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OPTIMIZATION MODEL FOR LONG RANGE PLANNING IN THE CHEMICAL INDUSTRY

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Abstract—In this paper a multiperiod MILP model is presented for the optimal selection and expansion of processes given time varying forecasts for the demands and prices of chemicals over a long range horizon. To reduce the computational expense of solving this long range planning problem, several strategies are investigated, including branch and bound, the use of integer cuts, strong cutting planes, Benders decomposition and heuristics. These procedures, which have been implemented in the program MULPLAN, are illustrated with several example problems. As is shown, the proposed model is especially useful for the study of a variety of different scenarios.

INTRODUCTION

Chemical companies are increasingly concerned with the development of planning techniques for their process operations (see Hirshfeld, 1987). The incentive for doing so derives from the interaction of several factors. Recognizing the potential benefits of new resources when these are used in conjunction with existing processes is the first factor. Another major factor is the dynamic nature of the economic environment. Companies must assess the potential impact on their business of important changes in the external environment. Included are changes regarding demand, prices, technology, capital, markets and competition. Hence, due to technology obsolescence, increasing competition, and fluctuating prices and demands of chemicals, there is an increasing need of quantitative techniques for planning the selection of new processes, the expansion and shut-down of existing processes, and the production of chemicals.

A rather large number of papers has been reported in the operations research literature on capacity expansion problems in several areas of application. A recent survey can be found in Luss (1982). In the chemical engineering literature, dynamic programming (see Roberts, 1964) has been applied to chemical plant expansions, but this decomposition technique becomes quite ineffective for large-scale problems. Alternative approaches include the NLP formulation by Himmelblau and Bickel (1980), the multiperiod MILP formulation by Grossmann and Santibanez (1980), the goal programming approach of Shimizu and Takamatsu (1985) and the recursive MILP technique by Jimenez and Rudd (1987). However, these approaches are often limited in the size of problems that they can handle.

It is the purpose of this paper to present a multiperiod MILP model for long-range planning in the chemical process industries. For a network of processes and chemicals that consists of existing as well as potentially new processes, the major objective in this model is to determine the selection of new processes and the capacity expansion and shut-down policies for all processes, given forecasts of prices and demands of the chemicals over a long-range horizon. Several solution strategies, including the use of integer cuts, strong cutting planes and Benders decomposition, are investigated for reducing the computational expense of solving the MILP problem. These strategies, which have been implemented in the computer program MULPLAN, will be illustrated with several example problems.

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PROBLEM STATEMENT

The specific problem that is addressed in this paper assumes that a network of processes and chemicals is given. This network includes an existing system as well as potential new processes and chemicals. Also given are forecasts for prices and demands of chemicals, as well as investment and operating costs over a finite number of time periods within a long range horizon. The problem then consists of determining the following items that will maximize the net present value over the given time horizon:

(a) capacity expansion and shut-down policy for existing processes;
(b) selection of new processes and their capacity expansion policy;
(c) production profiles;
(d) sales and purchases of chemicals at each time period.

Linear models are assumed for the mass balances in the processes, while fixed-charge cost models are used for the investment cost. Also, limits on the investment cost at each time period can be specified, as well as constraints on the sales and purchases. No inventories will be considered since the length of each time period is assumed to be rather long (e.g. 1 yr). It will be shown in the next section that the above problem can be formulated as a multiperiod MILP problem.

MULTIPERIOD MILP MODEL

A network consisting of a set of NP chemical processes that can be interconnected in a finite number of ways is assumed to be given. The network also involves a set of NC chemicals which include raw materials, intermediates and products. This network can then be represented by two types of nodes: one for the processes and another for the chemicals. These nodes will be interconnected by a total of n streams to represent the different alternatives that are possible for the processing and the purchases and sales from different markets.

Also, a finite number of NT time periods is considered during which prices and demands of chemicals, and investment and operating costs of the processes can vary. The objective function to be maximized is the net present value of the project over the specified horizon consisting of NT time periods.

It will be assumed that the material balances in each process can be expressed linearly in terms of the production rate of a main product, which in turn defines the capacity of the plant. As for the investment costs of the processes and their expansions, it will be considered that they can be expressed linearly in terms of the capacities with a fixed charge cost to account for the economies of scale.

In the formulation of this problem, the variable Q_{it} represents the total capacity of the plant of process i that is available in period t, $t = 1, NT$. The parameter Q_{i0} represents the existing capacity of process at time $t = 0$. QE_{it} represents the capacity expansion of the plant of process i which is installed in period t. If y_{it} are the 0–1 binary variables which indicate the occurrence of the expansions for each process i at each time period t, the constraints that apply are:

$$\left.\begin{array}{r} y_{it} QE^{\mathrm{L}}_{it} \leqslant QE_{it} \leqslant QE^{\mathrm{U}}_{it} y_{it} \\ y_{it} = 0, 1 \end{array}\right\} \quad i = 1, NP, \quad t = 1, NT, \tag{1}$$

$$Q_{it} = Q_{i,t-1} + QE_{it} \quad i = 1, NP, \quad t = 1, NT. \tag{2}$$

In equation (1), QE^{L}_{it} and QE^{U}_{it} are lower and upper bounds for the capacity expansions. A zero-value of the binary variables y_{it} forces the capacity expansion at period t to zero, i.e. $QE_{it} = 0$. If the binary variable is equal to one, the capacity expansion is performed. Equation (2) simply defines the total capacity Q_{it} that is available at each time period t.

The amounts of the chemicals being consumed and produced in period t of the plant of process i are represented by the variables:

$$W_{kt} \geqslant 0 \quad k \in L_i \quad i = 1, NP \quad t = 1, NT, \tag{3}$$

where L_i is the index of the subset of n streams corresponding to inputs and outputs of process i, and $\bigcup_{i=1}^{NP} L_i = \{1, 2, \ldots n\}$. Let stream $m_i \in L_i$ correspond to the main product produced by process i. Then the amount produced of that product cannot exceed the installed capacity; that is:

$$Q_{it} \geqslant W_{m_i t} \quad i = 1, NP \quad t = 1, NT. \tag{4}$$

The case of shut-down of an existing plant results when the variable $W_{m_i t}$ takes a value of zero after a given time period t.

The material balances in each plant are given by the linear relations:

$$W_{kt} = \mu_{ik} W_{m_i t} \quad k \in L_i \quad i = 1, NP \quad t = 1, NT, \tag{5}$$

where μ_{ik} are positive constants characteristic of each process i.

As for the raw materials, intermediates and products, they will be represented by NC nodes of chemicals where purchases and sales are considered on one of several markets, $l = 1, NM$. If the corresponding variables are represented, respectively, in each period by the variables $P^l_{jt}, S^l_{jt}, j = 1, NC$, they must satisfy the inequalities:

$$\left.\begin{array}{r} a^{l\mathrm{L}}_{jt} \leqslant P^l_{jt} \leqslant a^{l\mathrm{U}}_{jt} \\ d^{l\mathrm{L}}_{jt} \leqslant S^l_{jt} \leqslant d^{l\mathrm{U}}_{jt} \end{array}\right\} \quad j = 1, NC, \quad t = 1, NT, \quad l = 1, NM, \tag{6}$$

where $a^{l\mathrm{L}}_{jt}, a^{l\mathrm{U}}_{jt}$ are lower and upper bounds on the availabilities, and $d^{l\mathrm{L}}_{jt}, d^{l\mathrm{U}}_{jt}$ are lower and upper bounds on the demands.

Defining $I(j)$ as the index set of output streams of plants that produce chemical j, and $O(j)$ as the index set of input streams of plants that consume chemical j, the mass balances on these chemicals' nodes will be given by:

$$\sum_{l=1}^{NM} P^l_{jt} + \sum_{k \in I(j)} W_{kt} = \sum_{l=1}^{NM} S^l_{jt} + \sum_{k \in O(j)} W_{kt} \quad j = 1, NC \quad t = 1, NT. \tag{7}$$

Finally, the net present value of the project is given by:

$$\begin{aligned} \mathrm{NPV} = & -\sum_{i=1}^{NP} \sum_{t=1}^{NT} (\alpha_{it} QE_{it} + \beta_{it} y_{it}) \\ & -\sum_{i=1}^{NP} \sum_{t=1}^{NT} \delta_{m_i t} W_{m_i t} \\ & +\sum_{l=1}^{NM} \sum_{j=1}^{NC} \sum_{t=1}^{NT} (\gamma^l_{jt} S^l_{jt} - \Gamma^l_{jt} P^l_{jt}), \end{aligned} \tag{8}$$

where the parameters α_{it}, β_{it} represent, respectively, the variable and fixed terms for the investment cost, $\delta_{m_i t}$ is the unit operating cost, and $\gamma^l_{jt}, \Gamma^l_{jt}$ are the prices of sales and purchases of the chemical j in market l, $l = 1, NM$. All these parameters are discounted at the specified interest rate and include the effect of taxes in the net present value.

In order to determine the optimal planning of the network, the multiperiod MILP model consists of maximizing the objective function in (8), subject to the constraints (1–7).

