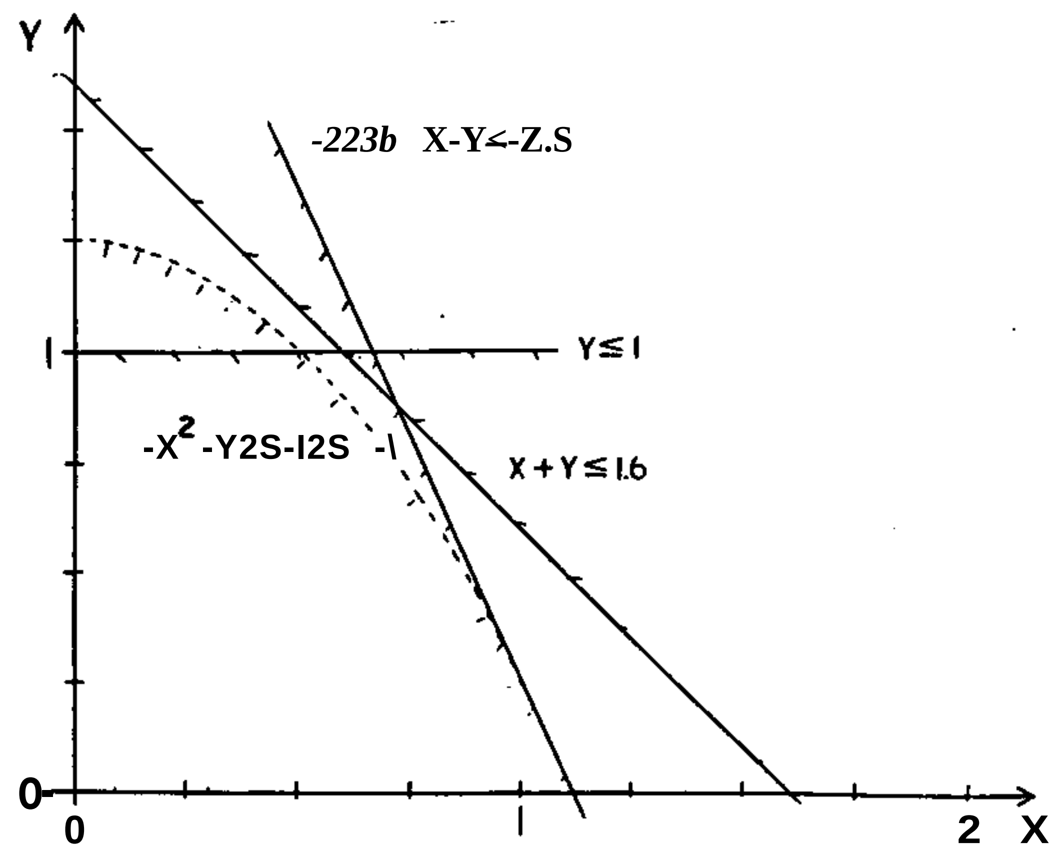


Figure 2. Steps in Two-Phase Strategy

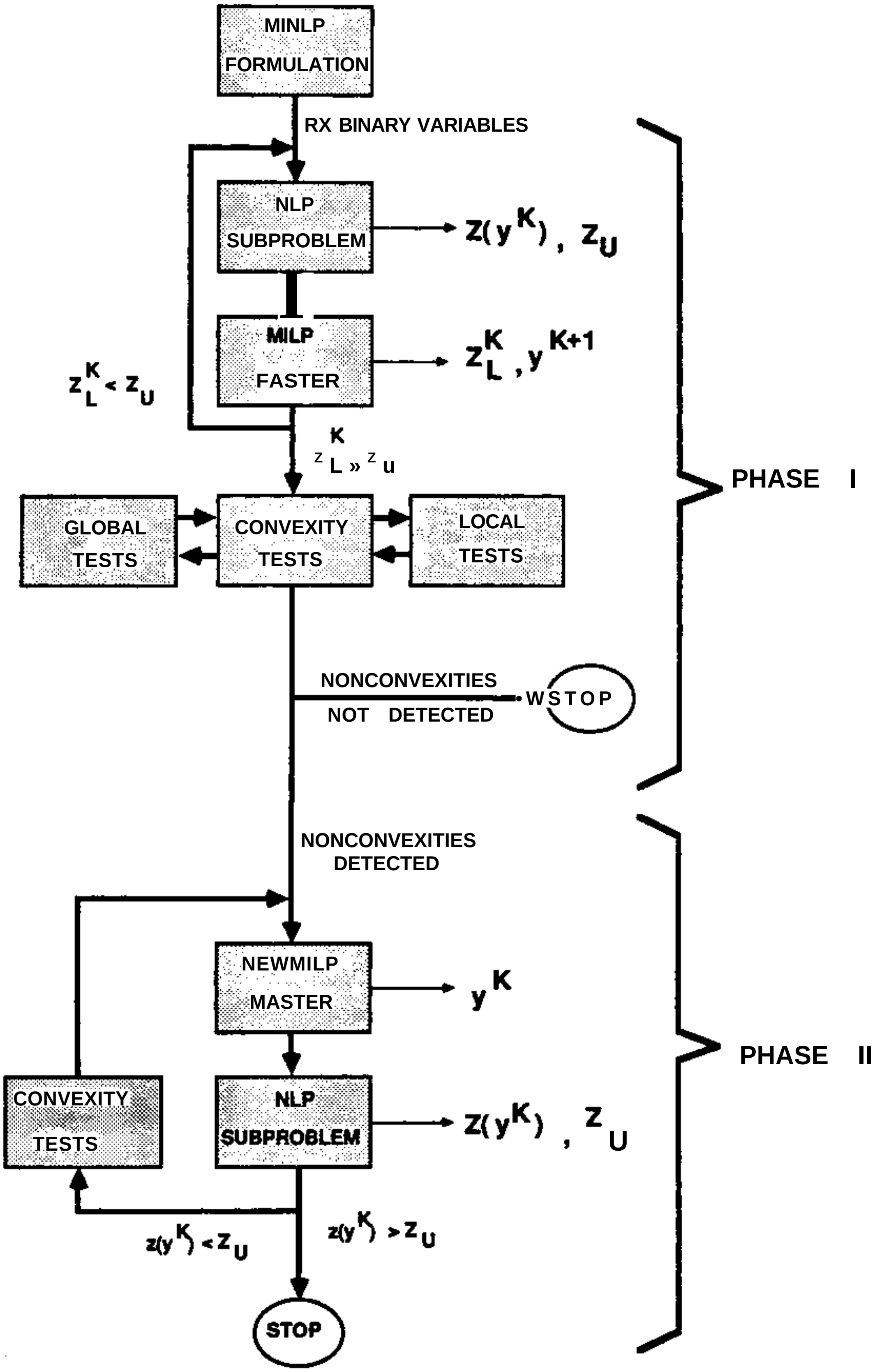


Figure 3. Nonlinear Constraint Linearization, **and** Relaxed Linearization in (EX-3)

