This article was downloaded by:[University of Oklahoma Libraries] On: 22 September 2007 Access Details: [subscription number 731942891] Publisher: Taylor & Francis Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



# Chemical Engineering Communications

Publication details, including instructions for authors and subscription information: http://www.informaworld.com/smpp/title~content=t713454788

A GLOBAL OPTIMIZATION APPROACH TO RATIONALLY CONSTRAINED RATIONAL PROGRAMMING

Vasilios Manousiouthakis <sup>a</sup>; Dennis Sourlas <sup>a</sup> <sup>a</sup> Chemical Engineering Department, University of California, Los Angeles, CA

Online Publication Date: 01 January 1992 To cite this Article: Manousiouthakis, Vasilios and Sourlas, Dennis (1992) 'A GLOBAL OPTIMIZATION APPROACH TO RATIONALLY CONSTRAINED RATIONAL PROGRAMMING ', Chemical Engineering Communications, 115:1, 127 -147

To link to this article: DOI: 10.1080/00986449208936033 URL: <u>http://dx.doi.org/10.1080/00986449208936033</u>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.informaworld.com/terms-and-conditions-of-access.pdf

This article maybe used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

Chem. Eng. Comm. 1992, Vol. 115, pp. 127-147 Reprints available directly from the publisher. Photocopying permitted by license only. © 1992 Gordon and Breach Science Publishers S.A. Printed in the United States of America

# A GLOBAL OPTIMIZATION APPROACH TO RATIONALLY CONSTRAINED RATIONAL PROGRAMMING<sup>†</sup><sup>‡</sup>

# VASILIOS MANOUSIOUTHAKIS\*, and DENNIS SOURLAS

**Chemical Engineering Department** University of California Los Angeles, CA 90024-1592

(Received January 2, 1991; in final form November 5, 1991)

The rationally constrained rational programming (RCRP) problem is shown, for the first time, to be equivalent to the quadratically constrained quadratic programming problem with convex objective function and constraints that are all convex except for one that is concave and separable. This equivalence is then used in developing a novel implementation of the Generalized Benders Decomposition (GBDA) which, unlike all earlier implementations, is guaranteed to identify the global optimum of the RCRP problem. It is also shown, that the critical step in the proposed GBDA implementation is the solution of the master problem which is a quadratically constrained, separable, reverse convex programming problem that must be solved globally. Algorithmic approaches to the solution of such problems are discussed and illustrative examples are presented.

KEYWORDS Global Optimization Decomposition Reverse convex.

#### I. INTRODUCTION

The class of rationally constrained rational programming (RCRP) problems and its subclass of polynomially constrained polynomial programming (PCPP) problems are often encountered in chemical engineering applications. The heat exchanger network synthesis problem can be formulated as a mixed integer nonlinear programming problem (Grossmann, 1990) that can be further transformed into a PCPP through the introduction of additional nonlinear constraints and the use of polynomial approximations of the objective function. Indeed, the requirement that a variable  $\delta$  be binary is equivalent to the quadratic equality  $\delta(\delta - 1) = 0$ , where  $\delta$  is assumed to be continuous. The robust controller design problem can be formulated as a minimax optimization problem. The latter has been shown to be equivalent to a linear programming problem with several additional quadratic equality constraints (Manousiouthakis and Sourlas, 1990). Global solution of such optimization problems is being pursued by several chemical engineering researchers (Manousiouthakis et al., 1990, Swaney, 1990. Visweswaran and Floudas, 1990).

<sup>†</sup> Part of this work was first presented at the 1990 Annual AIChE Meeting at Chicago, Paper No. 22d.

<sup>&</sup>lt;sup>‡</sup> Part of this work will be presented at the 1992 ORSA Meeting in Orlando, Florida. <sup>\*</sup> To whom correspondence should be addressed.

An optimization problem that belongs to one of these classes has several local minima (or maxima). There are special cases (i.e. minimization problems with convex objective and convex constraints such as: linear programming, positive semidefinite quadratic programming, etc.) where the objective value at all local minima is the same, hence any local minimum is also global. As a result, for this subclass of problems efficient large scale optimization algorithms have been developed.

However, most RCRP problems do not enjoy this property, namely not all local minima are global, and are thus more difficult to solve. In the case of the negative definite quadratic programming problem (NDQP) it has been established that the global optima are among the extreme points of the feasible region (which in this case is a convex polyhedron) (Charnes & Cooper, 1961). For the indefinite quadratic programming problem (IDQP) it has been established that the global optima lie on the feasible region's boundary (Mueller, 1970).

Another class of problems that has the same extreme point property is the class of concave minimization (or convex maximization) problems over a polyhedral feasible region. One can identify the global solution to this problem by total enumeration of the extreme points of the feasible region. These methods become computationally intensive for large scale problems. In this spirit, Cabot and Francis (1970) combined extreme point ranking techniques (Murty, 1969) with underestimating techniques to solve the quadratic concave minimization problem. Cutting plane methods have also been employed for the solution of the concave minimization problem. In that regard, Tuy (1964) introduced a cone splitting procedure (Tuy cuts) which was later demonstrated by Zwart (1973) to exhibit convergence problems. Zwart (1974) later presented a modified algorithm that is computationally finite. Several researchers have generalized the idea of Tuy cuts. Jacobsen (1981) proposed a similar algorithm and provided proof for its convergence. Glover (1973) extended the notion of the Tuy cuts and introduced so called convexity cuts.

In addition to the extreme point enumeration and the cutting plane methods, branch and bound techniques have also been used. Falk and Soland (1969) and Soland (1971) proposed algorithms applicable to separable problems. Horst (1976) presented an algorithm that can be used to solve nonseparable problems as well. Hoffman (1981) also presented a global optimization algorithm based on underestimating techniques. Pardalos and Rosen (1986) give an excellent review on the subject of concave minimization.

The extreme point property is also satisfied by the class of reverse convex programming (RCP) problems. A constraint  $g(x) \ge 0$  is called reverse convex when g(x) is quasiconvex (i.e.  $g(\lambda x_1 + (1 - \lambda)x_2) \le \max\{g(x_1), g(x_2)\}$  for all  $\lambda \in [0, 1]$ ). An optimization problem that involves reverse convex constraints and pseudo concave objective is a RCP problem. Using (1972) proposed a combinatorial procedure that yields the global optimum of RCP problems, when the objective function is strictly concave and the constraints are convex. For the solution of the general RCP problem, Hillestad and Jacobsen (1980a) proposed a cutting plane algorithm which however could exhibit convergence to infeasible points, as they demonstrated. Finally, for the special RCP problem of linear

programming with one reverse convex constraint, Hillestad and Jacobsen (1980b) proposed a finite algorithm.

Linear Programming with one reverse convex constraint can also be viewed as a special case of convex minimization problems with an additional reverse convex constraint. For this general class of problems Tuy (1987) proposed a method that reduces the problem to a sequence of convex maximization problems that can be solved globally with the techniques mentioned in the previous paragraph. Tuy (1986) also established connections between this type of problems and the so called d.c. programming (DCP) problem. In fact, he demonstrated that any nonlinear programming (NLP) problem can, in principle, be approximated by a DCP problem which in turn can be further transformed, in principle, into a convex programming problem with an additional reverse convex constraint.

In this paper, it is demonstrated that the RCRP problem is equivalent to a convex quadratically constrained quadratic programming problem with an additional reverse convex, quadratic and separable constraint. It is shown, that one can *exactly* transform the former into the latter by the use of variable transformations and the introduction of new variables. Furthermore, a novel implementation of the Generalized Benders' Decomposition Algorithm (GBDA) is proposed for the solution of the latter problem. It is shown that this implementation of GBDA is *always guaranteed* to identify the global optimum of the general RCRP problem. The critical step in this procedure is the solution of the master problem, which is shown to be a quadratic, separable, RCP problem.