Additional constraints that can be considered include:

(a) limit on the number of expansions of some processes:

$$\sum_{t=1}^{NT} y_{it} \leqslant NEXP(i) \quad i \in I' \subseteq \{1, 2, \dots NP\}; \quad (9)$$

(b) limit on the capital available for investment during some time periods:

$$\sum_{i=1}^{NP} (\bar{\alpha}_{it} QE_{it} + \bar{\beta}_{it} y_{it}) \leqslant CI(t)$$

$$t \in T' \subseteq \{1, 2, \dots NT\}; \quad (10)$$

where $\bar{\alpha}_{it}$, $\bar{\beta}_{it}$ are nondiscounted cost coefficients corresponding to period t.

Finally, for the case when the economics of shutdowns are modelled explicitly, the constraints discussed in Appendix A can be included.

SOLUTION STRATEGIES

The MILP model given in the previous section can typically be solved directly with branch and bound enumeration procedures (Little *et al.*, 1963; Garfinkel and Nemhauser, 1972; Schrijver, 1986; Nemhauser and Wolsey, 1988) such as the ones that are implemented in standard computer packages (e.g. MPSX, APEX, LINDO, ZOOM). For large networks, however, the computational expense can be high. For example, a network with 40 processes, 50 chemicals, two markets and five time periods would involve 200 binary variables, and approx. 1000 continuous variables and 1200 constraints. Since most of the alternatives embedded in such a model are feasible, a large number of branches must usually be examined. Therefore, there is a clear incentive to develop efficient computational strategies and approximate procedures since this then allows the examination of a greater variety of scenarios with the planning model. In the following section four numerical schemes will be described.

BOUNDING AND INTEGER CONSTRAINTS

In this section it will be assumed that there are no limitations on the capital investment at each time period. A simple bounding constraint that can then be generated for the MILP problem is to solve the relaxed LP and determine the two following solutions that correspond to lower bounds to the net present value:

LB_1—relaxed LP solution with nonzero binaries set to one;

LB_2—relaxed LP solution with nonzero binaries of first active period set to one, and with the corresponding capacities set to the minimum required in order to serve demand during all subsequent active time periods in the relaxed LP solution.

In other words LB_1 corresponds to a feasible solution where expansions are performed as determined by the relaxed LP solution. LB_2 corresponds to a feasible solution where only one expansion is considered at the first active period determined from the relaxed LP. These bounds, which are very easy to determine, can then be incorporated into the MILP with the following inequality:

$$\text{NPV} \geqslant \max\{\text{LB}_1, \text{LB}_2\}. \quad (11)$$

Additional constraints that can reduce the computational effort in the branch and bound procedure are integer constraints that place a limit on the number of expansions in a process. Again, assuming no limitation in the investment cost, the maximum number of expansions $NEXP(i)$ can be determined by calculating the maximum number of expansions whose cost is less than or equal to the maximum cost (in the worst-case sense) of any given expansion. This then leads to the following MILP problem for each process i:

$$NEXP(i) = \max \sum_{t=1}^{NT} y_{it}, \quad (12)$$

st.

$$\sum_{t=1}^{NT} (\alpha_{it} QE_{it} + \beta_{it} y_{it}) \leqslant \alpha_{i\,\max} Q_{i\,\max} + \beta_{i\,\max},$$

$$\sum_{t=1}^{NT} QE_{it} = Q_{i\,\max},$$

$$0 \leqslant QE_{it} \leqslant QE^{U} y_{it} \quad i = 1, NP, \quad t = 1, NT,$$

$$y_{it} = 0, 1 \quad i = 1, NP, \quad t = 1, NT,$$

where QE^{U} is a large positive quantity.

Note that the first inequality simply states that the cost of the expansions cannot exceed the investment cost of process i at maximum capacity with the "worst" cost coefficients. Due to the discount factors, these usually correspond to period 1. As for the maximum capacity $Q_{i\,\max}$, this is a function of the upper bounds on demands and availabilities of chemicals, and it is equal to the minimum capacity required in order to serve the maximum possible demand. This demand, in turn, can be found by solving for each time period an LP that maximizes W_{mjt} subject to the material balance constraints (5), (6) and (7) in the whole network.

From the solution of the above small-scale MILPs in (12), the constraints in (9) can be added to the multiperiod MILP. Both constraints (9) and (11) will usually help in reducing the gap between the relaxed LP and MILP solutions so as to decrease the computational effort of the branch and bound method. However, for large-scale problems these provisions may not be sufficient. Furthermore, when the constraints (10) on capital investment are present or when $Q_{i\,\max}$ in (12) exceeds QE^{U}_{it}, the problem in (12) will often underestimate the maximum number of expansions. Therefore, it is worth considering the use of strong cutting planes that can strengthen the upper bound of the relaxed LP problem when the investment constraints in (10) are present and the expansion upper bounds in (1) are finite quantities with physical significance.

STRONG CUTTING PLANES

Recently, a new approach to the solution of large-scale ILP and MILP problems has emerged (Crowder *et al.*, 1983; Van Roy and Wolsey, 1987; Nemhauser and Wolsey, 1988). The idea of this approach is to try to generate from the relaxed LP tighter formulations of 0–1 polyhedra by adding cutting planes that describe facets or faces of high dimension of the convex hull of these polyhedra. The gap between the MILP and its LP relaxation is thereby often reduced (if not completely eliminated), and the subsequent use of branch and bound or any other algorithm is made computationally less expensive.

At each iteration the procedure starts by finding (x^*, y^*), the optimum values for the continuous and 0–1 variables of the LP relaxation of the current MILP formulation. Then a *separation problem* is solved by using only part of the model (corresponding to a combinatorial problem which has been studied extensively in the literature, e.g. some network flow type constraints) to generate additional valid inequalities which attempt to chop off the point (x^*, y^*) from the solution space of the LP relaxation polyhedron. The procedure is then repeated until an integer solution to the new LP relaxation is found, or else until there is a small improvement in strengthening the LP relaxation bound.

The above procedure, for which details can be found in Van Roy and Wolsey (1987), can be applied to the multiperiod MILP with capital investment constraints as follows. First, network substructures of the model are identified; namely, equations (1) and (10) for each time period t, $t = 1, NT$:

$$S_t = \left\{(QE, y): \sum_{i=1}^{NP} (\bar{\alpha}_{it} QE_{it} + \bar{\beta}_{it} y_{it}) \leq CI(t), \right.$$
$$\left. y_{it} QE^L_{it} \leq QE_{it} \leq QE^U_{it} y_{it},\; y_{it} \in \{0, 1\} \quad i = 1, NP \right\}. \tag{13}$$

To see the network structure, we substitute:

$$\left.\begin{aligned} x_{it} &= \bar{\alpha}_{it} QE_{it} + \bar{\beta}_{it} y_{it} \\ l_{it} &= \bar{\alpha}_{it} QE^L_{it} + \bar{\beta}_{it} \\ u_{it} &= \bar{\alpha}_{it} QE^U_{it} + \bar{\beta}_{it} \end{aligned}\right\} \quad i = 1, NP \tag{14}$$

and obtain:

$$S'_t = \left\{(x, y): \sum_{i=1}^{NP} x_{it} \leq CI(t), \right.$$
$$\left. l_{it} y_{it} \leq x_{it} \leq u_{it} y_{it},\; y_{it} \in \{0, 1\} \quad i = 1, NP \right\}. \tag{15}$$

For this structure two families of valid inequalities have been derived (Van Roy and Wolsey, 1986):

the simple generalized flow cover inequality:

$$\sum_{i \in C_t} [x_{it} + (u_{it} - \lambda_t)^+ (1 - y_{it})] \leq CI(t); \tag{16}$$

and the extended generalized flow cover inequality:

$$\sum_{i \in C_t} [x_{it} + (u_{it} - \lambda_t)^+ (1 - y_{it})]$$
$$+ \sum_{i \in R_t} [x_{it} + (\bar{u}_{it} - \lambda_t)^+ (1 - y_{it})] \leq CI(t), \tag{17}$$

where the notation Φ^+ stands for $\max(0, \Phi)$ and $C_t \subseteq \{1, 2, \ldots NP\}$ is a generalized cover, i.e.

$$\lambda_t = \sum_{i \in C_t} u_{it} - CI(t) > 0;$$

and

$$R_t \subseteq \{1, 2, \ldots NP\}; \quad \bar{u}_{it} = \max(\bar{u}_t, u_{it});$$

$$\bar{u}_t = \max_{i \in C_t} \{u_{it}\}, \quad \text{and } \bar{u}_t > \lambda_t > 0.$$

Note that u_{it} is given in (14).

The exact separation algorithms for the simple and the extended generalized cover inequalities correspond to Knapsack problems parameterized in λ_t, R_t, C_t that maximize the violation of the derived cut by the relaxed LP solution point (x^*, y^*). This leads to the following Knapsack problem for each time period t:

$$\max \zeta_t = \sum_{i=1}^{NP} \{-(1 - y^*_{it}) z_i\}, \tag{18}$$

$$\text{st.} \qquad \sum_{i=1}^{NP} u_{it} z_i > CI(t),$$

$$z_i \in \{0, 1\} \quad i = 1, NP,$$

where $z_i = 1$ if $i \in C_t$; $z_i = 0$ otherwise. The violated inequalities (16) and (17) are derived whenever $\zeta_t > -1$. The indices i that are included in the set R_t for the inequality in (17) must satisfy the condition: $x^*_{it} - (\bar{u}_{it} - \lambda_t)^+ y^*_{it} \geq 0$.

