



A Tabu Search Based Approach for Solving a Class of Bilevel Programming Problems in Chemical Engineering

RAJESH J., KAPIL GUPTA AND HARI SHANKAR KUSUMAKAR

Department of Chemical Engineering, Indian Institute of Technology, Mumbai, India

V.K. JAYARAMAN AND B.D. KULKARNI*

Chemical Engineering Division, National Chemical Laboratory, Pune, India

email: bdk@ems.ncl.res.in

Submitted in February 2000 and Accepted by Anthony Cox, Jr. in March 2003 after two revisions

Abstract

In this paper an approach based on the tabu search paradigm to tackle the bilevel programming problems is presented. The algorithm has been tested for a number of benchmark problems and the results obtained show superiority of the approach over the conventional methods in solving such problems.

Key Words: bilevel programming, tabu search

1. Introduction

Multilevel optimization and programming problems are frequently encountered in several branches of engineering. One of their important features is that a decision at one level of the hierarchy may be determined in part by decisions at other levels. Also, the optimization variables at one level may be used to control and manipulate the solution space of the optimization variables at the other levels. The bilevel programming problem (BLP) is a special case of the multilevel programming problem (MLP), where only two levels are involved. Here the inner level optimization problem(s) constrains the feasible region available for an outer level optimization. The original formulation for bilevel programming appeared in 1973 in a paper authored by Bracken and McGill (1973) although it was Candler and Norton (1977) who first used the terms “bilevel and multilevel programming”. It was only in the early eighties that these problems received the attention they deserved. Motivated by the game theory of Stackelberg (1952), several authors studied bilevel programming intensively and contributed to its wider use in the mathematical programming community. BLP problems find extensive applications in the domain of engineering design of transportation networks, process synthesis and economic planning, to name a few (Yang and Yagar, 1994;

* Author to whom correspondence should be addressed.

Bialas and Karwan, 1984; Brengel and Seider, 1992; Biegler et al., 1997). In chemical engineering, Clark and Westerberg (1990) have applied a BLP strategy to optimize chemical processes, while Sahin and Ciric (1998) have applied it to obtain the layout of a chemical plant.

A typical formulation of a bilevel optimization problem (Candler and Townsley, 1982) can be stated mathematically as,

$$\underset{x}{\text{Min}} A(x, y) \quad (1)$$

such that

$$B_i(x, y) \leq 0, \quad (i = 1, 2, \dots, n) \quad (2)$$

$$C_j(x, y) = 0 \quad (j = 1, 2, \dots, m) \quad (3)$$

while

$$\underset{y}{\text{Min}} D(x, y) \quad (4)$$

$$E_k(x, y) \leq 0, \quad (k = 1, 2, \dots, p) \quad (5)$$

$$F_l(x, y) = 0 \quad (l = 1, 2, \dots, q) \quad (6)$$

In the most general formulation, the constraints B , C , E and F may be linear or non-linear in nature, and the problem may or may not have integer variables.

In the above formulation, x and y are, the outer and the inner loop optimization variables respectively. For a certain value of the outer loop optimization variable, the inner loop is processed first to determine the feasible region for the optimal inner loop variable, subject to the given constraints. Within the feasible region, the inner loop objective function is then optimized. The optimized value of the inner loop variable is then sent to the outer loop. This constitutes one evaluation of the BLP problem. The same process is repeated for various other values of the outer loop optimization variable(s) with a view to reach an optimum (satisfying the constraints), for the outer loop objective function. The block diagram in figure 1 illustrates the above process. The theory of bilevel programming has been discussed by a number of authors (Dempe, 1992; Outrata, 1994) and its application to linear BP problem with a number of variables can be found in the work of Calamai and Vicente (1993). It has also been proven that even the linear BLP problem where all the involved functions are affine, is a strongly NP-hard problem (Hansen et al., 1992). A number of approaches for solving bilevel programming problems have been proposed in the literature (Bard, 1991; Clark and Westerberg, 1983). All these approaches essentially reduce the two-level optimization problem to a single level by means of suitable transformations on the inner objective function. This process, however, brings in nonconvexity into the problem and several methods have been reported to deal with it (Bard and Moore, 1990; Edmunds and Bard, 1991, 1992; Clark and Westerberg, 1990; Visweswaran et al., 1996). These solution techniques employ the Kuhn-Tucker strategy to reduce the two level problems. The approach, however, cannot handle discontinuous functions. Wen and Hsu (1991) have discussed a number of different methods of solving BLP problems to which the Kuhn-Tucker strategy cannot be applied. Some of these methods assume linearity and hence may