## **II. OPTIMIZATION PROBLEM EQUIVALENCE**

In this work we deal with several optimization problems which we consider expedient to present next.

The rationally constrained rational programming problem (P1) can be stated as follows:

$$\min_{z \in \mathbb{R}^n} \frac{f^0(z)}{g^0(z)} \tag{P1}$$

subject to,

$$\frac{f^{i}(z)}{g^{i}(z)} \leq 0, \qquad j=1,\ldots,k$$

where,

$$f^{j}(z) \triangleq \alpha_{0}^{j} + \sum_{i_{1}=1}^{n} \alpha_{i}^{j} z_{i_{1}} + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \alpha_{i_{1}i_{2}}^{j} z_{i_{1}} z_{i_{2}} + \cdots$$

$$+ \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \cdots \sum_{i_{m} \ge i_{m-1}}^{n} \alpha_{i_{1}i_{2}\cdots i_{m}}^{j} z_{i_{1}} z_{i_{2}} \cdots z_{i_{m}} \qquad j = 0, \dots, k,$$

$$g^{j}(z) \triangleq \beta_{0}^{j} + \sum_{i_{1}=1}^{n} \beta_{i_{1}}^{j} z_{i_{1}} + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \beta_{i_{1}i_{2}}^{j} z_{i_{1}} z_{i_{2}} + \cdots$$

$$+ \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \cdots \sum_{i_{m} \ge i_{m-1}}^{n} \beta_{i_{1}i_{2}\cdots i_{m}}^{j} z_{i_{1}} z_{i_{2}} \cdots z_{i_{m}}, \qquad j = 0, \dots, k$$

and

$$z = [z_1, z_2, \ldots, z_n] \in \mathbb{R}^n$$

Similarly, the polynomially constrained polynomial programming problem (P2) can be stated as follows:

$$\min_{z \in \mathbb{R}^{n}} \left\{ \alpha_{0}^{0} + \sum_{i_{1}=1}^{n} \alpha_{i_{1}}^{0} z_{i_{1}} + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \alpha_{i_{1}i_{2}}^{0} z_{i_{1}} z_{i_{2}} + \dots + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \cdots \sum_{i_{m} \ge i_{m-1}}^{n} \alpha_{i_{1}i_{2}\dots i_{m}}^{0} z_{i_{1}} z_{i_{2}\dots z_{i_{m}}} \right\}$$
(P2)

subject to,

$$\alpha_{0}^{1} + \sum_{i_{1}=1}^{n} \alpha_{i_{1}}^{1} z_{i_{1}} + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \alpha_{i_{1}i_{2}}^{1} z_{i_{1}} z_{i_{2}} + \dots + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \cdots \sum_{i_{m} \ge i_{m-1}}^{n} \alpha_{i_{1}i_{2}\dots i_{m}}^{1} z_{i_{1}} z_{i_{2}} \cdots z_{i_{m}} \le 0$$

$$\cdots$$

$$\alpha_{0}^{k} + \sum_{i_{1}=1}^{n} \alpha_{i_{1}}^{k} z_{i_{1}} + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \alpha_{i_{1}i_{2}}^{k} z_{i_{1}} z_{i_{2}} + \dots + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \cdots \sum_{i_{m} \ge i_{m-1}}^{n} \alpha_{i_{1}i_{2}\dots i_{m}}^{k} z_{i_{1}} z_{i_{2}\dots z_{i_{m}}} \le 0$$

This problem formulation encompasses all polynomial programming problems since equality constraints can also be expressed as pairs of inequality constraints.

In turn, the quadratically constrained quadratic programming problem (P3) can also be stated as follows:

$$\min_{x_1,\ldots,x_n} \alpha_0^0 + \sum_{i_1=1}^n \alpha_{i_1}^0 x_{i_1} + \sum_{i_1=1}^n \sum_{i_2 \ge i_1}^n \alpha_{i_1 i_2}^0 x_{i_1} x_{i_2}$$
(P3)

subject to,

$$\alpha_{0}^{1} + \sum_{i_{1}=1}^{n} \alpha_{i_{1}}^{1} x_{i_{1}} + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \alpha_{i_{1}i_{2}}^{1} x_{i_{1}} x_{i_{2}} \le 0$$
  
$$\cdots$$
$$\alpha_{0}^{k} + \sum_{i_{1}=1}^{n} \alpha_{i_{1}}^{k} x_{i_{1}} + \sum_{i_{1}=1}^{n} \sum_{i_{2} \ge i_{1}}^{n} \alpha_{i_{1}i_{2}}^{k} x_{i_{1}} x_{i_{2}} \le 0$$
  
By defining  $x \triangleq [x_{1}x_{2} \cdots x_{n}]^{T}$ ,  $c_{j} \triangleq \alpha_{0}^{j}$ ,  $b_{j} \triangleq [\alpha_{1}^{j} \alpha_{2}^{j} \cdots \alpha_{n}^{j}]^{T}$ ,

$$A_{j} \triangleq \begin{bmatrix} \alpha_{11}^{l} & 0.5 \, \alpha_{12}^{l} & \cdots & 0.5 \, \alpha_{1n}^{l} \\ 0.5 \, \alpha_{12}^{l} & \alpha_{22}^{l} & \cdots & 0.5 \, \alpha_{2n}^{l} \\ \vdots & \vdots & \vdots & \vdots \\ 0.5 \, \alpha_{1n}^{l} & 0.5 \, \alpha_{2n}^{l} & \cdots & \alpha_{nn}^{l} \end{bmatrix}$$

we can also represent (P3) as follows:

$$\min_{x} x^{T} A_{0} x + b_{0}^{T} x + c_{0}$$
(P3)

subject to,

$$x^{T}A_{j}x + b_{j}^{T}x + c_{j} \leq 0 \qquad j = 1, \ldots, k$$

Let us finally state the quadratically constrained quadratic programming problem with the following special features:

(i) the objective function is convex ( $A_0$  is positive semi-definite)

.

(ii) all the constraints, except the last one, are convex  $(A_j, j = 1, ..., k - 1$  are p.s.d.)

(iii) the last constraint is concave and separable  $(A_k \text{ diagonal and negative s.d.})$ 

We refer to this problem as (P4), and state it next.

$$\min_{x \in B^n} x^T A_0 x + b_0^T x + c_0 \qquad (A_0 \text{ p.s.d.})$$
(P4)

subject to,

$$x^{T}A_{j}x + b_{j}^{T}x + c_{j} \le 0 \qquad j = 1, \dots, k - 1 \qquad (A_{j} \text{ p.s.d.})$$
$$x^{T}A_{k}x + b_{k}^{T}x + c_{k} \le 0 \qquad (A_{k} \text{ diagonal and n.s.d.})$$

The four aforementioned programming problems (P1), (P2), (P3), (P4) will be shown to be equivalent to each other, in the sense that a problem of one type can be exactly transformed to a problem of the other type through the use of variable transformations and the introduction of new variables. In that respect, the following theorem is proved.

#### Theorem 1:

P1⇔P2⇔P3⇔P4

#### **Proof:**

 $P1 \Rightarrow P2$ 

Define  $\gamma \triangleq f^0(z)/g^0(z)$ . Then the optimization problem (P1) can be rewritten in the following form:

 $\min_{z \in R''} \gamma$ 

subject to,

$$f^{0}(z) - \gamma g^{0}(z) \leq 0$$
  
-f^{0}(z) + \gamma g^{0}(z) \le 0  
f^{j}(z) \cdot g^{j}(z) \le 0, j = 1, \dots, k

This is a (P2) type problem.

.