The cutting plane algorithm is then as follows:

Step 0. Solve the LP relaxation of the multiperiod MILP. Set NPV′ = NPV (optimum from relaxed LP).

Step 1. For each time period t, solve the separation problem (18). Here the problem is only approximately solved using some form of the greedy heuristic (see Appendix B). From the solution to the Knapsack problem, determine the cover C_t and add the violated inequalities (16) and (17) to the current MILP formulation.

Step 2. Solve the new LP relaxation. If (NPV′ − NPV)/NPV′ > tolerance, then set NPV′ = NPV and repeat Steps 1 and 2.

Otherwise, start the branch and bound procedure or any other algorithm to find the optimum to the current formulation.

The algorithm has the advantage that no attempt is made to generate all the facets of the 0–1 polyhedron at once, which is an *NP*-hard problem. Instead, cuts are added at each iteration in an attempt to reduce the LP relaxation gap. On the other hand, it must be pointed out that it suffers from the following. First, the information is extracted only from an isolated part of the model and secondly, the separation problem has been relaxed to a computationally effective form which might not always generate an optimum cut. Therefore, it is to be expected that the LP relaxation gap will not be completely eliminated. Nevertheless, since the method is computationally very cheap and at the same time effective in the initial iterations, it can be used to reformulate the initial multiperiod MILP model to one which is more easily solved by other methods like branch and bound and decomposition schemes.

BENDERS DECOMPOSITION

A standard decomposition technique that can be applied to the multiperiod MILP problem is Benders decomposition method (Benders, 1962; Geoffrion, 1972) which has been found to be very effective for the solution of a static, multiproduct, multifacility distribution system design problem (Geoffrion and Graves, 1974). In this algorithm the MILP problem is solved through a sequence of LP subproblems and MILP master problems, with the former providing lower bounds to the net present value and the latter providing upper bounds. The definition of the LP subproblems and master problems depends, however, on the partitioning of variables that is used.

In its most natural form the variables of the multiperiod MILP are partitioned as follows:

(a) complicating variables for the master problem: y_{it};

(b) remaining variables for the LP subproblem:

$$u = [Q_{it}, QE_{it}, S^l_{jt}, P^l_{jt}, W_{kt}].$$

The basic steps in Benders decomposition method are as follows:

Algorithm B-I

Step 1. Select y^1_{it}; set $\mathrm{NPV}^U = +\infty$, $\mathrm{NPV}^L = -\infty$, $R = 1$.

Step 2. (a) Fix the variables y^R_{it} and solve the multiperiod MILP problem as an LP to determine NPV^R and u^R;

(b) update the lower bound by setting $\mathrm{NPV}^L = \max\{\mathrm{NPV}^L, \mathrm{NPV}^R\}$.

Step 3. To determine new values y^{R+1}_{it} for the 0–1 variables and an upper bound to NPV, solve the pseudo-integer master problem:

$$\mathrm{NPV}^U = \max_{y_{it}, \mu} \mu, \tag{19}$$

st.

$$\mu \leqslant \mathrm{L}^r(y_{it}) \quad r = 1, R,$$

$$\mu \in \mathcal{R}^1, \quad y_{it} = 0, 1 \quad i = 1, NP, \quad t = 1, NT,$$

where the Lagrangian:

$$\mathrm{L}^r(y_{it}) = \mathrm{NPV}(y_{it}, u^r) + \sum_{i=1}^{NP} \sum_{t=1}^{NT} [\lambda^{U,r}_{it}(QE^t_{it} - QE^U_{it} y_{it}) + \lambda^{L,r}_{it}(QE^L_{it} y_{it} - QE^t_{it})] \tag{20}$$

and $\mathrm{NPV}(y_{it}, u^r)$ is the NPV function with all continuous variables u^r fixed (but not the y_{it}) and $\lambda^{L,r}_{it}, \lambda^{U,r}_{it}$ are the Lagrange multipliers of constraints (1) in the LP solution of Step 2.

Step 4. If $\mathrm{NPV}^L = \mathrm{NPV}^U$, stop. Otherwise set $R = R + 1$, and return to Step 2.

Although the above algorithm has the advantage of involving an integer programming problem with only one continuous variable μ in the master problem of Step 3, the disadvantage is that this problem is often too relaxed. As a result, the algorithm has the tendency to yield initially very high values for the upper bound NPV^U, and hence requires a large number of iterations.

In order to strengthen the bounds predicted by the master problem, one can redefine the partitioning as follows:

(a) complicating variables for the master problem: y_{it}, Q_{it}, QE_{it};

(b) remaining variables for the LP:

$$u = [S^l_{jt}, P^l_{jt}, W_{kt}].$$

In this way the basic steps in Algorithm B-II for this partitioning are similar to Algorithm B-I except for the following:

(a) in Step 2a, $y^R_{it}, Q^R_{it}, QE^R_{it}$ are fixed to solve the LP in which constraints (1) and (2) can be removed;

(b) in Step 3, the master problem corresponds to the following MILP problem:

$$\mathrm{NPV}^U = \max_{y_{it}, Q_{it}, QE_{it}, \mu} \mu, \tag{21}$$

st.

$$\mu \leqslant \mathrm{L}^r(y_{it}, Q_{it}, QE_{it}, u^r) \quad r = 1, R,$$

$$\left.\begin{array}{c} y_{it} QE^L_{it} \leqslant QE_{it} \leqslant QE^U_{it} y_{it} \\ Q_{it} = Q_{i,t-1} + QE_{it} \\ Q_{it}, QE_{it} \geqslant 0, y_{it} = 0, 1 \end{array}\right\} \quad i = 1, NP, \quad t = 1, NT,$$

$$\mu \in \mathcal{R}^1$$

where:

$$\mathrm{L}^r(y_{it}, Q_{it}, QE_{it}, u^r) = \mathrm{NPV}(y_{it}, Q_{it}, QE_{it}, u^r) + \sum_{i=1}^{NP} \sum_{t=1}^{NT} \rho^r_{it}(W_{mt} - Q_{it})$$

and $NPV(y_{it}, Q_{it}, QE_{it}, u^r)$ is the NPV function with the variables u^r fixed, and ρ^r_{it} are the Lagrange multipliers of constraint (4).

As will be shown later in the results, Algorithm B-II predicts stronger upper bounds and hence requires fewer iterations. In addition, the subproblems can be now solved as a sequence of independent problems (one for each time period).

HEURISTIC PROCEDURE WITH BOUNDS

The purpose of the procedures in the previous sections is to determine the exact solution of the multiperiod MILP model. It is useful, however, to also consider heuristic methods for which the quality of the solution can be established as shown in this section.

Due to the effect of the discount factors, many instances of the optimal solution of the multiperiod MILP problems involve only one expansion, especially if there are no limits on the capital investment. Such a solution corresponds often to the lower bound LB_2 described previously in the paper. Since this bound is easy to obtain, as is in fact the lower bound LB_1, the higher of these two can be used as a heuristic estimate of the optimal solution. The question that then arises, however, is how good these estimates are.

In order to answer the above question, a tight upper bound must be generated. An easy to compute upper bound is the solution of the relaxed LP, which will be denoted by UB_1. Since this bound might not be very strong, the following procedure can be used to generate a second bound, UB_2. Consider that only one expansion will be performed at period 1 but with the lowest coefficients of the investment cost $\alpha_{i\,min}, \beta_{i\,min}$ (usually the ones of the last time period). The multiperiod MILP can then be simplified as follows for this upper bound:

$$UB_2 = \max\left\{-\sum_{i=1}^{NP}(\alpha_{i\,min} QE_i + \beta_{i\,min} y_i) - \sum_{i=1}^{NP}\sum_{t=1}^{NT}\delta_{m_it} W_{m_it} + \sum_{l=1}^{NM}\sum_{j=1}^{NC}\sum_{t=1}^{NT}(\gamma^t_{jl} S^t_{jl} - \Gamma^t_{jl} P^t_{jl})\right\}, \quad (22)$$

st.

$$\left.\begin{aligned} Q_i &= Q_0 + QE_i \\ QE^L y_i &\leqslant QE_i \leqslant QE^U y_i \\ y_i &= 0, 1 \end{aligned}\right\} \quad i = 1, NP,$$

$$Q_i \geqslant W_{m_it} \quad i = 1, NP \quad t = 1, NT.$$

Constraints (3), (5), (6) and (7).

Note that the above MILP involves only NP 0–1 variables instead of $(NP)(NT)$ and it has $NP(NT-1)$ fewer constraints. Therefore, this MILP is easier to solve than the multiperiod MILP given by (1–8). In addition, since the solution to this problem is a feasible solution of the multiperiod MILP [at least when there are no constraints for investment limits (10)], it corresponds to a new lower bound LB_3 for which we only have to evaluate the objective function value.

Having determined UB_2 from (22), the heuristic solution can be set to:

$$NPV^H = \max\{LB_1, LB_2, LB_3\} \quad (23)$$

and the upper bound to

$$UB = \min\{UB_1, UB_2\} \quad (24)$$

Hence the maximum gap of the heuristic solution with respect to the optimal MILP solution will be given by:

$$\text{gap} = \frac{UB - NPV^H}{UB}. \quad (25)$$

This gap can be expected to be small in many instances.