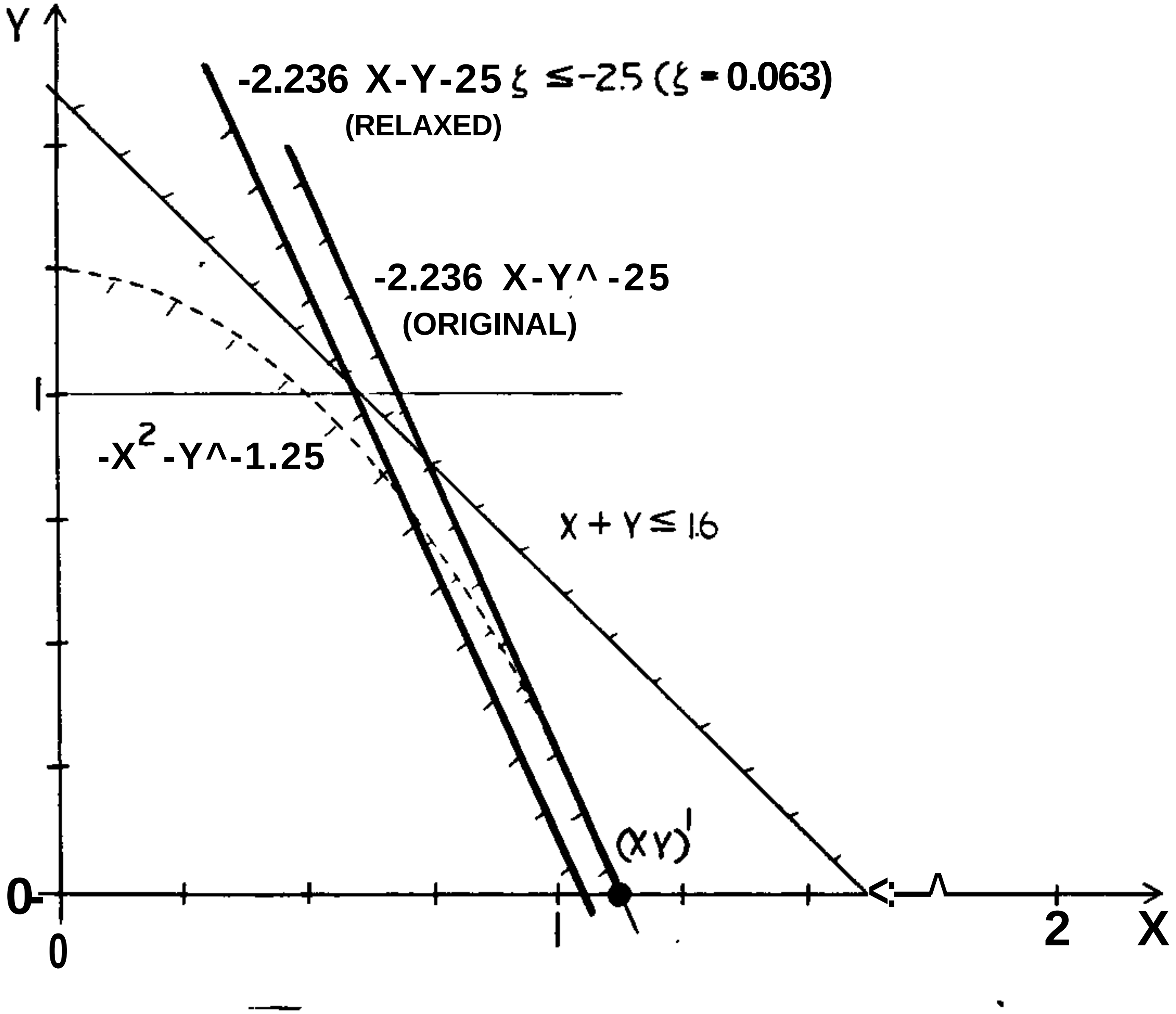