 $P2 \Rightarrow P3$ Define:

$$y_{i_1,i_2} \triangleq z_{i_1} z_{i_2}, \quad i_1 = 1, \dots, n, \quad i_2 = i_1, \dots, n,$$
  
$$y_{i_1,i_2,i_3} \triangleq y_{i_1,i_2} z_{i_3}, \quad i_1 = 1, \dots, n, \quad i_2 = i_1, \dots, n, \quad i_3 = i_2, \dots, n,$$
  
$$y_{i_1,i_2,\dots,i_m} \triangleq y_{i_1,i_2,\dots,i_{m-1}} z_{i_m},$$
  
$$i_1 = 1, \dots, n, \quad i_2 = i_1, \dots, n, \dots, i_m = i_{m-1}, \dots, n.$$

Under these transformations the objective function and the constraints of (P2) become linear. The only nonlinearity in the resulting optimization problems stems from the equality constraints defining the y variables. Since these constraints are quadratic in nature and since equality constraints can be replaced by inequality constraints  $(f = 0 \Leftrightarrow -f \leq 0, f \leq 0)$  the resulting optimization problem is of the form (P3).

#### P3⇒P4

Let  $A_j = W_j \Lambda_j W_j^T$  denote the eigendecomposition of  $A_j$  ( $A_j$  is a symmetric matrix and thus  $\Lambda_j$  is real,  $W_j$  is orthogonal and  $W_j^{-1} = W_j^T$ ). Let also

$$\Lambda_{j} = \operatorname{diag}(\{\lambda_{j_{i}}^{+}\}_{i=1}^{n}, \{\lambda_{j_{i}}^{-}\}_{i=n_{j}+1}^{n})$$
$$\Lambda_{j}^{+} = \operatorname{diag}(\{\lambda_{j_{i}}^{+}\}_{i=1}^{n}, \{0\}_{i=n_{j}+1}^{n})$$
$$\Lambda_{j}^{-} = \operatorname{diag}(\{0\}_{i=1}^{n_{j}}, \{\lambda_{j_{i}}^{-}\}_{i=n_{j}+1}^{n})$$

where

$$\lambda_{j_i}^+ \ge 0$$
  $i = 1, ..., n_j, \quad j = 0, ..., k$   
 $\lambda_{j_i}^- < 0$   $i = n_j + 1, ..., n, \quad j = 0, ..., k$ 

Then  $A_j = W_j \Lambda_j W_j^T = W_j (\Lambda_j^+ + \Lambda_j^-) W_j^T = W_j \Lambda_j^+ W_j^T + W_j \Lambda_j^- W_j^T \Delta A_j^+ + A_j^-$  where  $A_j^+$  is p.s.d. and  $A_j^-$  is n.s.d.. As a result, (P3) becomes

$$\min_{x} x^{T} A_{0}^{+} x + x^{T} A_{0}^{-} x + b_{0}^{T} x + c_{0}$$

subject to,

$$x^{T}A_{j}^{+}x + x^{T}A_{j}^{-}x + b_{j}^{T}x + c_{j} \leq 0$$
  $j = 1, ..., k$ 

Let J be the set of indices j (j = 0, ..., k) for which  $A_j^-$  has at least one nonzero eigenvalue and let  $n_i$  be the cardinality of this set. We now introduce  $n_i$  nonnegative variables  $t_i$ ,  $j \in J$  defined as follows:

$$t_i \triangle - x^T A_i^- x, \qquad j \in J$$

These equalities are equivalent to the following set of inequalities

$$x^{T}(-A_{j})x - t_{j} \leq 0, \qquad j \in J$$
$$\sum_{i \in J} (t_{j} + x^{T}A_{j}x) \leq 0.$$

By construction,  $\sum_{j \in J} A_j^-$  is symmetric. Let  $\sum_{j \in J} A_j^- = W_{\Sigma} \Lambda_{\Sigma} W_{\Sigma}^T$  be an eigendecomposition of  $\sum_{j \in J} A_j^-$ , where  $\Lambda_{\Sigma}$  is a diagonal n.s.d. matrix and  $W_{\Sigma}$  is orthogonal  $(W_{\Sigma}^{-1} = W_{\Sigma}^T)$ . Let  $n_y$  be the number of strictly negative eigenvalues of  $\sum_{j \in J} A_j^-$  (the other  $n - n_y$  eigenvalues are zero). Without loss of generality the following structure can be assumed for  $\Lambda_{\Sigma}$ :

$$\Lambda_{\Sigma} = \begin{bmatrix} \Lambda_{\Sigma 1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where  $\Lambda_{\Sigma 1}$  is a  $n_y \times n_y$ , diagonal, n.d. matrix (contains only the strictly negative diagonal elements of  $\Lambda_{\Sigma}$ ). Based on this partition the matrix  $W_{\Sigma}$  of eigenvectors of  $\sum_{i \in J} A_i^-$  can be written as:

$$W_{\Sigma} = \begin{bmatrix} W_{\Sigma 1} & W_{\Sigma 2} \end{bmatrix}$$

where,

- $W_{\Sigma 1}$   $n \times n_y$  real matrix containing as columns the eigenvectors associated with the strictly negative eigenvalues of  $\sum_{j \in J} A_j^-$ .
- $W_{\Sigma 2}$   $n \times (n n_y)$  real matrix.

Then  $\sum_{i \in J} A_i^-$  can be written as:

$$\sum_{j \in J} A_j^- = W_{\Sigma} \Lambda_{\Sigma} W_{\Sigma}^T = W_{\Sigma 1} \Lambda_{\Sigma 1} W_{\Sigma 1}^T$$

and the inequalities defining the variables  $t_j$ ,  $(j \in J)$  take the form:

$$x^{T}(-A_{j}^{-})x - t_{j} \leq 0, \qquad j \in J,$$
$$\left(\sum_{j \in J} t_{j}\right) + x^{T}W_{\Sigma 1}\Lambda_{\Sigma 1}W_{\Sigma 1}^{T}x \leq 0.$$

Define the vector  $y \in \mathbb{R}^{n_y}$  as:

$$y \triangleq W_{\Sigma 1}^T x$$

As a result the problem (P3) is tranformed to

$$\min_{\substack{x \\ t \\ y}} x^{T} A_{0}^{+} x - e_{0}^{T} t + b_{0}^{T} x + c_{0}$$
(1)

subject to,

$$x^{T}A_{j}^{+}x + b_{j}^{T}x + c_{j} \leq 0, \qquad j \notin J$$

$$x^{T}A_{j}^{+}x - t_{j} + b_{j}^{T}x + c_{j} \leq 0, \qquad j \in J$$

$$x^{T}(-A_{j}^{-})x - t_{j} \leq 0, \qquad j \in J$$

$$y - W_{\Sigma 1}^{T}x \leq 0$$

$$-y + W_{\Sigma 1}^{T}x \leq 0$$

$$y^{T}\Lambda_{\Sigma 1}y + \sum_{j \in J} t_{j} \leq 0.$$

where,  $e_0 \in \mathbb{R}^{n_i}$  is identically zero if  $j = 0 \notin J$  and is such that  $e_0^T t = t_0$  otherwise. Also  $\Lambda_{\Sigma 1} = \text{diag}\{\lambda_{\Sigma,i}\}_{i=1}^{n_y}, \lambda_{\Sigma,i} < 0, i = 1, ..., n_y$ . As a result,  $\Lambda_{\Sigma 1}$  is a negative definite diagonal matrix and the last constraint is a quadratic, separable, reverse convex constraint. Since the remaining constraints are quadratic and convex it follows that the last optimization problem belongs to the class (P4).

 $(P4) \Rightarrow (P1)$  obvious. O.E. $\Delta$ .

Having established that (P1), (P2), (P3) and (P4) are equivalent, we now proceed to the discussion of solution methodologies for (P4) type problems.