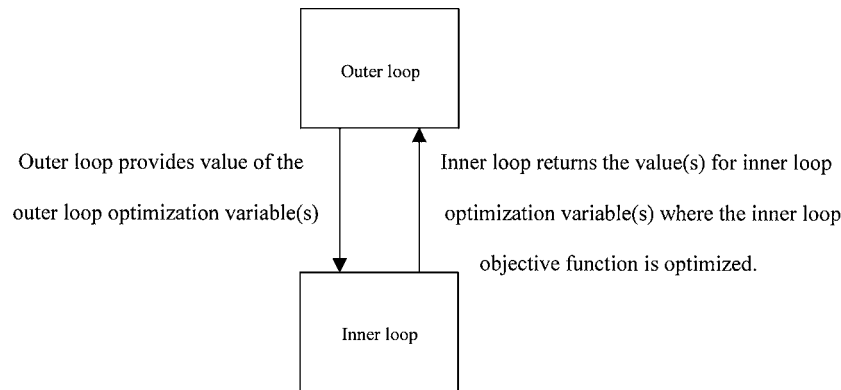


Figure 1. Block diagram illustrating the evaluation of objective functions in a bilevel programming problem.

not be of much use in real-world applications where equations are highly nonlinear (Wen and Hsu, 1991; Clark and Westerberg, 1990).

Intelligent metaheuristic algorithms like the “*Tabu Search*” and the “*Ant Colony Optimization*” have been proposed as viable alternatives for solving optimization problems (Glover et al., 1993; Bonabeau et al., 2000). In this paper, an approach based on the tabu search to tackle the BLP problems is presented. The algorithm has been tested on several problems taken from literature and the results obtained show the superiority of the approach in solving such problems.

2. Tabu search—the algorithm

Proposed by Glover (1986, 1989, 1990), the tabu search is an intelligent metaheuristic search procedure that has found very wide applications in a variety of diverse fields. The basic tabu search algorithm and its hybrids with other heuristic and algorithmic procedures have succeeded in finding superior solutions to problems in spin glass systems, sequencing, scheduling, assignment problems, etc. (Laguna et al., 1993, 1999; Laguna, 1995a, 1995b). The widespread successes of these methods, coupled with more rigorous and robust formulations, have catalyzed their rapid growth and application potential. Exhaustive surveys of the status of the tabu search procedures can be found in Glover and Laguna (1997). The premise underlying the tabu search is that the improving moves, that is the moves from the current point that lead to better values of the objective function do not necessarily lead us to the better solution; on the contrary valuable knowledge can be gained about the nature of the problem (and the objective function) by looking at the ‘worsening’ moves (moves from the current point which lead to immediate deterioration of the objective function). The most impressive features making the tabu search very attractive are its adaptive memory structure and responsive exploration capabilities. While exploring the problem domain, the tabu search algorithm employs both short term and long-term memory structures. This ensures that the search doesn’t deteriorate into a random search process. The short-term

memory is managed by creating one or more tabu lists to keep a note of solutions (and their attributes) that have been visited in the recent past. Such points acquire a 'tabu' status that is kept active for a certain duration called the 'tabu tenure'. The 'tabu' status, however, is overridden when certain aspiration conditions are fulfilled. This is done to ensure that the 'tabu' status of a move doesn't deter us from choosing it, if it offers a solution better than any of the previously encountered moves. The short-term memory produces optimal solutions, which are further improved using the long-term memory feature of the algorithm. Two very important long-term memory aspects of tabu search are the intensification and the diversification strategies (Kelly et al., 1994; Laguna et al., 1999). Intensification strategies are formulated to encourage moves and solutions in the neighborhood of historically promising regions. A simple intensification approach is to keep an elite list of the best solutions, and add new promising solutions during the course of the iterations. The diversification strategies are designed to propel the search into unexplored new regions. In machine scheduling problems, a frequency-based memory of all the previously-generated solutions has proved to be a very successful diversification strategy (Glover, 1989, 1990). The tabu search procedure has been well developed for combinatorial optimization problems, and several problem-specific variants of the basic algorithm are reported in literature. The bilevel problems considered in the present study belong to the class of continuous function optimization and only a very few tabu search procedures are available (Battiti and Tecchiolli, 1996; Chelouah and Siarry, 2000; Cvijovic and Klinowski, 1995; Siarry and Berthiau, 1997). We found that the treatment of Cvijovic and Klinowski (1995) can be conveniently adapted to bilevel problems. This approach has the added advantage of being applicable to multimodal functions as well.