MULPLAN

In order to automatically formulate and solve the multiperiod MILP model, the computer program MULPLAN (MULtiperiod PLANning) has been developed. Given data on the structure of the network, mass balance coefficients and other economic information and constraints, the program formulates the problem using the modelling system GAMS (Kendrick and Meeraus, 1985). In its simplest form, the multiperiod MILP problem is solved directly using the branch and bound method. However, provisions are available in MULPLAN to use as alternate solution strategies the methods described previously in this paper. Also, a special version of the program can interface through MPS files with any MILP solver (e.g. MPSX, LINDO, ZOOM, APEX).

EXAMPLES

In the following sections two examples will first be presented to illustrate the application of the multiperiod MILP model. A comparison of the performance of the computational strategies will then be given in a later section.

Example 1

In Example 1, the network indicating all the alternatives is shown in Fig. 1. Product 3 is to be produced by process 2 or 3. The feedstock to processes 2 and 3 is either bought or manufactured in process 1. Process 2 has an existing capacity of 50 kton yr^{-1}. This problem spans over three periods of 2, 3 and 5 yr. Limits on investment are specified at each time period.

Three scenarios of this example are considered that differ from each other in the following ways: scenario 2 differs from scenario 1 by 20% reduction in sales prices of product 3; and scenario 3 differs from scenario 2 by reducing the investment bound in period 2 to 0, increasing by 20% the cost of chemical 1, and reducing by 20% the cost of chemical 2.

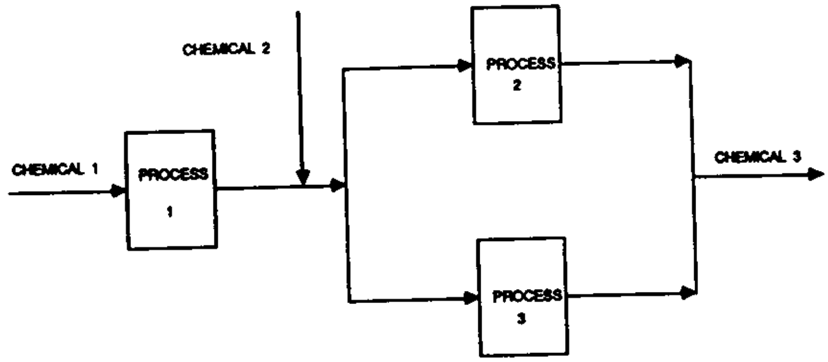

Fig. 1. Flow diagram for Example 1.

Table 1. Example 1, scenario 1. Selected processes and production profiles (kton yr^{-1})

Process		Period 1	2	3
1	Capacity	7.75	7.75	7.75
	Production	5.41	6.76	7.75
2	Capacity	50.0[a]	50.0[a]	50.0[a]
	Production	20.82	0.0	0.0
3	Capacity	0.0	35.95	35.95
	Production	0.0	30.72	35.95

[a]Existing capacity.

Table 3. Example 1, scenario 3. Selected processes and production profiles (kton yr^{-1})

Process		Period 1	2	3
1	Capacity	0.0	0.0	7.75
	Production	0.0	0.0	7.75
2	Capacity	50.0[a]	50.0[a]	50.0[a]
	Production	0.0	0.0	11.52
3	Capacity	51.14	51.14	51.14
	Production	38.10	45.57	51.14

[a]Existing capacity.

Scenario 3 also differs from 1 and 2 in that the upper bounds for the availability of chemical 2 were doubled. In both cases a maximum number of three expansions was considered with limits on investment cost at each time period. The economic data for all three scenarios and the constants for material balance equations and the demand for chemicals are given in Chathrathi (1986). The corresponding MILP problem involves nine binary variables, 42 continuous variables and 58 rows.

Some of the results of the three scenarios obtained with MULPLAN are presented in Tables 1–4. The analysis of these results indicates that the optimal solution of scenario 1 involves shutting down process 2 in periods 2 and 3 and installing process 3 in period 2 (see Fig. 2). Process 1 should be installed in period 1. As seen in Table 1, all processes operate below maximum capacity in periods 1 and 2. This illustrates the effect of economies of scale in the optimum solution: the cost of maintaining an idle (or partially used) process is outbalanced by the savings of a large installation (the more capacity that is purchased, the less the price *per unit* of capacity). The net present value for scenario 1 is $1697.61 $\times 10^5$. Though the results for scenario 2 are identical (see Fig. 3, Table 2), the net present value is reduced to $1063.01 $\times 10^5$, indicating the effect of the reduction in sales price. The optimal solution of scenario 3 involves installing process 1 in period 3, process 3 in period 1, and shutting down process 2 in periods 1 and 2 (see Fig. 4, Table 3). The net present value in this case is $2236.38 $\times 10^5$. This increase was mainly due to the larger availability of chemical 2, which allowed for larger production of chemical 3. Purchases and sales for the three scenarios are given in Table 4.

Table 2. Example 1, scenario 2. Selected processes and production profiles (kton yr^{-1})

Process		Period 1	2	3
1	Capacity	7.75	7.75	7.75
	Production	5.41	6.76	7.75
2	Capacity	50.0[a]	50.0[a]	50.0[a]
	Production	20.82	0.0	0.0
3	Capacity	0.0	35.95	35.95
	Production	0.0	30.72	35.95

[a]Existing capacity.

Example 2

Example 2 involves a larger chemical complex which is a network of 10 processes. None of these processes is assumed to have an existing capacity. The network showing all the alternatives for this complex is shown in Fig. 5. Product 6 is to be produced in four

Table 4. Example 1, purchases and sales (kton yr^{-1})

Chemical	Period 1	2	3
Scenario 1—purchases			
1	6.0	7.5	8.6
2	20.0	25.5	30.0
Sales			
3	20.82	30.72	35.95
Scenario 2—purchases			
1	6.0	7.5	8.6
2	20.0	25.5	30.0
Sales			
3	20.82	30.72	35.95
Scenario 3—purchases			
1	0.0	0.0	8.6
2	40.0	51.0	60.0
Sales			
3	38.1	48.54	62.66

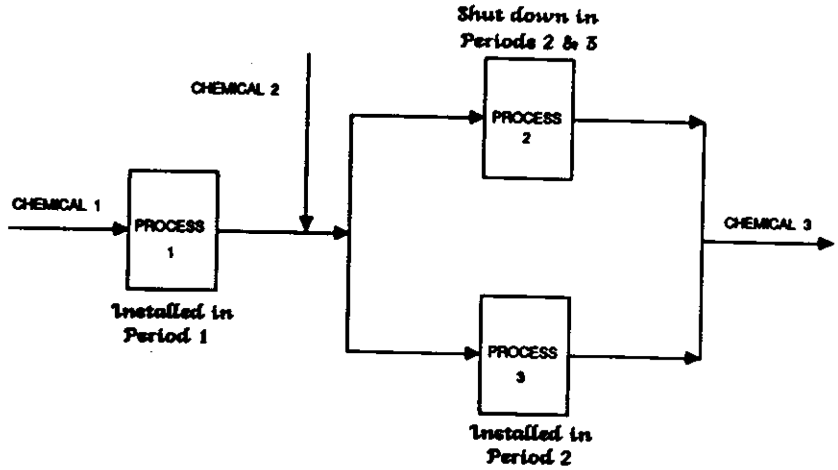

Fig. 2. Example 1: optimum for scenario 1. Net present value = $\$1697.6 \times 10^5$.

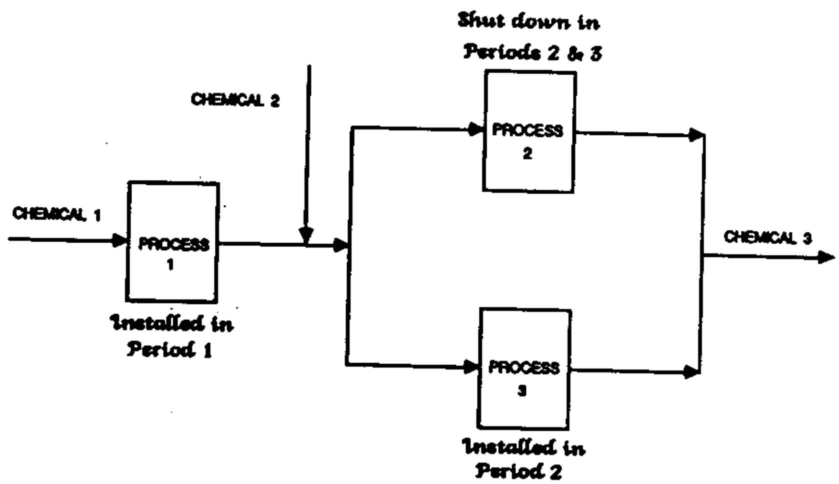

Fig. 3. Example 1: optimum for scenario 2. Net present value = $\$1063 \times 10^5$.