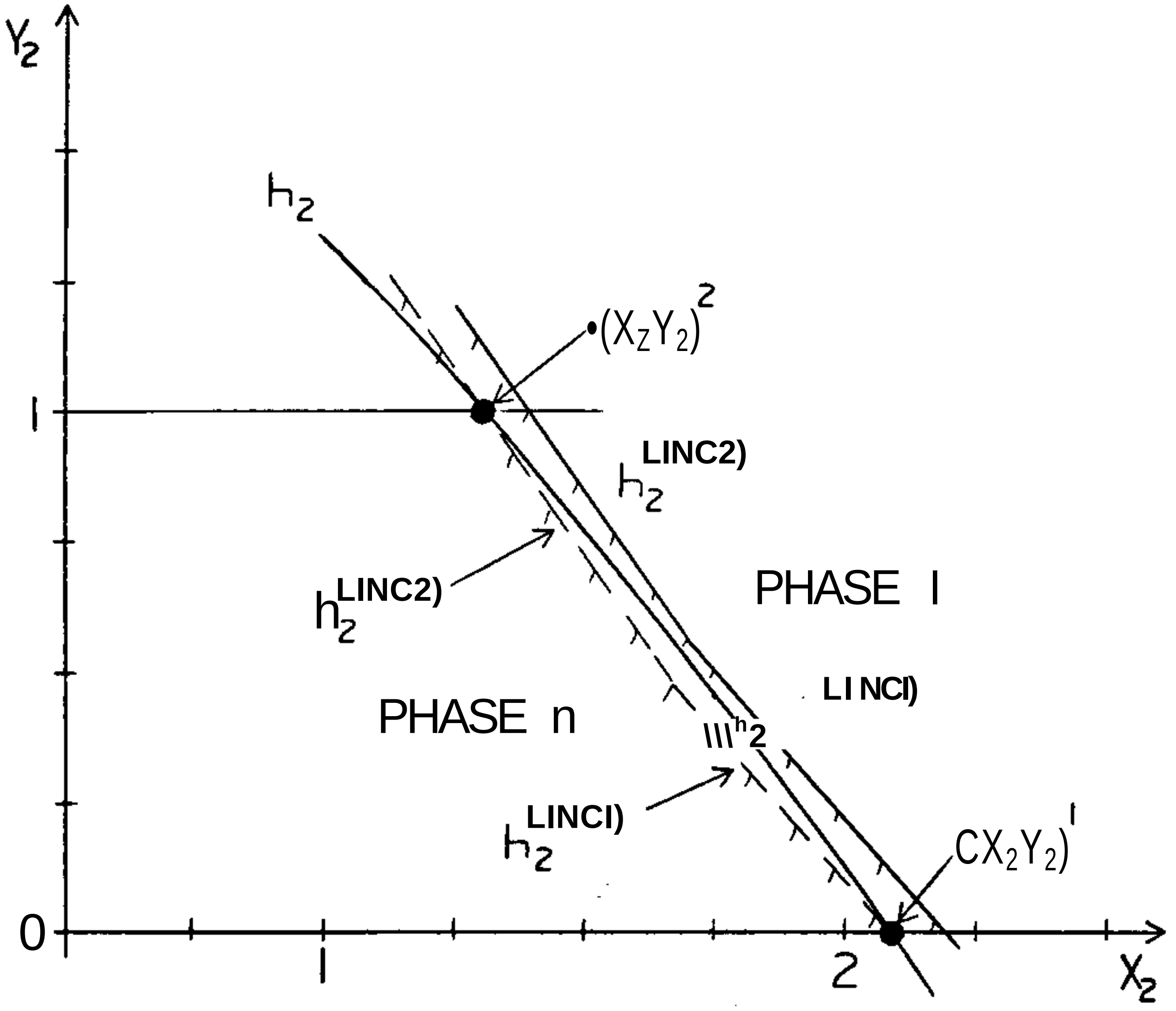