2.1. Tabu search algorithm as used in the current study

The method of discretizing or partitioning the search space is illustrated in figure 2(a) where the search intervals for the variables x_1 , x_2 and x_3 are divided into 3, 2 and 3 sub-intervals, respectively. The number of sub-intervals is called the *partition parameter*. Such a partitioning facilitates the division of the problem domain into different cells. A *cell* can be identified by its address as shown in figure 2(b) where a cell with the address 123 has been shown. In this cell the ranges of variable x_1 , x_2 and x_3 are in the subintervals 1, 2 and 3, respectively. The search is initiated by picking $10n$ cells and by choosing any n_s sample points from each of them to calculate best function value, f . An elite list is then created with a view to keep a record of the best solutions (L in number) obtained since the beginning of the search until the current point of the search. To keep track of the location of the function values, the cell addresses are also stored. A tabu list that stores the most recent tabu moves (say, T , in number) is created and kept empty initially. Whenever a move is made from a cell $C(s)$ to $C(s')$, the cell $C(s)$ is added to the tabu list to replace the oldest cell in the list. At each iteration, n_c cells are randomly chosen and n_s samples are randomly drawn from each of the cells. The algorithm accepts, at a given iteration step, the non-tabu move with the best function value f . A move becomes tabu if it is: (1) in the tabu list or (2) if the move results in a function value worse than a (problem specific) predetermined value. The tabu status of a move is nullified if the move satisfies the aspiration condition. An aspiration function

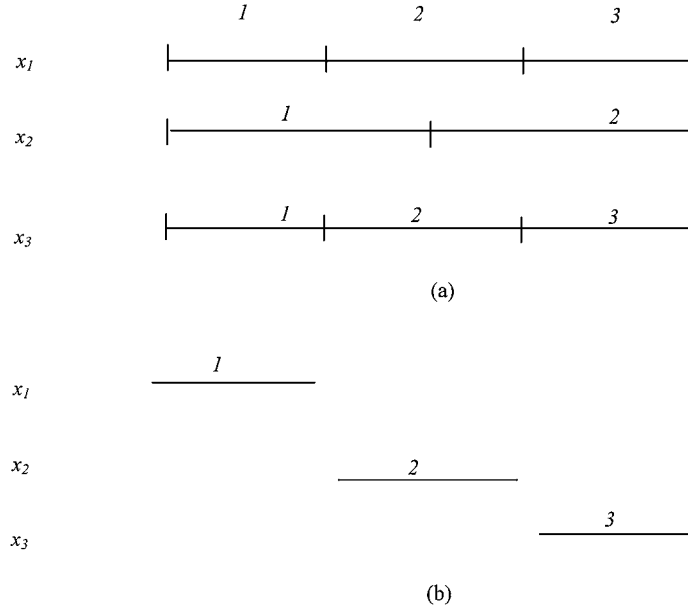


Figure 2. An illustration of partitioning of the problem domain.

(AF) can be defined in many ways, but in the present work, the aspiration function at any iteration step is taken as the best function value encountered so far. Thus, the tabu status of a move is cancelled if the move results in a value better than the current best function value. If the move results in a value worse than the worst function value in memory, the search is intensified by randomly picking a cell from the elite list and searching n_s sample points in the chosen cell. The step-by-step description of the algorithm is given below.

Step 1 (Initialization). Pick $(10 * n)$ cells (n is the dimension of the problem). Take n_s sample points in each cell and find f , the best function value (out of $10n * n_s$ sample points). Also, find the local best function value in each cell. Initialize the search at the location of the best function value, f .

Step 2 (Filling up the elitelist, creating tabu list, determining AF & worst function value). Fill up the elitelist with the best L solutions along with the corresponding cell addresses. Find the best and worst solutions from all the cells examined. Create an empty tabu list, which can accommodate T cells. The best value of the solution obtained so far is the aspiration function AF , and the worst solution obtained is the worst function value.

Step 3 (Start iterations). Pick up n_c cells and take n_s sample points from each cell.

Step 4 (Check with tabu list). If the best function value, f (out of $n_c * n_s$ sample points) is in the tabu list, accept the move only if it is better than AF .

Step 5 (If the move occurs in a cell not in the tabu list). In this case, if f is worse than worst function value pick a cell from the elite list and sample n_s points in the cell and

find the local best function value. Position the current solution to this move. In case f is better than the worst function value, accept the move.

Step 6 (Update tabu list, AF , worst function value and elitelist). Compare the local best function value with the AF and update the AF . Also, update the elitelist. Do not update the tabu list if the current cell offers a solution better than the AF .

Repeat Steps 3–6 until the required number of iterations is carried out.

Figure 1 illustrates the strategy employed for solving the bilevel problems. In this procedure, the tabu search algorithm is run at both the levels for the inner and outer loops. This results in the outer loop picking a value for the independent variable, which is then sent to the inner loop tabu search algorithm. The inner loop algorithm returns to the outer loop the value (of the inner loop optimization variables) that optimizes the inner loop objective function. The outer loop algorithm then optimizes the outer loop objective function with these values as its domain.