#### **III. SOLUTION METHODOLOGIES FOR (P4)**

The globally optimal solution for optimization problems of the type (P4) can be obtained by several algorithms. Three such algorithms will be presented. They are iterative in nature and their  $\varepsilon$ -convergence to the globally optimal solution is guaranteed.

# Algorithm 1

This solution methodology is based on the Generalized Benders Decomposition Algorithm (GBDA) (Geoffrion, 1972). Floudas *et al.* (1989) proposed a GBDA implementation as a so called "global optimum search technique" for the solution of P2 type problems, namely NLP's and MINLP's. However, Bagajewicz and Manousiouthakis (1991) demonstrated that the proposed GBDA implementation is not guaranteed to identify the global solution for such problems. Nevertheless the following theorem holds:

#### Theorem 2:

The GBDA, if properly implemented, is guaranteed to identify the global optimum of the general RCRP problem (P1). Furthermore, global solution of (P1) is ascertained upon global solution of a series of separable, quadratically constrained, reverse convex programming (RCP) problems.

#### **Proof:**

It has been established in Theorem 1 that (P1) is equivalent to (P4) which can take the form:

$$\min_{\substack{x \in R^n \\ t \in R^{n_i} \\ y \in R^{n_y}}} F(x, t) = x^T A_0^+ x - e_0^T t + b_0^T x + c_0 \tag{1}$$

subject to,

$$G(x, t) \le 0$$
$$L(x, y) \le 0$$

 $y^T \Lambda_{\Sigma 1} y + \sum_{j \in J} t_j \leq 0$ 

where:

$$G(x, t) = \begin{bmatrix} x^T A_j^+ x + b_j^T x + c_j \le 0, & j \notin J \\ x^T A_j^+ x - t_j + b_j^T x + c_j \le 0, & j \notin J \\ x^T (-A_j^-) x - t_j \le 0, & j \notin J \end{bmatrix},$$

$$L(x, y) = \begin{bmatrix} y - W_{\Sigma 1}^T x \le 0 \\ -y + W_{\Sigma 1}^T x \le 0 \end{bmatrix},$$

$$\Lambda_{\Sigma 1} = \text{diag}\{\lambda_{\Sigma,i}\}_{i=1}^{n_y}, \quad \lambda_{\Sigma,i} < 0, \quad i = 1, \dots, n_y.$$
We vector 
$$\begin{bmatrix} x \\ t \end{bmatrix}$$
 be decomposed in two parts: the negative set of the set of the

Let the variable vector  $\begin{bmatrix} t \\ y \end{bmatrix}$  be decomposed in two parts: the noncomplicating variable vector  $\begin{bmatrix} x \\ t \end{bmatrix}$  and the complicating variable vector y. Based on this

variable vector  $\begin{bmatrix} t \end{bmatrix}$  and the complicating variable vector y. Based on this decomposition, (1) takes the form (Geoffrion, 1972):

$$\min_{y \in R^{n_y} \cap V} \phi(y) \tag{1a}$$

.

,

subject to,

$$\phi(y) = \begin{cases} \min_{\substack{x \in \mathbb{R}^n \\ t \in \mathbb{R}^{n_i}}} F(x, t) \\ s.t. \quad G(x, t) \le 0 \\ L(x, y) \le 0 \\ y^T \Lambda_{\Sigma 1} y + \sum_{j \in J} t_j \le 0 \end{cases}$$
(1b)  
$$V = \left\{ y : L(x, y) \le 0, \ y^T \Lambda_{\Sigma 1} y + \sum_{j \in J} t_j \le 0 \text{ for some } x, t \text{ satisfying } G(x, t) \le 0 \right\}$$

For each value of y, the internal optimization problem (1b) is a convex optimization problem. Therefore, based on the strong duality theorem (Luenberger, 1969, p. 224), the value of (1b) is equal to the value of its dual. Thus (1b) is equivalent to:

$$\phi(y) = \max_{u \ge o} \min_{x, t} \left[ F(x, t) + u_1^T G(x, t) + u_2^T L(x, y) + u_3 \left( y^T \Lambda_{\Sigma 1} y + \sum_{j \in J} t_j \right) \right] \quad (1c)$$

Based on the proposed variable transformations and the presented problem decomposition the following two subproblems are created.

# **Primal:**

$$v(\bar{y}) = \min_{\substack{x \in R^n \\ t \in R^{n_i}}} F(x, t) = x^T A_0^+ x - e_0^T t + b_0^T x + c_0$$
(2)

subject to,

$$G(x, t) \le 0$$
$$L(x, \bar{y}) \le 0$$
$$\bar{y}^T \Lambda_{\Sigma 1} \bar{y} + \sum_{i \in J} t_i \le 0$$

where  $\bar{y}$  is fixed.

Master:

$$\min_{\substack{y_0 \in R \\ y \in R^{n_y}}} y_0$$
(3)  
subject to,  
$$L^*(y, u) = \min_{x, t} \left[ F(x, t) + u_1^T G(x, t) + u_2^T L(x, y) + u_3 \left( y^T \Lambda_{\Sigma 1} y + \sum_{j \in J} t_j \right) \right] \le y_0,$$
  
for all  $u \ge 0$ .  
$$L_*(y, v) = \min_{x, t} \left[ v_1^T G(x, t) + v_2^T L(x, y) + v_3 \left( y^T \Lambda_{\Sigma 1} y + \sum_{j \in J} t_j \right) \right] \le 0,$$

for all  $v \in N$ 

where  $u = (u_1^T u_2^T u_3)^T$ ,  $v = (v_1^T v_2^T v_3)^T$ ,  $N = \{v \ge 0, ||v||_1 = 1\}$ . In this formulation,  $L_*(y, v) \le 0$  is equivalent to the requirement that  $y \in V$ .

For each value of  $\bar{y}$  the primal subproblem, (2) is an upper bound to the global minimum of (1). The global solution of the master (3) is equal to the global solution of (1). By creating a relaxed version of (3) one can develop an iterative procedure for the global solution of (1) as follows:

**Step 1:** Identify a feasible point  $\bar{y} \in R^{n_y} \cap V$ . Solve (2) and obtain a multiplier vector  $\bar{u}$  and the optimal variable vector  $[\bar{x}^T \bar{t}^T]^T$ . Set p = 1, r = 0,  $u^1 = \bar{u}$ ,  $[x^{1T}t^{1T}]^T = [\bar{x}^T \bar{t}^T]^T$  and  $UBD = \phi(\bar{y})$ . The separability of the function  $L^*(y, u^p)$  in y, allows its evaluation as follows:

$$L^{*}(y, u^{p}) = \min_{x,t} \left[ F(x, t) + u_{1}^{pT}G(x, t) + u_{2}^{pT} \begin{bmatrix} y - W_{\Sigma_{1}}^{T}x \\ -y + W_{\Sigma_{1}}^{T}x \end{bmatrix} \right] \\ + u_{3}^{p} \left( y^{T} \Lambda_{\Sigma_{1}} y + \sum_{j \in J} t_{j} \right) \right] \\ = \min_{x,t} \left[ F(x, t) + u_{1}^{pT}G(x, t) + u_{2}^{pT} \begin{bmatrix} -I \\ I \end{bmatrix} W_{\Sigma_{1}}^{T}x + u_{3}^{p} \sum_{j \in J} t_{j} \right] \\ + u_{2}^{pT} \begin{bmatrix} I \\ -I \end{bmatrix} y + u_{3}^{p} y^{T} \Lambda_{\Sigma_{1}} y \Rightarrow L^{*}(y, u^{p}) \\ = F(x^{p}, t^{p}) + u_{1}^{pT}G(x^{p}, t^{p}) + u_{2}^{pT} \begin{bmatrix} -I \\ I \end{bmatrix} W_{\Sigma_{1}}^{T}x^{p} \\ + u_{3}^{p} \sum_{j \in J} t_{j}^{p} + u_{2}^{pT} \begin{bmatrix} I \\ -I \end{bmatrix} y + u_{3}^{p} y^{t} \Lambda_{\Sigma_{1}} y.$$
(4)

The last equality is a result of the saddle point property that holds for the Langrangian of the primal (Luenberger, 1969, p. 219).