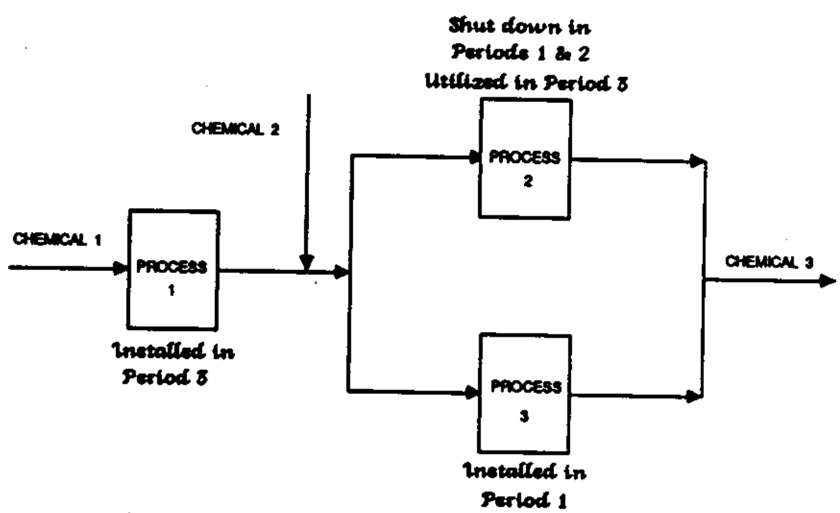

Fig. 4. Example 1: optimum for scenario 3. Net present value = $\$2236.4 \times 10^5$.

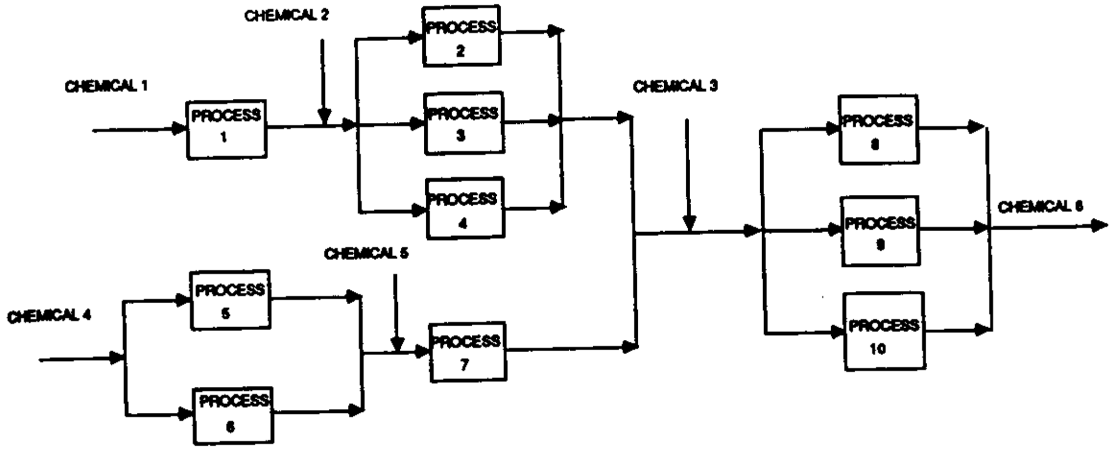

Fig. 5. Flow diagram for Example 2.

periods, each having a length of 2 yr and various constraints on the chemical demands and prices.

The alternatives presented in Fig. 5 are as follows: product 6 can be produced by processes 8, 9 and 10 which use chemical 3 as raw material. Chemical 3 can be purchased or produced by processes 2, 3 and 4 using chemical 2 as raw material, or by process 7 using chemical 5 as raw material. Chemicals 2 and 5 can be purchased or produced by process 1, and 5 or 6, respectively. Process 1 uses chemical 1 as raw material, and processes 5 and 6 use chemical 4 as raw material. Two scenarios are considered in this example; the first has no investment bounds, and the second scenario has investment bounds. Also, in both cases a maximum number of two expansions per process was considered. The economic data and chemical prices, the constants for the material balance equations, and the demand for chemicals are given in Chathrathi (1986). The corresponding MILP model involves 40 binary variables, 174 continuous variables and 198 rows.

Some of the results of the problem that were obtained with MULPLAN are presented in Tables 5–8 for both scenarios. These results indicate that the optimum net present value of $51,027.1 × 10^5$ can be obtained for scenario 1 by using the following configuration as seen in Table 5; the optimal configuration does not use processes 2, 3, 5 and 10; and the capacities of processes 7 and 8 are expanded in period 2. In this configuration, process 6 operates below maximum capacity in period 4; and process 9 would be shut down in periods 2 and 3, and reused in period 4. This optimal configuration is shown in Fig. 6, and the sales and purchases in Table 6.

The optimum NPV for the second scenario with the bounds on investment costs at each time period

Table 6. Example 2, scenario 1. Purchases and sales (kton yr^{-1})

Chemical	Period 1	2	3	4
Purchases				
1	45.0	75.0	99.0	110.0
2	35.67	0.0	0.0	0.0
3	0.0	0.0	0.0	0.0
4	45.0	75.0	75.0	27.92
5	45.0	59.64	64.73	110.0
Sales				
6	145.0	175.0	199.0	210.0

Table 5. Example 2, scenario 1. Selected processes and production profiles (kton yr^{-1})

Process		Period 1	2	3	4
1	Capacity	99.1	99.1	99.1	99.1
	Production	40.54	67.57	89.19	99.1
2	Capacity	0.0	0.0	0.0	0.0
	Production	0.0	0.0	0.0	0.0
3	Capacity	0.0	0.0	0.0	0.0
	Production	0.0	0.0	0.0	0.0
4	Capacity	94.38	94.38	94.38	94.38
	Production	74.48	64.35	84.94	94.38
5	Capacity	0.0	0.0	0.0	0.0
	Production	0.0	0.0	0.0	0.0
6	Capacity	67.57	67.57	67.57	67.57
	Production	40.54	67.57	67.57	25.16
7	Capacity	100.0	128.72	128.72	128.72
	Production	81.47	121.15	126.0	128.72
8	Capacity	100.0	200.0	200.0	200.0
	Production	81.47	175.0	199.0	200.0
9	Capacity	45.0	45.0	45.0	45.0
	Production	45.0	0.0	0.0	10.0
10	Capacity	0.0	0.0	0.0	0.0
	Production	0.0	0.0	0.0	0.0

Table 7. Example 2, scenario 2. Selected processes and production profiles (kton yr^{-1})

Process		Period 1	2	3	4
1	Capacity	0.0	67.57	99.1	99.1
	Production	0.0	67.57	89.19	99.1
2	Capacity	0.0	0.0	0.0	0.0
	Production	0.0	0.0	0.0	0.0
3	Capacity	0.0	53.2	53.2	53.2
	Production	0.0	53.2	42.08	51.52
4	Capacity	42.86	42.86	42.86	42.86
	Production	42.86	42.86	42.86	42.86
5	Capacity	0.0	0.0	0.0	0.0
	Production	0.0	0.0	0.0	0.0
6	Capacity	0.0	0.0	34.56	34.56
	Production	0.0	0.0	34.56	26.47
7	Capacity	54.63	54.63	129.97	129.97
	Production	42.86	54.63	127.2	129.97
8	Capacity	100.0	175.0	175.0	175.0
	Production	100.0	175.0	175.0	175.0
9	Capacity	0.0	0.0	35.0	35.0
	Production	0.0	0.0	24.0	35.0
10	Capacity	0.0	0.0	0.0	0.0
	Production	0.0	0.0	0.0	0.0

is $45,244.50 × 10^5. This configuration does not use processes 2, 5 and 10. The details of the capacity expansions and production profiles are shown in Tables 7 and 8 and Fig. 7. Note that due to the investment bounds, this second scenario features three processes with expansions vs the two for the first scenario.

Table 8. Example 2, scenario 2. Purchases and sales (kton yr^{-1})

Chemical	Period 1	2	3	4
Purchases				
1	0.0	75.0	99.0	110.0
2	45.0	33.29	0.0	0.0
3	20.29	34.82	0.0	0.0
4	0.0	0.0	38.36	29.38
5	45.0	57.36	99.0	110.0
Sales				
6	100.0	175.0	199.0	210.0

COMPUTATIONAL RESULTS

The three scenarios of Example 1 were solved with MULPLAN using the following techniques as seen in Table 9a: branch and bound, strong cutting planes followed by branch and bound, Benders decomposition (Algorithms B-I and B-II), strong cutting planes followed by Algorithm B-II of Benders decomposition. It can be seen that branch and bound required the smallest CPU times. The explanation of this is the fact that Example 1 is a relatively small multiperiod problem. However, the following general trends can be identified.

First, the strong cutting planes reduce the gap between the relaxed LP solution (Z_{LP}) and the optimal MILP solution (Z_{IP}) as seen in Table 10. Although in Example 1, the benefits of this reduction were rather marginal in terms of reduction at branches and pivot operations, scenario 2 of Example 2, which is a larger MILP model, exhibits a substantial reduction in both items. Also note from Table 9b that the CPU time with the use of cutting planes followed by branch and bound is more than 50% lower than that of direct branch and bound.