3. Results and discussion

The tabu search algorithm was tested on nine examples taken from literature. The examples were chosen in a manner to illustrate the ability of the algorithm to handle a variety of problem conditions and complexities (the choice of problems is discussed later in this paper). In all subsequent occurrences the term ‘optimum,’ implies the neighborhood of the true optimum—a region defined within 0.1% of the value reported in the literature.

There are two critical issues involved in the optimization process using tabu search algorithm. The first one concerns the choice of initial parameters. For example, to ensure that an accurate solution is reached, it may be necessary to give a large value for the partition parameter (for each variable). The large number of options available in picking up the cells suggests that there is a good possibility of the region of interest not being chosen at all. In this case, a poor solution may be obtained. On the other hand, too small a partition parameter results in inaccurate solutions, essentially due to the fact that very close to the optimum may remain unexplored. Hence, it is important to realize the existence of an appropriate range for the partition parameter. A similar argument may be used to identify the existence of an appropriate length of the tabu list, which determines the number of iterations for which a move remains ‘tabu’. Also, the choice of number of sample points and cells must be made judiciously, keeping in mind the partition parameter set chosen. It is necessary to realize that the choice of parameters is problem-specific and to some extent, guided by heuristics.

In the examples solved, the aim is to find the outer loop objective function’s global optimum subject to the condition that the inner loop objective function is also at its global optimum. It is possible that any straying of the inner loop objective function from its global optimum may result in an apparently better value of the outer loop global optimum as compared to the true one. Hence, there is a genuine need to drive the inner objective function to its global optimum. To achieve the same, a large number of inner loop iterations are performed (nearly 10 times that of the outer loop).

The description of the nine BLP problems tested (and their sources) is presented in Table 1. For the sake of choosing problems with differing levels of complexities these have

Table 1. Bilevel programming test problems.

Sr. no.	Problem description	Global optimum
1	$\begin{aligned} &\text{Max}_x \quad F = x + 3y_1 - 2y_2 \\ &\text{s.t.} \quad 0 \leq x \leq 8, \\ &\text{Max}_{y_1 y_2} \quad (y) \\ &\text{s.t.} \quad 2x - y_1 - 4y_2 \geq -16, \quad -8x - 3y_1 + 2y_2 \geq -48, \\ &\quad 2x - y_1 + 3y_2 \geq 12, \quad 0 \leq y_1 \leq 4. \end{aligned}$	$F = 13 \ (x, y_1, y_2) \equiv (5, 4, 2)$
2	$\begin{aligned} &\text{Min}_x \quad F = (x - 3)^2 + (y - 2)^2 \\ &\text{s.t.} \quad 0 \leq x \leq 8. \\ &\text{Min}_y \quad (y - 5)^2 \\ &\text{s.t.} \quad 2x - y \geq -1, \quad -x + 2y \geq 2, \\ &\quad -x - 2y \geq -14. \end{aligned}$	$F = 5 \ (x, y) \equiv (1, 3)$
3	$\begin{aligned} &\text{Min}_x \quad F = (x - 3)^2 + (y - 2)^2 \\ &\text{s.t.} \quad 2x - y \geq -1, \quad -x + 2y \geq 2, \\ &\quad -x - 2y \geq -14, \quad 0 \leq x \leq 8, \\ &\text{Min}_y \quad F = (y - 5)^2 \end{aligned}$	$F = 9 \ (x, y) \equiv (3, 5)$
4	$\begin{aligned} &\text{Max}_x \quad F = -2x + 11y \\ &\text{s.t.} \\ &\text{Max}_y \quad (-x - 3y) \\ &\text{s.t.} \quad x - 2y \leq 4, \quad 2x - y \leq 24, \\ &\quad 3x + 4y \leq 96, \quad x + 7y \leq 126, \\ &\quad -4x + 5y \leq 65, \quad x + 4y \geq 8, \\ &\quad x, y \geq 0. \end{aligned}$	$F = 85.0909$ $(x, y) \equiv (17.4545, 10.90909)$
5	$\begin{aligned} &\text{Max}_{x_1} \quad F = x_2 \\ &\text{s.t.} \\ &\text{Max}_{x_2} \quad (-x_2) \\ &\text{s.t.} \quad -x_1 - 2x_2 \leq -10, \quad x_1 - 2x_2 \leq 6, \\ &\quad 2x_1 - x_2 \leq 21, \quad x_1 + 2x_2 \leq 38, \\ &\quad -x_1 + 2x_2 \leq 18, \quad x_1, x_2 \geq 0. \end{aligned}$	$F = 11 \ (x_1, x_2) \equiv (16, 11)$
6	$\begin{aligned} &\text{Min}_x \quad F = (x - 5)^2 + (2y + 1)^2 \\ &\text{s.t.} \quad x \geq 0 \\ &\text{Min}_y \quad (y - 1)^2 - 1.5xy \\ &\text{s.t.} \quad -3x + y \leq -3, \quad x - 0.5y \leq 4 \\ &\quad x + y \leq 7, \quad y \geq 0 \end{aligned}$	$F = -17 \ (x, y) \equiv (1, 0)$
7	$\begin{aligned} &\text{Max}_x \quad F = x^2 + (y - 10)^2 \\ &\text{s.t.} \quad x \leq 15, \quad -x + y \leq 0, \quad -x \leq 0 \\ &\text{Max}_y \quad [(x + 2y - 30)^2] \\ &\text{s.t.} \quad x + y \leq 20, \quad 0 \leq y \leq 20 \end{aligned}$	$F = 100 \ (x, y) \equiv (10, 10)$