#### Step 2: Solve globally the relaxed master problem:

subject to,  $\begin{array}{c} \min_{\substack{y_0 \in R \\ y \in R^{n_y}}} y_0 \qquad (5) \\ L^*(y, u^i) \leq y_0, \quad i = 1, \dots, p \\ L_*(y, v^j) \leq 0, \quad j = 1, \dots, r \end{array}$ 

The value of  $L_*(y, v^j)$  is calculated according to the procedure presented in step (3b). Let  $(\hat{y}, \hat{y}_0)$  denote the global solution of the relaxed master. Then  $\hat{y}_0$  is a lower bound to the global minimum of (1). If UBD  $\leq \hat{y}_0 + \varepsilon$ , where  $\varepsilon$  is a convergence tolerance, then terminate. Otherwise continue to the next step.

- Step 3: Solve (2) for  $\bar{y} = \hat{y}$ . Then there are two possibilities: the primal is either feasible or infeasible.
  - (a) The primal is feasible: if  $\phi(\hat{y}) \le \hat{y}_0 + \varepsilon$  then terminate. Otherwise determine a new optimal multiplier vector  $\bar{u}$  and set p = p + 1 and  $u^p = \bar{u}$ . If  $\phi(\hat{y}) < \text{UBD}$  then set  $\text{UBD} = \phi(\hat{y})$ . Then evaluate the function  $L^*(y, u^p)$  and return to step 2.

(b) *The primal is infeasible*: Then solve the following infeasibility minimization problem:

$$\min_{\substack{x,t\\a\in R}} a \tag{6}$$

subject to,

$$\begin{bmatrix} G(x, t) \\ L(x, \tilde{y}) \\ \tilde{y}^T \Lambda_{\Sigma 1} \tilde{y} + \sum_{j \in J} t_j \end{bmatrix} - a\mathbf{1} \leq 0.$$

where  $1[1 \ 1 \ \cdots \ 1]^{T}$ .

Since the primal is infeasible the solution of (6) is positive. Based on the Kuhn-Tucker necessary conditions for this problem the optimal multiplier vector  $\bar{v}$  can be shown to satisfy the relations:  $\bar{v} \ge 0$ ,  $1 - ||\bar{v}||_1 = 0$ . Hence  $v \in N$ . Once  $\bar{v}$  is determined, set r = r + 1,  $v' = \bar{v}$  and evalute the function  $L_*(y, v')$ . Similarly to  $L^*(y, u^p)$ , the minimum in the definition of  $L_*(y, v')$  can be calculated independently of y, directly from the solution of (6):

$$L_{*}(y, v') = v_{1}^{rT}G(x', t') + v_{2}^{rT}\begin{bmatrix} -I\\ I \end{bmatrix} W_{\Sigma_{1}}^{T}x' + v_{3}^{r}\sum_{j \in J}t_{j}'$$
$$+ v_{2}^{rT}\begin{bmatrix} I\\ -I \end{bmatrix} y + v_{3}^{r}y^{T}\Lambda_{\Sigma_{1}}y.$$

where  $[x^{r^T}t^{r^T}]^T$  is the solution of (6) that corresponds to  $v^r$ . Then return to step 2.

This procedure is guaranteed to create a nondecreasing sequence of lower bounds for the global optimum of (1) iff each relaxed master is solved globally. Furthermore, since the primal is convex, and thus there is no gap between (1b) and (1c), this sequence will converge to the global optimum of (1) (Geoffrion, 1972, Bagajewicz and Manousiouthakis, 1991).

Therefore, the global solution of (1) (equivalently P1) is obtained through the global solution of a series of relaxed master problems (5). Based on (4), (7) each relaxed master problem is a separable, quadratically constrained, reverse convex programming (RCP) problem since  $\Lambda_{\Sigma 1}$  is diagonal, n.d. and  $u_3^i$ ,  $v_3^i$  are positive. O.E. $\Delta$ .

**Remark 1:** It has been shown, that the GBDA implementation we have proposed, can be used to identify the global optimum of the general RCRP problem. The unique features of this implementation are:

- The primal is convex, therefore there is no dual gap between the primal and its dual.
- The functions  $L^*(y, u)$ ,  $L_*(y, v)$  are such that the minimization problems in their definition can be solved independently of y. Furthermore, the solution to these optimization problems is readily obtained from the solution of the related

primal. The resulting relaxed master problem is a separable quadratically constrained RCP problem.

Because of its characteristics the proposed GBDA implementation coverges to the global optimum.

**Remark 2:** As mentioned above, each relaxed master problem may have several local minima. Thus, its global solution can be obtained only through the use of special algorithms. Several algorithms for the solution of such problems have been developed. Ueing (1972) proposed a combinatorial procedure for the solution of RCP problems and Hillestad and Jacobsen (1980) proposed a cutting plane method that utilizes Tuy type cuts but may converge to infeasible points. The separability of the relaxed master's constraints allows also application of Soland's (1971) algorithm which guarantees  $\varepsilon$ -convergence in a finite number of iterations and is described later as algorithm 2.

The relaxed master problem can be stated as follows:

$$\min_{y,y_0} y_0 \tag{M}$$

subject to,

$$f_i(y) - y_o \le 0,$$
  $i = 1, 2, ..., K_f$   
 $g_j(y_0) \le 0,$   $j = 1, 2, ..., K_i$ 

where  $y \in \mathbb{R}^{n_y}$  and  $y_0 \in \mathbb{R}$ , and  $f_i(y)$ ,  $g_j(y)$  are concave real valued functions of the complicating variables.

To apply Ueing's algorithm it is essential that the objective function be strictly concave. This requirement can be satisfied by a slightly perturbed objective that results in the following modified master:

$$\min_{y,y_0} y_0 - \alpha \left[ \sum_{m=1}^{n_y} y_m^2 + y_0^2 \right]$$
 (M1)

subject to,

$$f_i(y) - y_0 \le 0,$$
  $i = 1, 2, ..., K_f$   
 $g_j(y) \le 0,$   $j = 1, 2, ..., K_i$ 

where  $\alpha$  is an arbitrarily small constant. Then at every local minimum  $(y, y_0)$  of this modified problem at least  $n_y + 1$  constraints are active. Furthermore each local minimum can be identified as the solution of a concave maximization problem that has the same objective as the modified master and involves only  $(n_y + 1)$  of the (p + r) constraints of the modified master with reversed sign (Ueing, 1972):

$$\max_{y,y_0} y_0 - \alpha \left[ \sum_{m=1}^{n_y} y_m^2 + y_0^2 \right]$$
 (M2)

subject, to

$$-f_i(y) + y_0 \le 0,$$
  $i = 1, 2, ..., p_1$   
 $-g_j(y) \le 0,$   $j = 1, 2, ..., r_1$ 

where:  $p_1 + r_1 = n_y + 1$ . This concave maximization over a convex set (note that all the constraints are convex) has naturally a unique global maximum. If, for that maximum, all the constraints of (M2) are active and all the constraints of (M1) are satisfied then this maximum is also a local minimum of the modified master (M1). Using this procedure one can determine all the local minima of the modified master, and in the limit ( $\alpha \rightarrow 0$ ) of the master itself. Since there is only a finite number of local minima the global minimum can be recovered in a finite number of steps.