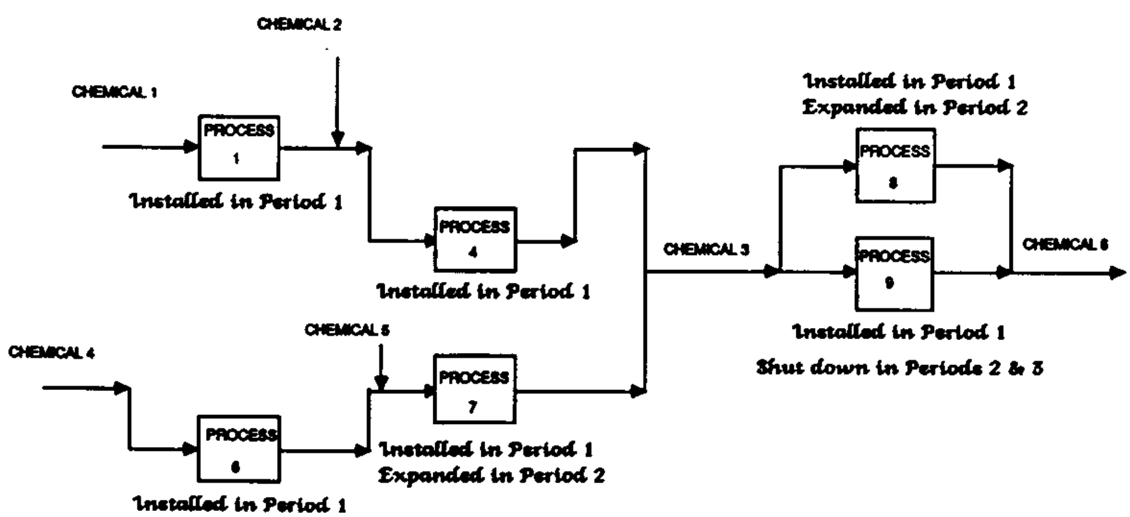

Fig. 6. Example 2: optimum for scenario 1. Net present value = $51,027.1 × 10^5.

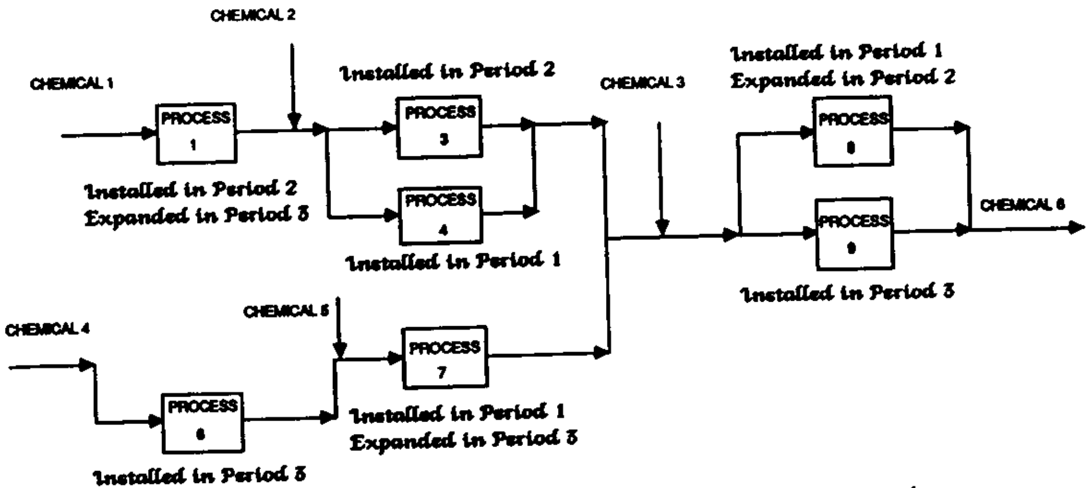

Fig. 7. Example 3: optimum for scenario 2. Net present value $45,244.5 × 10^5$.

As for Benders decomposition, even though all provisions were taken so as to restart the subproblems at each iteration from the previous solution, the performance is not very encouraging as seen in Tables 9a, 11 and 12. However, it is clear that the modified formulation of Algorithm B-II is much better than the one in Algorithm B-I as it requires almost 40% fewer iterations due to the modified master problem. Also, the reduction of time is roughly 35% as seen in Table 9. In this case the use of the strong cutting planes has a modest, but significant, effect in speeding up the solution of Algorithm B-II. It is also interesting to note that Algorithm B-I of Benders has the tendency of introducing far too many expansions in the initial iterations as seen in Table 12.

Although the above computational results are somewhat limited, they clearly indicate that the use of strong cutting planes followed by branch and bound

Table 9. CPU times[a] for Examples 1 and 2

(a) Example 1	Scenario 1	Scenario 2	Scenario 3
Branch and bound	2.62	3.0	2.55
Branch and bound/cuts	4.39	4.43	4.37
Benders decomposition I	68.2	76.79	49.81
Benders decomposition II	43.32	48.7	35.33
Benders decomposition II/cuts	39.15	43.81	31.82

(b) Example 2	Scenario 1	Scenario 2
Branch and bound	7.81	102.6
Branch and bound/cuts	NA[b]	47.4

[a]CPUs on IBM-3083. MILP and LP solver: MPSX.
[b]Cut generation technique not applicable to this example.

Table 10. Effect of addition of cuts on branch and bound[a]

		Branch and bound			Branch and bound/cuts		
	Z_{IP} (\$$10^5$)	Z_{LP} (\$$10^5$)	No. branches	No. pivots	Z_{LP} (\$$10^5$)	No. branches	No. pivots
Example 1							
Scenario 1	1697	1898	11	145	1874	11	160
Scenario 2	1063	1246	13	142	1223	12	159
Scenario 3	2236	2540	7	151	2472	6	96
Example 2							
Scenario 2	45,248	46,248	183	8580	46,236	140	5182

[a]LINDO computer code.

Table 11. Number of iterations of Benders decomposition for Example 1

	Benders I	Benders II	Benders II/cuts	Z_{LP}	Z_{IP}
Scenario 1	17	11	10	1898	1697
Scenario 2	19	12	10	1246	1063
Scenario 3	12	9	9	2540	2236

Table 12. Iterations for alternative Benders decomposition schemes in Example 1, scenario 2[a]

Iteration No.	Benders decomposition I Z_L	Z_U	Selected y's	Benders decomposition II Z_L	Z_U	Selected y's	Benders decomposition II/cuts Z_L	Z_U	Selected y's
0	$-\infty$	$+\infty$		$-\infty$	$+\infty$		$-\infty$	$+\infty$	
1	684.5	1246.5	y_{11}	684.5	1246.5	y_{13}	684.5	1223.2	y_{11}
2	899.7	1246.5	y_{32}	746.8	1246.5	y_{31}, y_{32}	892	1223.2	y_{11}, y_{32}
3	899.7	1246.5	y_{13}, y_{33}	746.8	1246.5	y_{11}, y_{33}	892	1223.2	y_{11}, y_{13}, y_{31}, [illegible]
4	899.7	1246.5	y_{12}, y_{32}	914.8	1246.5	y_{12}, y_{31}	892	1223.2	y_{11}, y_{32}
5	980	1246.5	y_{12}, y_{31}	1033.8	1163	y_{11}, y_{32}	1027	1184.3	y_{12}, y_{31}
6	1057	1246.5	y_{11}, y_{21}, y_{31}	1033.8	1075.5	y_{11}	1033	1071.4	y_{12}, y_{31}
7	1057	1246.5	y_{11}, y_{31}	1033.8	1069.5	y_{12}, y_{31}	1033	1067.2	y_{11}, y_{32}
8	1057	1246.5	y_{11}, y_{31}, y_{32}	1033.8	1067.5	y_{11}, y_{32}	1040.9	1065.5	y_{11}, y_{32}
9	1057	1246.5	y_{11}, y_{13}, y_{31}	1039.5	1065.5	y_{11}, y_{32}	1054.4	1063	y_{11}, y_{32}
10	1057	1246.5	$y_{11}, y_{13}, y_{31}, y_{32}$	1054.4	1063.8	y_{13}, y_{31}	1063		
11	1057	1246.5	y_{11}, y_{12}, y_{31}	1054.4	1063	y_{11}, y_{32}			
12	1057	1246.5	$y_{11}, y_{12}, y_{31}, y_{32}$	1063					
13	1057	1246.5	$y_{11}, y_{12}, y_{31}, y_{33}$						
14	1057	1246.5	$y_{11}, y_{12}, y_{13}, y_{32}, y_{33}$						
15	1057	1246.5	y_{11}, y_{32}						
16	1063	1105	y_{11}, y_{33}						
17	1063	1095.4	y_{13}, y_{32}						
18	1063	1091.7	y_{13}, y_{31}						
19	1063	1063							

[a]Optimum $Z^* = 1063$, $y_{11} = y_{32} = 1$.

is a more promising technique for solving larger multiperiod MILP problems than Benders decomposition. Also, for the second example, the use of strong cutting planes exhibited better performance than the direct use of branch and bound. This trend is maintained in a much larger example as will be shown in the next section where the use of heuristic techniques and other bounds is also illustrated.