(Continued on next page.)

Table 1. (Continued).

Sr. no.	Problem description	Global optimum
8	$\begin{aligned} &\text{Max}_x \quad F = x + y \\ &\text{s.t.} \quad x \geq 0 \\ &\text{Max}_y \quad 5x + y \\ &\text{s.t.} \quad -x - 0.5y \leq -2, \quad -0.25x + y \leq 2 \\ &\quad \quad x - 2y \leq 2, \quad y \geq 0 \end{aligned}$	$-3.111 (x, y) \equiv (0.889, 2.222)$
9	<p>Micropore</p> $\frac{d^2 C_i}{dX^2} + \frac{2}{X} \frac{dC_i}{dX} = \frac{\phi^2 C_i}{K_m + C_i} \text{ (Michaelis-Menten Kinetics)}$ <p>s.t. $\left(\frac{dC_i}{dX}\right) = 0$ at $X = 0$ $C_i = C_a$ at $X = 1$</p>	$F = 0.0 \quad C_{ma}(0) = 0.630083$
9	<p>Macropore</p> $\frac{d^2 C_a}{dY^2} + \frac{2}{Y} \frac{dC_a}{dY} = \alpha \left(\frac{dC_i}{dX}\right)_{x=1}$ <p>s.t. $\left(\frac{dC_a}{dY}\right) = 0$ at $Y = 0$, $C_a = 1$ at $Y = 1$ $\phi = 1, \quad \alpha = 5, \quad \overline{K_m} = 1$</p> <p>Reformulated optimization problem</p> <p>Min $\text{abs}(1 - C_{ma}(1))$ Min $\text{abs}(C_{mi}(1) - C_{ma}(0))$ $0 \leq C_{mi} \leq 1$ $0 \leq C_{ma} \leq 1$</p>	

been selected from different sources. For each problem, at least 25 runs were taken. This was done to ensure that the choice of seed values for the random number generator used did not have a major influence on the solution obtained. All simulations were carried out on a Sun Enterprise 450 server.

Problems 1, 2 and 3 are examples taken from Clark and Westerberg (1990). In problem 1, the outer loop optimization variable is x , while y_1 and y_2 are the inner loop optimization variables. The inner loop is linearly constrained. The domain of the optimization variables x and y_1 is specified in the problem, while that of y_2 may be obtained from the constraints. The value of the global optimum obtained for the outer loop objective function was 12.9539, which is in the vicinity (within 0.4%) of the global optimum reported earlier. Problems 2 and 3 illustrate the effect of constraints on the inner and outer loop. The problems involve quadratic objective functions with linear constraints. The variables x and y lie in the domain $[0, 8]$. For both the problems, the respective values of the outer loop objective functions obtained were very close (within 0.02%) to the value reported by Clark and Westerberg.

Problem 4 (Wen and Hsu, 1991) involves a large number of linear constraints, which considerably reduce the solution space for the problem. The domain for x and y is relatively

wide [5, 15] and hence a larger value of the partition parameter (as compared to the earlier problems) was used for the variables. The algorithm converged to a value of 84.898, which is within 0.2% of the global optimum reported by the authors. Problem 5 is an application of bilevel programming in planning operations. It is a two-level resource control problem from Bialas and Karwan (1984). With a domain of [5, 15] for both x and y , the algorithm gave a value for the outer objective function close to (within 0.1%) the reported global optimum of 11.

The CPU requirements for the present study along with the CPU requirements for the earlier works are provided in Table 2. Although a direct comparison is difficult to make due to differences in computational platforms, it can be mentioned that the requirements in the present study are very nominal.