Figure 4. Global Test and Relaxed Linearizations in Problem (EX-3)



Figures. Superstructure for Problem (EX-5)

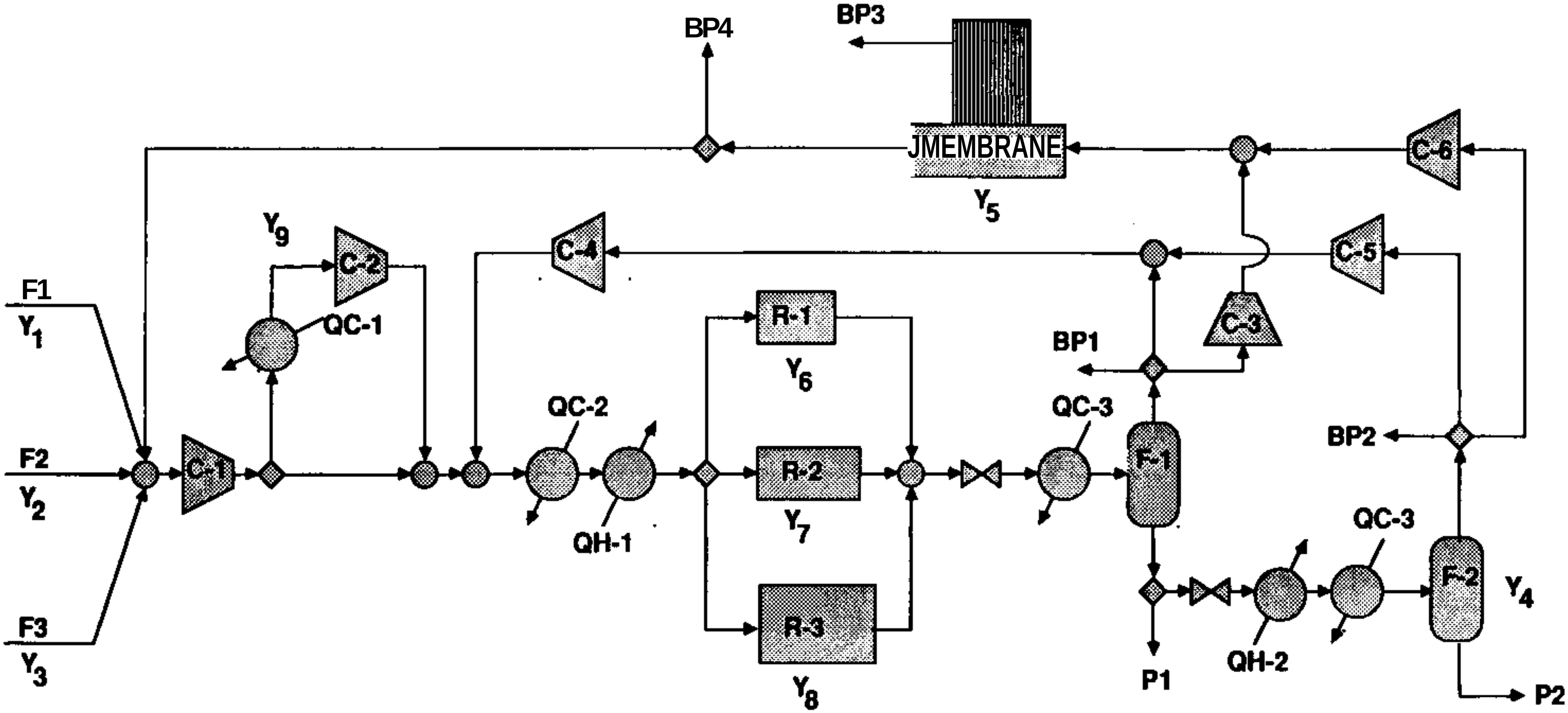


Figure 6. Optimal Flowsheet Structure in (EX-5)