Example 3. A petrochemical complex

The network of a proposed petrochemical complex is shown in Fig. 8. Four time periods of 2 yr each are considered. Processes 12, 13, 16 and 38 are assumed to exist with capacities 39.9, 25, 300 and 200 kton yr^{-1}, respectively. These processes are assumed to have possibilities of expansion starting in period 2, while all the other nonexisting processes could be installed starting in period 1. There are a total of 38 processes and 25 chemicals. The economic data and the constants for the material balance equations are given in Fornari and Grossmann (1986). We consider two different scenarios. Limits on the number of expansions and bounds for the investment cost are specified in scenario 2 but they are not present in scenario 1.

First we consider scenario 1, in which case the problem has 148 integer variables, 961 continuous variables and 785 constraints. Due to the large size of this MILP, the heuristic procedure with bounds was first applied. From the analysis of the solution of the relaxed problem, lower bounds were obtained for the objective function. These lower bounds are $LB_1 = \$420.1 \times 10^6$ (obtained by solving the relaxed problem and setting all the nonzero binary variables to 1) and $LB_2 = \$488.2 \times 10^6$ by installing all the processes selected in the relaxed problem, but by making only one expansion for each of them. Clearly, the latter yields a better lower bound.

The relaxed LP problem solution yields a valid upper bound for the optimum solution: $UB_1 = \$648.6 \times 10^6$; hence the gap with respect to the lower bound of $\$488.2 \times 10^6$ is 24.7%. This gap can be reduced by obtaining a tighter upper bound from problem MILP (22) assuming only initial expansions and with lowest investment cost coefficients. This problem yields a lower upper bound $UB_2 = \$569.8 \times 10^6$ and the corresponding feasible solution a lower bound $LB_3 = 512.9 \times 10^6$. Now the gap is reduced to 10%. The solution corresponding to the lower bound $LB_3 = \$512.9 \times 10^6$ is as follows. The selected processes are: 4, 5, 6, 8, 14, 17, 26, 28, 32, 34, 35 and 36. All these processes are installed in period 1 with an initial capacity that remains constant throughout the four periods.

The problem was also solved to optimality with the MPSX code on the IBM-3090 supercomputer at the Cornell Theory Center. The optimum solution requires that processes 8, 14, 28 and 32 are selected during the first period. The optimum NPV is 529.8×10^6, differing by only 3.2% from the heuristic solution (LB_3). This clearly illustrates the usefulness of the heuristic procedure.

The computational requirements to solve the problem to optimality are shown in Table 13. Using straightforward branch and bound, it was not possible to verify the global optimum for scenario 1 (no limits on capital investment) after 92 min of CPU time. The procedure crashed due to the extremely large size of the search tree. It is here where the importance of the integer cuts [constraints (9) and (11)] becomes evident. Results from the MILP problem (12) showed that the maximum number of expansions for all processes is one, except for processes 2 and 10, for which two is the maximum number of expansions. After adding constraints (9) and (11), it was possible to find *and* verify the global optimum for this scenario in 35 min of CPU time.

It was also found that the branch and bound

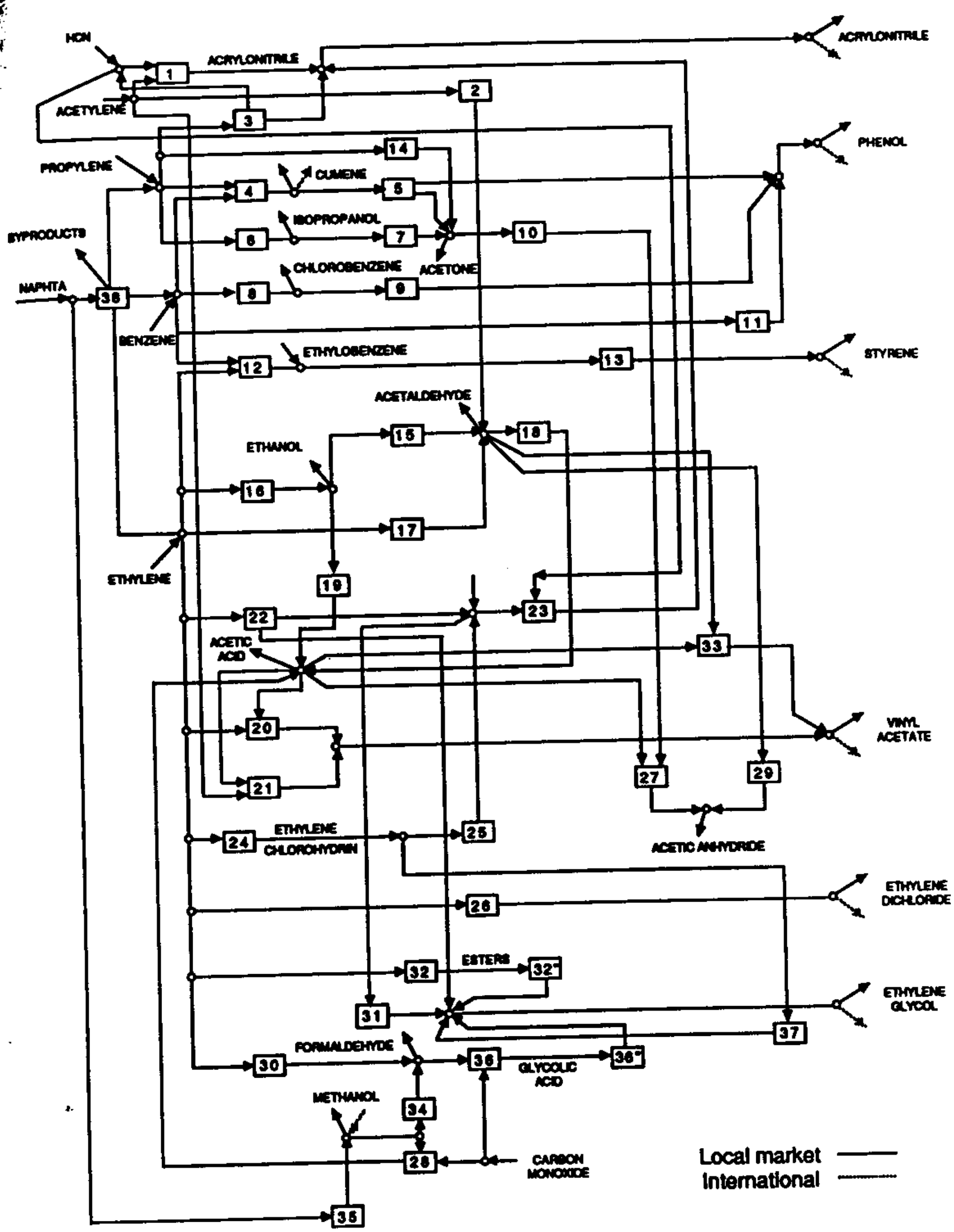

Fig. 8. Petrochemical complex.

requirements were 9.5 min after addition of constraints (10) for limits of investment cost (scenario 2), although the optimum solution did not change. For this scenario, the application of the strong cutting plane algorithm followed by the branch and bound reduced the computing time to 8 min. These results are also summarized in Table 13.

The computational experience with this example shows that for large multiperiod MILP models it is important to include the suggested integer constraints and bounds, and that the use of strong cutting planes followed by branch and bound is a promising technique.

CONCLUSIONS

This paper has presented a multiperiod MILP model for long-range planning of capacity expansions

Table 13. Effect of integer cuts and strong cutting planes on the solution[a] of a large scale problem (148 binaries, 961 continuous variables, 785 constraints)

	Z_{LP}	No. branches	No. pivots	Minutes
Scenario 1				
Branch and bound (BB)	648.6	NA[b]	>356,609[b]	>92[b]
BB/integer cuts (BBI)	648.6	28,897	134,440	35
Scenario 2				
Branch and bound (BB)	631	4530	32,713	9.5
BB/strong cutting planes	629	4618	29,683	8

[a]Integer optimum solution: $Z_{IP} = 529.8$, MPSX/MIP-370 computer code, IBM-3090.
[b]Procedure terminated with a lower bound of 529.8 and an upper bound of 561.

and process selection. The incorporation of this model in the computer program MULPLAN makes this model especially useful for the study of different scenarios as was illustrated in the example problems.

A number of solution strategies have been presented to reduce the computational burden of solving the corresponding MILP problems. Based on the results obtained in this paper, it would seem that for large-scale problems a combination of integer cuts, strong cutting plane generation and branch and bound is the most promising strategy for solving these problems to optimality. However, the strong cutting planes used here can only be generated based on constraints that limit the capital investment, which are not always present in the MILP formulation of the planning problem. Nevertheless, when their generation is possible, it is also computationally cheap and reduces the branch and bound requirements. Benders decomposition in its various forms would seem to have little promise. The master problem is unable to predict tight bounds, and the procedure requires the solution of many subproblems. Finally, the last example illustrates the usefulness of the heuristic procedure for which the quality of the solution can be predicted.

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REFERENCES

Beale E. M. L., Branch and bound methods for mathematical programming systems. *Ann. Discrete Math.* **5**, 201–210 (1979).

Benders J. F., Partitioning procedures for solving mixed-variables programming problems. *Numer. Math.* **4**, 238–252 (1962).

Chathrathi M., Computer system for long range planning in the chemical industry. M.S. Thesis, Carnegie Mellon University (1986).