The test cases 6, 7 and 8 were taken from a computational study of the modified GOP algorithm proposed by Visweswaran et al. (1996). In case 6, the outer loop and the inner loop objective functions are quadratic in nature. For this problem, the CPU time required by them was 3.3 seconds on a SPARC 10 system. The well-known solver GAMS was used for solving the primal and dual sub problems in arriving at the global optimum. With the tabu search algorithm, the CPU time for obtaining the global optimum (outer loop) of 17 was 0.04 seconds. Case 7 presents a problem involving quadratic objective functions at both levels. The present approach required 0.08 seconds to reach the global optimum of 100 (for the outer loop objective). For the same problem, Visweswaran et al. (1996) report a CPU time of 0.12 seconds on a HP-730 system, again using the GAMS solver for the primal and dual sub problems. The case 8 tested was a linear programming problem originally proposed by Bard (1983) involving several constraints at the inner level, but no constraints at the outer level. The tabu search algorithm was able to reach the global optimum consistently (in each of the 25 runs) within 0.05 seconds of CPU time. No CPU times have been reported for this problem in the literature. In order to ascertain the efficiency of the tabu search algorithm, it was decided to increase the search space for the variables, in steps of 10, from 10 to 50 for each variable (with zero as the lower limit in each case). The study revealed the ability of the algorithm to track the global optimum even in a very large solution space within 0.07 s of CPU time.

The next example was that of a reaction diffusion equation of an isothermal pellet. Pellets with a biporous structure emerge when powdered particles are pelletized (Ors and Dogu, 1979; Jayaraman et al., 1981; Jayaraman, 1993). The governing mass balance equations along with the boundary conditions are included as case example 9 in Table 1. The reacting gas has to diffuse through the macropores and then further through the micropores to react with the catalyst located on the inner walls of the micropore. As can be seen from the Table 1, this problem can be described by two second order ordinary differential equations, one each for the micro and macro regions, respectively. The macropore is coupled to the micropore region through the boundary condition at the surface of the micropores. Such a coupling makes the solution procedure difficult. Using different solution strategies like transformation of variables and shooting methods, researchers have earlier solved this problem (Jayaraman et al., 1981; Jayaraman, 1993). This problem can be posed as an optimization problem by reformulating the boundary conditions at the surface of the micropores and macropores as objective functions. The reformulated optimization problem is an example of a bilevel

Table 2. BLP problems—performance measures.

Prob. no.	Problem source	Properties [@]	Search interval	Global optimum		CPU time (in sec)		Computational platform	
				Literature	This study	Literature	This study	Literature	This study
1	Clark and Westerberg, 1990	Linear	$x \in [0, 8], y_1 \in [0, 4], y_2 \in [0, 8]$	13	12.953	44.58	0.02	Sun ultra 2 workstation	Sun enterprise 450
2	Clark and Westerberg, 1990	Quadratic, 3 local optima (1, 3), (3, 5), (4.4, 4.8)	$x \in [0, 8], y \in [0, 8]$	5	4.999	(0.67–230.26)*	0.07	Sun ultra 2 workstation	Sun enterprise 450
3	Clark and Westerberg, 1990	Quadratic	$x \in [0, 8], y \in [0, 8]$	9	8.997	199.38	0.03	Sun ultra 2 workstation	Sun enterprise 450
4	Wen and Hsu, 1991	Linear	$x \in [5, 15], y \in [5, 15]$	85.0909	84.898	–	0.18	–	Sun enterprise 450
5	Bialas and Karwan, 1984	Linear	$x \in [5, 15], y \in [5, 15]$	11	10.990	–	0.08	–	Sun enterprise 450
6	Visweswaran et al., 1996	Quadratic, non-convex with local optima at (1, 0), (5, 2)	$x \in [0, 10], y \in [0, 10]$	17	17.071	3.3	0.04	SPARC-10	Sun enterprise 450
7	Visweswaran et al., 1996	Quadratic	$x \in [0, 15], y \in [0, 20]$	100	100.324	0.12	0.08	HP-730	Sun enterprise 450
8	Visweswaran et al., 1996	Linear	$x \in [0, 50], y \in [0, 50]$	3.11	–3.179	–	0.05	–	Sun enterprise 450
9	Jayaraman, 1993	Nonlinear	$C_{mi} \in (0, 1), C_{ma} \in (0, 1)$	0.0	0.0	–	10	–	Sun enterprise 450

[@] Indicates nature of the objective functions.

*In this case, the global optimum was obtained with only 20% of the times attempted in 0.67 sec; and with 80% success in 230.26 sec. With TS, the global optimum was obtained on all the runs without any convergence difficulties.