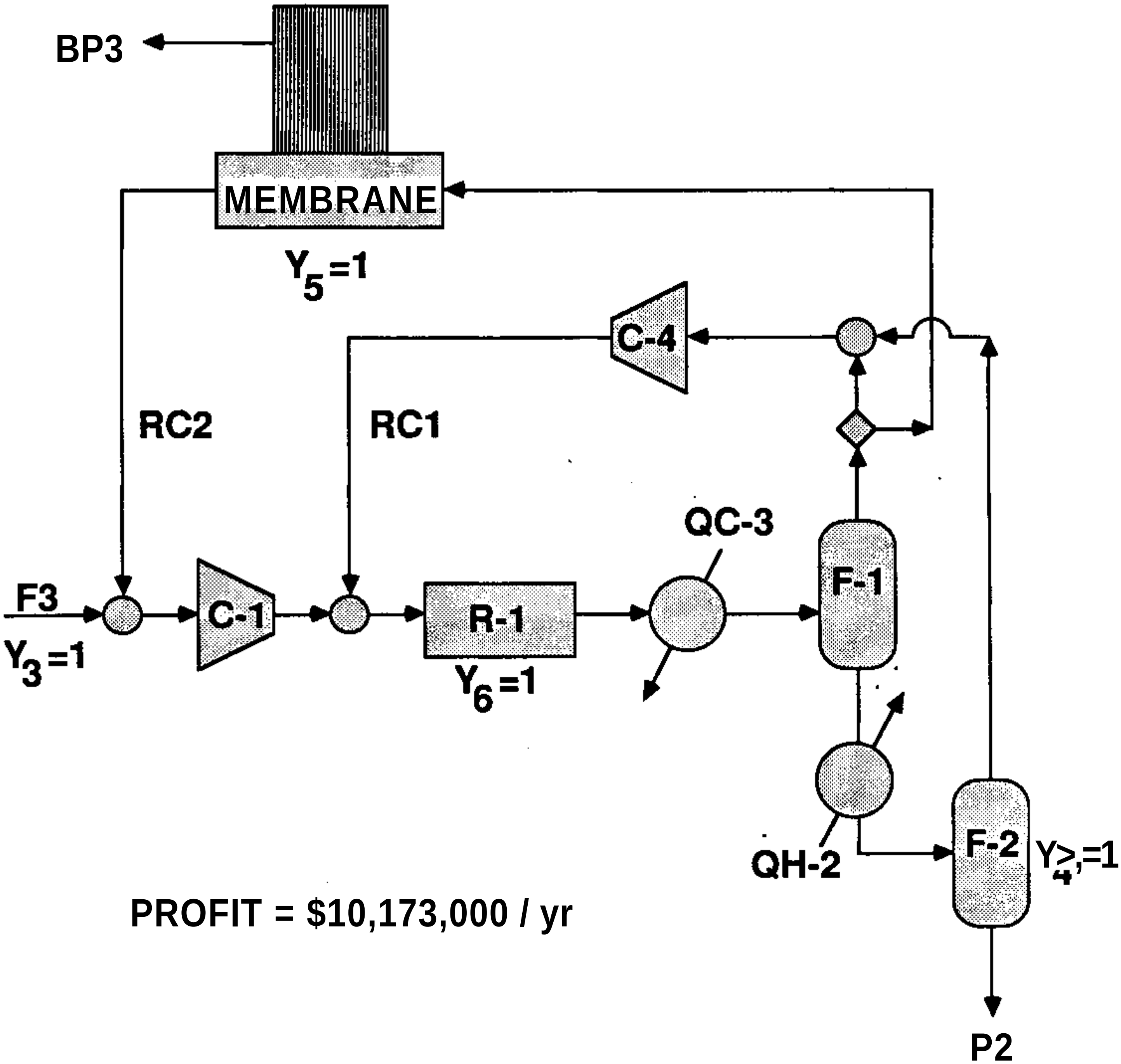
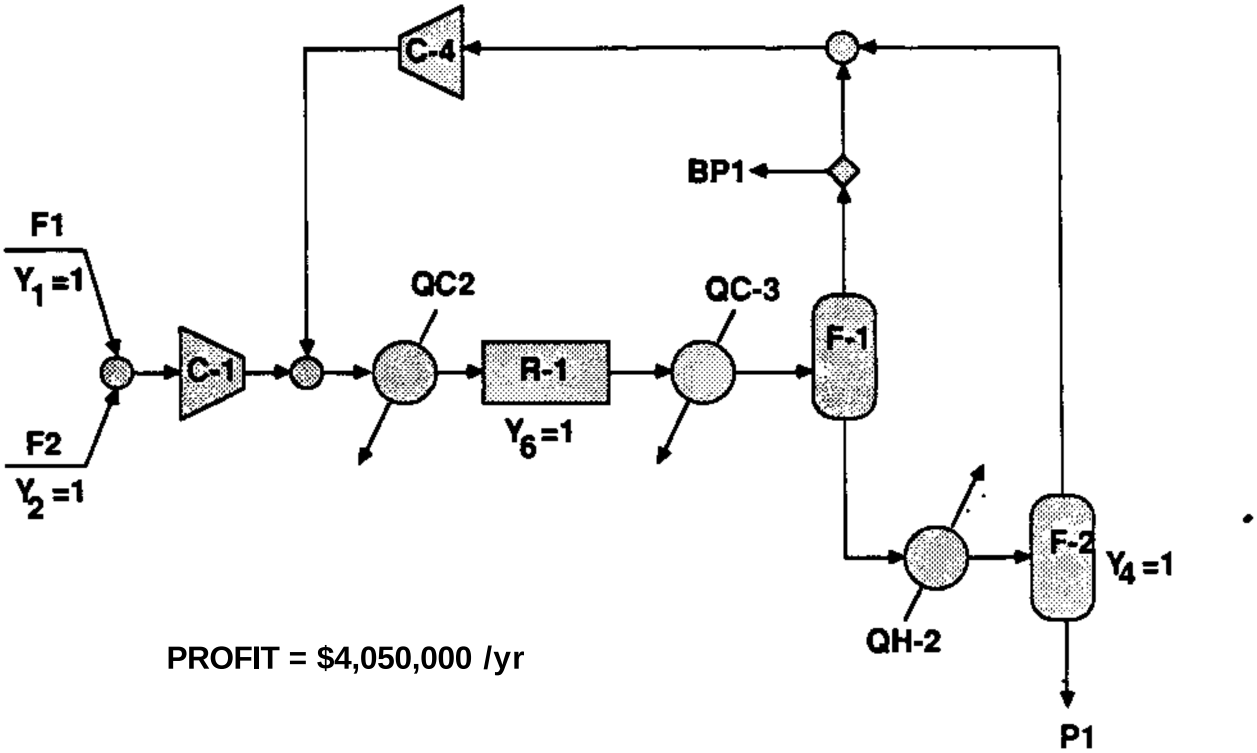
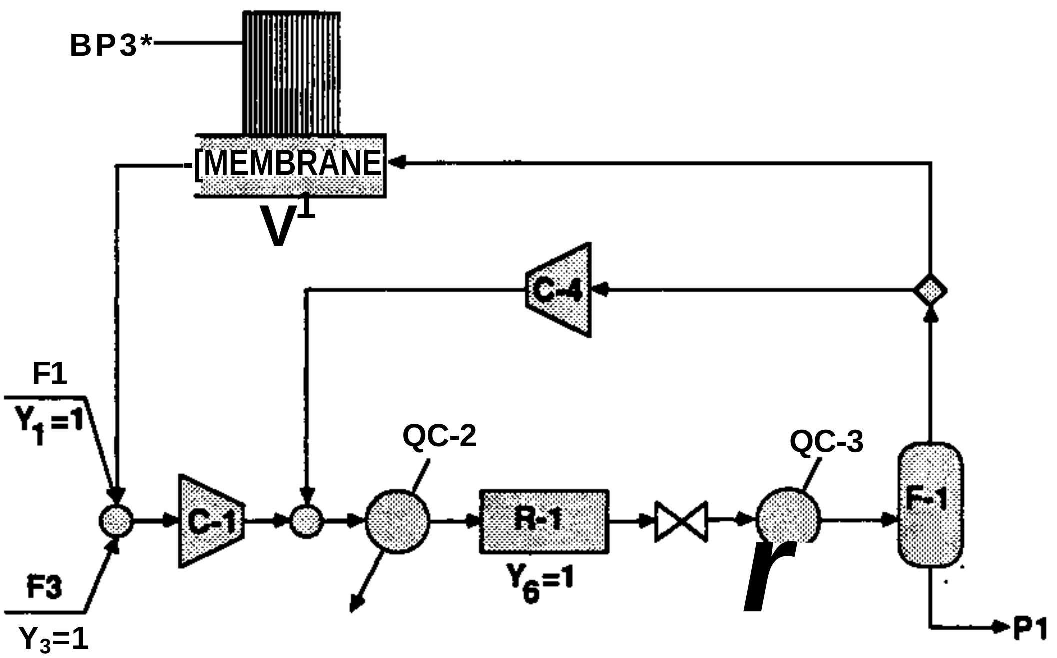


Figure 7. Initial Points in Problem (EX-5)

(a) $y^1 = [1,1,0,1,0,1,0,0,0]$



(b) $y^1 = [1,0,1,0,1,1,0,0,0]$



PRORT = $7,926,000 / yr