#### Algorithm 2

As stated earlier (P4) is a nonconvex optimization problem with a single reverse convex constraint,  $\phi(y, t)$ , that is separable:

$$\phi(y, t) = \sum_{i=1}^{n_y} \phi_i(y_i) + \sum_{i=1}^{n_t} t_i,$$

where  $y \in R^{n_y}$ ,  $t \in R^{n_t}$  and  $\phi_i(.)$  is a concave function in one variable. Furthermore, the master problem in the GBDA implementation is of the same type, that is it has linear objective and concave, separable constraints. For this type of problems Soland (1971) proposed an algorithm that can identify the globally  $\varepsilon$ -optimal solution in a finite number of steps.

The algorithm assumes the existence of a "rectangular" region C where the y variables lie:  $C = \{y \in R^{n_y}: l \le y \le L\}$ , with l and L being vectors of upper and lower bounds. Through solution of a series of convex programming problems, the algorithm generates a sequence of lower bounds to the global optimum of (P4). Each of the intermediate convex problems,  $(P4_k)$ , is obtained from (P4) through substitution of  $\phi_i(.)$  by its convex envelope for all  $i = 1, \ldots, n_y$  over a rectangular subset of C (Soland, 1971). To obtain  $(P4_{k+1})$  from  $(P4_k)$  a branch and bound technique is used: first C is refined into smaller rectangles, and then the objective is minimized over the intersection of each rectangle with the feasible set and a lower bound on the objective is determined. The sequence of lower bounds produced by this procedure is guaranteed to  $\varepsilon$ -converge to the global optimum of (P4) in a finite number of iterations.

#### Algorithm 3

Tuy (1987) proposed an algorithm for the solution of convex problems with an additional reverse convex constraint, that can be applied to solve (P4).

Let C be the convex set defined by the k-1 convex constraints of (P4). Then (P4) can be restated as:

$$\min_{x \in C} x^T A_0 x + b_0^T x + c_0$$
(P4)

subject to,

$$\phi(x) = x^T A_k x + b_k^T x + c_k \le 0$$

Let v be the global minimum to this problem. It has been established that the value of the following optimization problem is zero:

$$\max_{x \in C} x^T (-A_k) x - b_k^T x - c_k$$

subject to,

$$x^{T}A_{0}x + b_{0}^{T}x + c_{0} - v \le 0$$

The global solution to this convex maximization problem can be obtained by available algorithms (Hoffman, 1981, Horst, 1976). The complete algorithm for the solution of (P4) is comprised of the following steps:

- Solve (P4) without the reverse convex constraint and let w be the resulting global optimum. It is assumed that this optimum is finite, but this is rather a technicality than a restrictive assumption. If w satisfies the reverse convex constraint then it is the global optimum for (P4).
- If w is such that:  $\phi(w) > 0$  and  $w^T A_0 w + b_0^T w + c_0 < v$  identify a point  $x_i$  that belongs on the boundary of the set  $G = \{x \in \mathbb{R}^n : \phi(x) > 0\}$ . Then solve the following convex maximization subproblem:

$$\max_{x \in C} x^T (-A_k) x - b_k^T x - c_k$$

subject to,

$$x^{T}A_{0}x + b_{0}^{T}x + c_{0} - x_{i}^{T}A_{0}x_{i} - b_{0}^{T}x_{i} - c_{0} \le 0$$

Let  $z_i$  be the global solution to this problem. If  $\phi(z_i) = 0$  then the algorithm terminates. Otherwise a one dimensional search that identifies a new point  $x_i + 1$  belonging to the boundary of G is performed, and the same procedure is repeated.

The described algorithm provides a sequence of points  $z_{i_{i-1,\dots,\omega}}$ . This sequence converges to the solution of (P4), thus resulting in a globally  $\varepsilon$ -optimal solution in a finite number of steps. Within the same conceptual framework, there are several improvements that can help increase the speed of convergence of this algorithm (Tuy, 1987).

#### IV. EXAMPLES

subject to,

#### 1. Polynomially Constrained Polynomial Programming Problem

Consider the following nonconvex optimization problem:

$$\min_{x_1, x_2} x_1^4 - 14x_1^2 + 24x_1 - x_2^2$$
$$-x_1 + x_2 - 8 \le 0$$
$$x_1 - 10 \le 0$$
$$-x_2 \le 0$$
$$x_2 - x_1^2 - 2x_1 + 2 \le 0$$

This optimization problem has several local minima. The following table contains the values of the variables and the corresponding value of the objective at each local minimum.

 <i>x</i> <sub>1</sub>	<i>x</i> <sub>2</sub>	Objective	
0.84025	0.3865	10.631	
0.7320	0.0000	10.354	
2.7016	10.7016	-98.600	
-3.1736	1.7245	-118.705	

The problem was solved by both the first and the second algorithm.

#### Algorithm 1 (Benders Decomposition)

Employing the transformation  $x_3 = x_1^2$  and  $x_4 = x_2^2$  and introducing the variables  $y_1 = x_1$  and  $y_2 = x_2$  the original optimization problem is being transformed to the following:

The complicating variables for this problem are  $y_1$ , and  $y_2$ . Then the primal subproblem becomes:

$$\min_{\substack{x_1, x_2 \\ x_3, x_4}} x_3^2 - 14x_3 + 24\bar{y}_1 + x_4 \qquad (Primal)$$

$$x_2 - x_3 - 2\bar{y}_1 + 2 \le 0$$

$$x_1^2 - x_3 \le 0$$

$$x_2^2 - x_4 \le 0$$

$$\bar{y}_1 - x_1 = 0$$

$$\bar{y}_2 - x_2 = 0$$

$$- \bar{y}_1^2 + x_3 - \bar{y}_2^2 + x_4 \le 0$$

The primal subproblem is an evaluation step and a check for the feasbility of the vector  $[\bar{y}_1 \ \bar{y}_2]$ . The master subproblem has the following form:

$$\min_{y_0, y_1, y_2} y_0$$
 (Master)

subject to,

subject to,

$$\begin{aligned} -y_1 + y_2 - 8 &\leq 0 \\ y_1 - 10 &\leq 0 \\ -y_2 &\leq 0 \end{aligned}$$
$$(x_{3,i}^2 - 14x_{3,i} + 24y_1 - x_{4,i}) + \lambda_{1,i}(x_{2,i} - x_{3,i} - 2y_1 + 2) + \lambda_{2,i}(x_{1,i}^2 - x_{3,i}) \\ + \lambda_{3,i}(x_{2,i}^2 - x_{4,i}) + \lambda_{4,i}(y_1 - x_{1,i}) + \lambda_{5,i}(y_2 - x_{2,i}) \\ + \lambda_{6,i}(-y_1^2 + x_{3,i} - y_2^2 + x_{4,i}) &\leq y_0, \quad i = 1, \dots, K_f \end{aligned}$$
$$\mu_{1,j}(x_{2,j} - x_{3,j} - 2y_1 + 2) + \mu_{2,j}(x_{1,j}^2 - x_{3,j}) + \mu_{3,j}(x_{2,j}^2 - x_{4,j}) + \mu_{4,j}(y_1 - x_{1,j}) \\ + \mu_{5,j}(y_2 - x_{2,j}) + \mu_{6,j}(-y_1^2 + x_{3,j} - y_2^2 + x_{4,j}) \leq 0, \quad j = 1, \dots, K_i \end{aligned}$$

As expected, the master subproblem is a separable quadratically constrained RCP problem. The solution of an RCP problem can be obtained by several methods. In the following, a branch and bound method (Algorithm 2) is being used.