–Indicates that these values were not available in the literature.

programming problem. The boundary condition at the macropore surface ($y = 1$) can be rewritten as an objective function for the outer level problem as:

$$\text{Minimize } \text{abs}[1 - (C_{ma}(1))] \quad (7)$$

Similarly, the micropore boundary condition at the micropore-macropore junction can be written as the inner level objective function as:

$$\text{Minimize } \text{abs}[C_{mi}(1) - C_{ma}(y)] \quad (8)$$

For a fixed value of parameters α and ϕ , there is a unique value of the macropore concentration ($C_{ma}(0)$) which satisfies the macropore boundary condition. Similarly for each micropore there is a unique value of micropore concentration ($C_{mi}(0)$), which satisfies the micropore boundary condition. The macropore concentration, $C_{ma}(0)$ can be looked upon as the outer level variable while the micropore concentration, $C_{mi}(0)$ as the inner level variable. Thus for every trial value of $C_{ma}(0)$ supplied by the outer level tabu, the inner level tabu solves (assuming step size of 0.01 for the macropore length variable, y) 100 inner level (micropore) boundary value problems.

The tabu search algorithm was run for linear first order kinetics for several values of the governing parameters ϕ and α . The results are in perfect agreement with the analytical solution (Ors and Dogu, 1979). Results were also obtained for a non-linear Michaelis-Menten kinetic rate expression, and were compared with those reported in the literature (Jayaraman, 1993). The algorithm performs very well in terms of the quality of the solutions obtained. A representative result for the Michaelis-Menten kinetic expression (for $\phi = 1$, $\alpha = 5$) is shown in Table 2, along with the results obtained with the classical shooting method. It can be seen that both methods compare very well. It must, however, be pointed out that for the shooting method, several auxiliary differential equations have to be simultaneously solved, which is rather cumbersome. Also, the shooting method exhibits convergence difficulties if the initial guess is far away from the actual value.

4. Conclusions

Bilevel programming problems are commonly encountered in several branches of engineering. The solution of these problems is time consuming and requires accurate estimation of several inner level problems for each call of the outer level problem. Several earlier approaches require tedious transformations, which often bring in complications like non-convexities. Also, these cannot handle discontinuous functions. The challenge is to develop a dependable algorithm capable of solving a variety of bilevel programming problems such as linear, non-linear and problems having multiple optima. The tabu search algorithm described in this paper is able to provide quality solutions to hard problems with minimal computational effort. This is illustrated by considering a number of test examples with varying degrees of complexities. The algorithm can be suitably modified to incorporate more rigorous mechanisms to handle very large-scale bilevel and multilevel problems.

Acknowledgment

Financial support received from Unilever Port Sunlight, U.K. is gratefully acknowledged.

References

- Bard, J.F. (1991). "Some Properties of the Bilevel Programming Problem." *Journal of Optimization Theory and Applications* 2, 371–378.
- Bard, J.F. and J.T. Moore. (1990). "A Branch and Bound Algorithm for the Bilevel Programming Problem." *SIAM Journal of Scientific and Statistical Computing* 11, 281–292.
- Batti, R. and G. Tecchiolli. (1996). "The Continuous Reactive Tabu Search: Blending Combinatorial Optimization and Stochastic Search for Global Optimization." *Annals of Operations Research* 63, 53–188.
- Bialas, W.F. and M.H. Karwan. (1984). "Two-Level Linear Programming." *Management Science* 30, 1004–1020.
- Biegler, L.T., I.E. Grossman, and A.W. Westerberg. (1997). *Systematic Methods of Chemical Process Design*. New Jersey: Prentice Hall PTR.
- Bonabeau, E., M. Dorigo, and G. Theraulaz. (2000). "Inspiration for Optimization from Social Insect Behavior." *Nature* 406, 39–42.
- Bracken, J. and J. McGill. (1973). "Mathematical Programs with Optimization Problems in the Constraints." *Operations Research* 21, 37–44.
- Bregel, D.D. and W.D. Seider. (1992). "Coordinated Design and Control Optimization of Nonlinear Processes." *Computers and Chemical Engineering* 16, 861–886.
- Calamai, P. and L. Vicente. (1993). "Generating Linear and Linear-Quadratic Bilevel Programming Problems." *SIAM Journal on Scientific and Statistical Computing* 14, 770–782.
- Candler, W. and R. Norton. (1977). "Multilevel Programming." Technical Report 20, World Bank Development Center, Washington, D.C.
- Candler, W. and R. Townsley. (1982). "A Linear Two-Level Programming Problem." *Computers and Operations Research* 9, 59–76.
- Chelouah, D. and P. Siarry. (2000). "Tabu Search Applied to Global Optimization." *European Journal of Operations Research* 123, 256–270.
- Clark, P.A. and A. Westerberg. (1983). "Optimization for Design Problems Having More than One Objective." *Computers and Chemical Engineering* 7, 259–278.
- Clark, P.A. and A. Westerberg. (1990). "Bilevel Programming for Chemical Process Design: Fundamentals and Algorithms." *Computers and Chemical Engineering* 14, 87–97.
- Cvijovic, D. and J. Klinowski. (1995). "Tabu Search: An Approach to the Multiple Minima Problem." *Science* 267, 664–666.
- Dempe, S. (1992). "A Necessary and a Sufficient Optimality Condition for Bilevel Programming Problems." *Optimization* 25, 341–354.
- Edmunds, T.A. and J.F. Bard. (1991). "Algorithms for Nonlinear Bilevel Mathematical Programs." *IEEE Transactions on Systems, Man and Cybernetics* 21, 83–89.
- Edmunds, T.A. and J.F. Bard. (1992). "An Algorithm for the Mixed Integer Nonlinear Bilevel Programming Problem." *Annals of Operations Research* 34, 149–162.
- Glover, F. (1986). "Future Paths for Integer Programming and Links to Artificial Intelligence." *Computers and Operations Research* 13, 533–549.
- Glover, F. (1989). "Tabu Search-Part I." *ORSA Journal on Computing* 1, 190–206.
- Glover, F. (1990). "Tabu Search-Part II." *ORSA Journal on Computing* 2, 4–32.
- Glover, F., M. Laguna, E. Taillard, and D. de Werra. (1993). "Users Guide to Tabu Search." *Annals of Operations Research* 41, 3–28.
- Glover, F. and M. Laguna. (1997). *Tabu Search*. Boston: Kluwer Academic Publishers.
- Hansen, P., B. Jaumard, and G. Savard. (1992). "New Branch-and-Bound Rules for Linear Bilevel Programming." *SIAM Journal on Scientific and Statistical Computing* 13, 1194–1217.
- Jayaraman, V.K., B.D. Kulkarni, and L.K. Doraiswamy. (1981). "A Simple Method of Solution for a Class of Reaction Diffusion Problems." *AIChE Journal* 29, 521–523.

- Jayaraman, V.K. (1993). "An Algorithm for Solving Bidisperse Catalyst Pellet Problems." *Computers and Chemical Engineering* 17, 639–642.
- Kelly, J., M. Laguna, and F. Glover. (1994). "A Study on Diversification Strategies for the Quadratic Assignment Problem." *Computers and Operations Research* 22, 885–893.
- Laguna, M., J. Barnes, and F. Glover. (1993). "Intelligent Scheduling with Tabu Search: An Application to Jobs with Linear Delay Penalties and Sequence Dependent Setup Costs and Times." *Journal of Applied Intelligence* 3, 159–172.
- Laguna, M. and P. Laguna. (1995a). "Applying Tabu Search to the Two-Dimensional Ising Spin Glass." *International Journal of Modern Physics-C* 6, 11–23.
- Laguna, M., J. Kelly, J. González-Velarde, and F. Glover. (1995b). "Tabu Search for the Multilevel Generalized Assignment Problem." *European Journal of Operational Research* 82, 176–189.
- Laguna, M., R. Martí, and V. Campos. (1999). "Intensification and Diversification with Elite Tabu Search Solutions for the Linear Ordering Problem." *Computers and Operations Research* 26, 1217–1230.
- Ors, N. and T. Dogu. (1979). "Effectiveness of Bidisperse Porous Catalysts." *AIChE J.* 25, 723–725.
- Outrata, J. (1994). "On Optimization Problems with Variational Inequality Constraints." *SIAM Journal on Optimization* 4, 340–357.
- Sahin, H.K. and R.A. Ciric. (1998). "A Dual Temperature Simulated Annealing Approach for Solving Bilevel Programming Problems." *Computers and Chemical Engineering* 23, 11–25.
- Siarry, P. and G. Berthiau. (1997). "Fitting of Tabu Search to Optimize Functions of Continuous Variables." *International Journal for Numerical Methods in Engineering* 40, 2449–2457.
- Stackelberg, H. (1952). *The Theory of Market Economy*. Oxford University Press.
- Visweswaran, V., C. Floudas, M. Ierapetritou, and E. Pistikopoulos. (1996). "A Decomposition Based Global Optimization Approach for Solving Bilevel Linear and Nonlinear Quadratic Programs." In Floudas and Pardalos (eds.), *State of the Art in Global Optimization: Computational Methods and Applications*. Kluwer Academic Publishers.
- Wen, U. and S. Hsu. (1991). "Linear Bilevel Programming Problems—A Review." *Journal of the Operations Research Society* 42, 125–133.
- Yang, H. and S. Yagar. (1994). "Traffic Assignment and Traffic Control in General Freeway-Arterial Corridor Systems." *Transportation Research* 28B, 463–486.