The point  $(\bar{y}_1, \bar{y}_2) = (-8, 0)$  was chosen as the initial point for the Benders iterations. For  $\varepsilon = 0.001$  the global optimum was identified at  $(x_1, x_2) = (-3.1749, 1.7301)$  with objective value -118.706 in 43 Benders iterations. MINOS was used to solve the primal subproblem and the subproblems that were generated by the branch and bound procedure. On the average, the solution of each master required about 30 branch and bound iterations.

#### Algorithm 2 (Branch and Bound)

subject to,

Employing the transformation  $x_3 = x_1^2$  and  $x_4 = x_2^2$  the original optimization problem is transformed to the following:

 $\min_{\substack{x_1, x_2 \\ x_3, x_4}} x_3^2 - 14x_3 + 24x_1 - x_4$  $-x_1 + x_2 - 8 \le 0$  $x_1 - 10 \le 0$  $-x_2 \le 0$  $x_2 - x_3 - 2x_1 + 2 \le 0$  $x_1^2 - x_3 \le 0$  $x_2^2 - x_4 \le 0$  $-x_1^2 + x_3 - x_2^2 + x_4 \le 0$ 

In this form, the problem has become a convex quadratically constrained quadratic programming problem with a reverse convex quadratic and separable constraint and therefore algorithm 2 can be employed. The optimization package MINOS was used for the solution of the intermediate convex subproblems. For  $\varepsilon = 0.001$  the global optimum was identified as  $(x_1, x_2) = (-3.173, 1.721)$  and the corresponding objective value was -118.705. The execution time for this particular problem was approximately 5.2 cpu seconds on a IBM-4381 computer. The solution required 35 branch and bound iterations.

# 2. Indefinite Quadratic Programming Problem

Consider the following indefinite quadratic optimization problem (V. Visweswaran and C.A. Floudas, 1990):

$$\min_{\mathbf{x},\mathbf{y}} \Phi_1(\mathbf{x}) + \Phi_2(\mathbf{y})$$

subject to,

$$A_{1}\mathbf{x} + A_{2}\mathbf{y} \le b$$
  

$$x_{i} \ge 0, \qquad i = 1, 2, \dots, 10,$$
  

$$y_{i} \ge 0, \qquad i = 11, 12, \dots, 20.$$
  

$$\Phi_{1}(\mathbf{x}) = \frac{-1}{2} \sum_{i=1}^{10} C_{i}(x_{i} - \bar{x}_{i})^{2}$$

where

$$\Phi_{2}(\mathbf{y}) = \frac{1}{2} \sum_{i=1}^{20} C_{i}(y_{i} - \bar{y}_{i})^{2}$$

The data for this problem are:

C = (63, 15, 44, 91, 45, 50, 89, 58, 86, 82, 42, 98, 48, 91, 11, 63, 61, 61, 38, 26) $\bar{\mathbf{x}} = (-19, -27, -23, -53, -42, 26, -33, -23, 41, 19)$  $\bar{\mathbf{y}} = (-52, -3, 81, 30, -85, 68, 27, -81, 97, -73)$ 5 5 6 4 4 5 6 4 4  $A_{1} = \begin{bmatrix} 3 & 5 & 5 & 6 & 4 & 4 & 5 & 6 & 4 & 4 \\ 5 & 4 & 5 & 4 & 1 & 4 & 4 & 2 & 5 & 2 \\ 1 & 5 & 2 & 4 & 7 & 3 & 1 & 5 & 7 & 6 \\ 3 & 2 & 6 & 3 & 2 & 1 & 6 & 1 & 7 & 3 \\ 6 & 6 & 6 & 4 & 5 & 2 & 2 & 4 & 3 & 2 \\ 5 & 5 & 2 & 1 & 3 & 5 & 5 & 7 & 4 & 3 \\ 3 & 6 & 6 & 3 & 1 & 6 & 1 & 6 & 7 & 1 \\ 1 & 2 & 1 & 7 & 8 & 7 & 6 & 5 & 8 & 7 \\ 8 & 5 & 2 & 5 & 3 & 8 & 1 & 3 & 3 & 5 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$ 1 1 1 1 1 1 1 1 1 1 **F8 2 4 1 1 1 2 1 7** 31 3 6 1 7 7 5 8 7 2 1 1 7 2 4 7 5 3 4 1 2  $A_2 = \begin{cases} 1 & 7 & 2 & 4 & 7 & 5 & 3 & 4 & 1 & 2 \\ 7 & 7 & 8 & 2 & 3 & 4 & 5 & 8 & 1 & 2 \\ 7 & 5 & 3 & 6 & 7 & 5 & 8 & 4 & 6 & 3 \\ 4 & 1 & 7 & 3 & 8 & 3 & 1 & 6 & 2 & 8 \\ 4 & 3 & 1 & 4 & 3 & 6 & 4 & 6 & 5 & 4 \\ 2 & 3 & 5 & 5 & 4 & 5 & 4 & 2 & 2 & 8 \end{cases}$ 4 5 5 6 1 7 1 2 2 4 1 1 1 1 1 1 1 1 1

$$b = (380, 415, 385, 405, 470, 415, 400, 460, 400, 200)$$

In this optimization problem the function  $\Phi_1(\mathbf{x})$  is concave while the function  $\Phi_2(\mathbf{y})$  is convex. Employing the transformation  $z_i = x_i^2$ , i = 1, 2, ..., 10 the following reverse convex programming problem is obtained:

 $\min_{\mathbf{z},\mathbf{x},\mathbf{y}} \left\{ \frac{-1}{2} \sum_{i=1}^{10} C_i (z_i - 2x_i \bar{x}_i + \bar{x}_i^2) + \frac{1}{2} \sum_{i=11}^{20} C_i (y_i - \bar{y}_i)^2 \right\}$ 

subject to,

$$A_{1}\mathbf{x} + A_{2}\mathbf{y} \le b$$

$$x_{i}^{2} - z_{i} \le 0, \qquad i = 1, 2, ..., 10$$

$$\sum_{i=1}^{10} (z_{i} - x_{i}^{2}) \le 0$$

$$x_{i} \ge 0, \qquad i = 1, 2, ..., 10,$$

$$y_{i} \ge 0, \qquad i = 11, 12, ..., 20.$$

As in the previous example, the original nonconvex optimization problem has been transformed into an optimization problem with objective function that is quadratic and convex, and constraints that are also quadratic and convex except one that is quadratic, reverse convex and separable. For  $\varepsilon = 0.001$  the  $\varepsilon$ -global optimum was identified at:

$$\mathbf{x}_{opt} = (0, 0, 0, 62.609, 0, 0, 0, 0, 0, 0)$$
$$\mathbf{y}_{opt} = (0, 0, 0, 0, 0, 0, 4.348, 0, 0, 0),$$

the objective value was 49318.078 and its determination required 4 branch and bound iterations. The execution time for this problem was 9.7 cpu seconds on an IBM-4381 computer.

#### 3. Reactor Sequence Design with Capital Cost Constraints

Consider the reaction sequence  $A \rightarrow B \rightarrow C$ . Assuming first order kinetics for both reactions, design a sequence of two reactors such that the concentration of B in the exit stream of the second reactor  $(c_{b2})$  is maximized and the investment cost does not exceed a given upper bound.

The values of the reaction constants for the first and the second reaction are given in the following table:

	Reactor 1	Reactor 2	
 k <sub>a</sub> k <sub>b</sub>	9.6540 10 <sup>-2</sup> s <sup>-1</sup> 3.5272 10 <sup>-2</sup> s <sup>-1</sup>	9.7515 10 <sup>-2</sup> s <sup>-1</sup> 3.9191 10 <sup>-2</sup> s <sup>-1</sup>	

The inlet concentration for B and C is zero. The inlet concentration for A is  $c_{a0} = 1.0 \text{ mol/l.}$ 

#### **Problem Formulation:**

Let  $V_1$ ,  $V_2$  be the residence times for the first and the second reactor respectively. Let  $k_{a1}$ ,  $k_{a2}$ ,  $k_{b1}$  and  $k_{b2}$  be the rate constants for the first and second reaction in the first and the second reactor respectively. Then the reactor design problem is formulated as a Nonlinear Programming Problem:

 $\max c_{b2}$ 

subject to,

$$(c_{a1} - c_{a0}) + k_{a1}c_{a1}V_1 = 0$$
  

$$(c_{a2} - c_{a1}) + k_{a2}c_{a2}V_2 = 0$$
  

$$(c_{b1} - c_{a1} - c_{a0}) + k_{b1}c_{b1}V_1 = 0$$
  

$$(c_{b2} - c_{b1} - c_{a2} + c_{a1}) + k_{b2}c_{b2}V_2 = 0$$

Assuming that the capital cost of a reactor is proportional to the square root of its residence time, the capital cost constraint can be written as:

$$V_1^{0.5} + V_2^{0.5} \le 4$$

Employing the transformation  $z_1^2 = V_1$  and  $z_2^2 = V_2$ , the capital cost constraint is replaced by the following set of constraints:

$$z_1 + z_2 \le 4$$
  
$$z_1^2 - V_1 = 0$$
  
$$z_2^2 - V_2 = 0$$

The resulting optimization problem belongs to the class (P2).

The problem has 2 local minima with objective values  $c_{b2} = 0.38810 \text{ mol/lt}$  and  $c_{b2} = 0.3746 \text{ mol/lt}$  respectively.

Using algorithm 2, the global optimum is identified as  $c_{b2} = 0.38810 \text{ mol/lt}$ . The total number of branch and bound iterations for this problem was 7950, and the execution time on an Apollo DN10000 was 7950 cpu seconds.

#### **V. CONCLUSIONS**

In this paper, it has been demonstrated that <u>any</u> rationally constrained rational programming problem can be <u>exactly</u> transformed into a convex, quadratically constrained, quadratic programming problem with an additional separable, quadratic, reverse convex constraint. One can generate the latter through variable transformations and introduction of new variables. The single reverse convex constraint has the additional feature of being separable, something that broadens the class of optimization algorithms that can be used for the solution of this problem.

A novel implementation of the GBDA which benefits from this problem equivalence has been shown to guarantee solution to global optimality for RCRP problems. Based on this result, the global solution of an RCRP problem has been translated to the global solution of a series of quadratically constrained and separable RCP problems. This in turn suggests that new, more efficient algorithmic approaches for the global solution of RCP problems will have an immediate positive impact on the global solution of RCRP problems.

# ACKNOWLEDGEMENTS

Financial support by the NSF-PYI CBT 88 57867 grant is gratefully acknowledged. Many helpful discussions with Dr. Stephen Jacobsen of the UCLA Electrical Engineering Dept. are also acknowledged.

#### REFERENCES

Bagajewicz, M., and Manousiouthakis, V., "On the Generalized Benders Decomposition", Comp. Chem. Eng., 15(10), 691-700 (1991).

Cabot, A.V., and Francis, R.L., "Solving nonconvex quadratic minimization problems by ranking the extreme points", Oper. Res., 18, 82-86 (1970).

Cabot, A.V., "Variations on a Cutting Plane Method for Solving Concave Minimization Problems with Linear Constraints", Naval. Res. Logist. Quart., 21, 265-274 (1974).

Charnes, A., and Cooper, W.W., "Management Models and Industrial Applications of Linear Programming", Wiley, NY, 1961. Falk, J.E., and Soland, R.M., "An Algorithm for Separable Nonconvex Programming Problems",

Management Sci., 15, 550-569 (1969).

Floudas, C.A., Aggarwal, A., and Ciric, A.R., "Global Optimum Search for Nonconvex NLP and MINLP problems", Comp. Chem. Engng., 13, 1117-1132 (1989). Glover, F., "Convexity Cuts and Cut Search", Oper. Res., 21, 123-134 (1973).

Grossmann, I.E., "MINLP Optimization Strategies and Algorithms for Process Synthesis", in Foundations of Computer-Aided Process Design, Siirola, J.J., Grossmann, J.E., Stephanopoulos, G. (editors), Elsevier Science, 1990.

Hadley, G., "Nonlinear and Dynamic Programming", Addison-Wesley, Reading, MA, 1964.

Hillestad, R.J., and Jacobsen, S.E., "Reverse Convex Constraint", Appl. Math. Optim., 6, 63-78 (1980a).

Hillestad, R.J., and Jacobsen, S.E., "Linear Programs with an Additional Reverse Convex Constraint", Appl. Math. Optim., 6, 257-269 (1980b).

Hoffman, K.L., "A Method for Globally Minimizing Concave Functions over Convex Sets", Math. Prog., 20, 22–23 (1981). Horst, R., "An Algorithm for Nonconvex Programming Problems", Mathematical Programming, 10,

312-321 (1976).

Jacobsen, S.E., "Convergence of a Tuy-type Algorithm for Concave Minimization Subject to Linear Inequality Constraints", Appl. Math. Opt., 7, 1-9 (1981).

Kough, F.P., "The Indefinite Quadratic Programming Problem", Operations Research 27(3), 516-533 (1978). Luenberger, "Optimization by vector space methods", John Wiley, New York, 1969.

Manousiouthakis, V., and Sourlas, D., "On I, Simultaneously Optimal Controller Design", Proc. ACC (1990), San Diego, CA.

Manousiouthakis, V. et al. "Total Annualized Cost Minimization for Heat/Mass Exchange Networks", Paper 22D, AIChE National Meeting 1990, Chicago, IL.

Mueller, R., "A Method for Solving the Indefinite Quadratic Programming Problem", Management Science 16(5), 333-339 (1970).

Murty, K., "Solving the Fixed Charge Problem by Ranking the Extreme Points", Oper. Res., 16, 268-279 (1969)

Pardalos, P.M., and Rosen, J.B., "Methods for Global Concave Minimization: A Bibliographic Survey", SIAM Rev., 28, 3, 367-378 (1986).

Ritter, K., "A Method for Sovling Maximum Problems with a Nonconcave Quadratic Objective Function", Z. Wahrscheinkchkeitstheorie 4, 340-351 (1966).

Soland R.M., "An Algorithm for Separable Nonconvex Programming Problems II: Nonconvex Constraints", Manag. Sci., 17, 759-773 (1971).

Swaney, R., "Global Solution of Algebraic Nonlinear Programs", Paper 22F, AIChE National Meeting 1990, Chicago, IL.

Tuy, H., "Concave Programming under Linear Constraints", Soviet Mathematics, 5, 1437-1440 (1964).

Tuy, H., "A General Deterministic Approach to Global Optimization via D.C. Programming" in Fermat Days 85: Mathematics for Optimization, J.B. Hiriart-Urruty (editor), Elsevier Science Publishers B.V., North Holland, 1986.

- Tuy, H., "Convex Programs with an Additional Reverse Convex Constraint", JOTA, 52, 463-486,
- (1987).
   Ueing, V., "A Combinatorial Method to Compute a Global Solution to Certain Nonconvex Optimization Problems", Numerical Methods for Nonlinear Optimization, F.A. Lootsma (ed.), Academic Press, 223-230 (1972).
- (ed.), Academic Press, 223-230 (1972).
  Visweswaran, V., and Floudas, C.A., "An Analytical Approach to Constrained Global Optimization", Paper 22C, AIChE National Meeting 1990, Chicago, IL.
  Zwart, P. B., "Nonlinear Programming: Counterexamples to two Global Optimization Algorithms", Oper. Res., 21, 1260-1266 (1973).
  Zwart, P. B., "Global Maximization of a Convex Function with Linear Inequality Constraints", Oper. Res., 22, 602-609 (1974).