Crowder H., E. L. Johnson and M. Padberg, Solving large-scale zero–one linear programming problems. *Opers Res.* **31**, 803 (1983).

Fornari R. E. and I. E. Grossmann, Long range planning models for process selection and capacity expansion in the chemical industry. Progress Report, Carnegie Mellon University (1986).

Garfinkel R. S. and G. L. Nemhauser, *Integer Programming*. Wiley, New York (1972).

Geoffrion A. M., Generalized Benders decomposition. *JOTA* **10**, 4 (1972).

Geoffrion A. M. and G. W. Graves, Multicommodity distribution system design by Benders decomposition. *Mgmt Sci.* **20**, 822–844 (1974).

Gondran M. and M. Minoux, *Graphs and Algorithms*. Wiley, New York (1986).

Grossmann I. E. and J. Santibanez, Application of mixed-integer linear programming in process synthesis. *Comput. chem. Engng* **4**, 205 (1980).

Himmelblau D. M. and T. C. Bickel, Optimal expansion of a hydrodesulfurization process. *Comput. chem. Engng* **4**, 101 (1980).

Hirshfeld D. S., Mathematical programming and the planning, scheduling and control of process operations. Paper presented at the *FOCAPO Conf.*, Park City (1987).

Jimenez A. G. and D. F. Rudd, Use of a recursive mixed-integer programming model to detect an optimal integration sequence for the Mexican petrochemical industry. *Comput. chem. Engng* **3**, 291 (1987).

Kendrick D. and A. Meeraus, GAMS–an introduction. *User's Manual for GAMS*. Development and Research Dept of the World Bank (1985).

Little J. D. C., K. G. Murty, D. W. Sweeney and C. Karel, An algorithm for the traveling salesman problem. *Opers Res.* **11**, 979–989 (1963).

Luss H., Operations research and capacity expansion problems: a survey. *Opers Res.* **30**, 907 (1982).

Nemhauser G. L. and L. A. Wolsey, *Integer and Combinatorial Optimization*. Wiley, New York (1988).

Padberg M. W., T. J. Van Roy and L. A. Wolsey, Valid linear inequalities for fixed charge problems. *Opers Res.* **33**, 842 (1985).

Roberts S. M., *Dynamic Programming in Chemical Engineering and Process Control*. Academic Press, New York (1964).

Schrijver A., *Theory of Linear and Integer Programming*. Wiley, New York (1986).

Shimizu Y. and T. Takamatsu, Applications of mixed-integer linear programming in multiterm expansion planning under multiobjectives. *Comput. chem. Engng* **9**, 367 (1985).

Van Roy T. J. and L. A. Wolsey, Valid inequalities for mixed 0–1 programs. *Discrete Appl. Math.* **14**, 199–213 (1986).

Van Roy T. J. and L. A. Wolsey, Solving mixed integer programs by automatic reformulation. *Opers Res.* **35**, 45–57 (1987).

APPENDIX A

Modelling Shut-Downs

It is sometimes desirable to account for a penalty (or profit) when a process is shut down or when an installed process is not operated for a period of time. In other cases it is desirable to operate an installed process at a minimum level of operation. In order to account for these considerations, let ϵ_{it} be a binary variable that will take the value 1 if process i is decided to be excluded from any further consideration (installation, expansion or operation) starting at the beginning of time period t. Also, let CP_{it} be equal to the available plant capacity at the time of shut-down (i.e. when $\epsilon_{it} = 1$).

The constraints that apply for ϵ_{it} and CP_{it} are:

$$CP_{it} \leq Q_{i,t-1} \quad i = 1, NP, \quad t = 1, NT+1, \tag{A1}$$

$$CP_{it} \leq U_{it}\epsilon_{it} \quad i = 1, NP, \quad t = 1, NT+1, \tag{A2}$$

$$Q_{it-1} \leq CP_{it} + U_{i,t-1}(1 - \epsilon_{it}) \quad i = 1, NP, \quad t = 1, NT+1, \tag{A3}$$

where $U_{it} = \Sigma_{T=1}^{t-1} QE_{iT}^{U}$. Equation (A2) will force CP_{it} to zero for as long as $\epsilon_{it} = 0$. When $\epsilon_{it} = 1$, equations (A1) and (A3) enforce $CP_{it} = Q_{it-1}$. Note that when a process is selected and not shut down at any time $\epsilon_{i,NT+1} = 1$, while for a process that is never selected $\epsilon_{i,1} = 1$. In addition, one has to include the following constraints that relate the variables ϵ_{it} to the rest of the model:

$$y_{iT} \leq 1 - \epsilon_{it} \quad i = 1, NP, \quad t = 1, NT+1, \quad T \geq t, \tag{A4}$$

$$W_{mit} \leq (U_{iT} + QE_{iT}^{U})(1 - \epsilon_{it}) \quad i = 1, NP, \quad t = 1, \quad NT+1, \; T \geq t. \tag{A5}$$

According to (A4), no expansion is allowed, and according to (A5) no operation is allowed once process i is decided not to be considered after time t.

In order to enforce operation of a process at a prespecified percentage of the installed capacity, the following simple constraint is sufficient:

$$W_{mit} \geq x_{it} Q_{it} \quad i = 1, NP, \quad t = 1, NT+1, \tag{A6}$$

where x_{it} is the prespecified percentage.

If it is desirable to operate an installed process i during time period t in such a way so as to process at least an amount of A_{it} units of the main product:

$$W_{mit} \geq A_{it}\left(1 - \sum_{T=1}^{t} \epsilon_{iT}\right) \quad i = 1, NP, \quad t = 1, NT, \quad \text{for } Q_{i0} > 0, \tag{A7}$$

$$W_{mit} \geq A_{it}\left(y_{iT} - \sum_{t_1=1}^{t} \epsilon_{it_1}\right) \quad i = 1, NP, \quad t = 1, NT, \quad T \leq t, \quad \text{for } Q_{i0} = 0. \tag{A8}$$

A penalty (or profit, e.g. when scrapping the process) term can be included in the objective as a function of the installed capacity at the time of shut-down:

$$\sum_{i=1}^{NP} \sum_{t=1}^{NT+1} (\alpha'_{it} CP_{it} + \beta'_{it}\epsilon_{it}),$$

where α'_{it} and β'_{it} are discounted cost coefficients. In the case of profit then $\alpha'_{it} \geq 0$ and $\beta'_{it} \geq 0$ and constraint (A3) is redundant for the maximization problem.

In the case where an installed process is not operated for a period of time, a penalty term can be included in the objective to account for the expenses of maintaining the idle plant:

$$\sum_{i=1}^{NP} \sum_{t=1}^{NT} \text{pen}_{it} QP_{it},$$

along with the following constraint:

$$QP_{it} \geq -U_{it} W_{mit} + Q_{it} - \sum_{T=1}^{t} CP_{iT} \quad i = 1, NP, \quad t = 1, NT, \tag{A9}$$

that will force QP_{it} to be equal to the installed capacity of the process. Here pen_{it} are again discounted (penalty) coefficients.

Finally, the decision to shut down a process is applied exactly once for each process, and therefore:

$$\sum_{t=1}^{NT+1} \epsilon_{it} = 1 \quad i = 1, NP, \tag{A10}$$

which gives rise to special ordered sets of type 1 (see Beale, 1979). Therefore, the additional computational requirements of the modelling presented in this appendix should not be excessive.

APPENDIX B

Solution to the Separation Problem

The separation problem has been shown to be the following Knapsack problem:

$$\max \zeta_i = \sum_{i=1}^{NP} \{-(1 - y_{it}^{*})z_i\}, \tag{B1a}$$

$$\text{st.} \sum_{i=1}^{NP} u_{it} z_i > CI(i), \tag{B1b}$$

$$z_i \in \{0, 1\} \quad i = 1, NP,$$

where $z_i = 1$ if $i \in C_i$, $z_i = 0$ otherwise. Here y_{it}^{*} corresponds to the solution from the relaxed LP and the u_{it} are given by (14).

The heuristic developed for the solution of this problem is a variation of the Greedy heuristic (see for example Gondran and Minoux, 1987) and it takes advantage of the fact that we are interested only in solutions for which $\zeta_i > -1$ (because only in this case a violated inequality is derived).

The algorithm is as follows:

Step 1. Set $z_i = 1$ for i such that $y_{it}^{*} = 1$. Set $z_i = 0$ for i such that $y_{it}^{*} = 0$. If constraint (B1b) is satisfied or all z_i are fixed, exit.

Step 2. Examine if by setting to 1 only one of the remaining z_i's, constraint (B1b) is satisfied. If so, set this to 1 and exit. Ties are broken by choosing the i for which $-(1 - y_{it}^{*})$ is the maximum coefficient in the objective (B1a).

Step 3. Apply the greedy heuristic in the following manner:
- (i) sort the remaining i's in order of decreasing $(1 - y_{it}^{*})/u_{it}$;
- (ii) select $z_i = 1$ one at a time in the order found in (i) until (B1b) is satisfied or all z_i are fixed.

In Step 1, the variables z_i are set to zero in order to avoid -1 terms in the objective (or else $\zeta_i < -1$ and no violated inequality will be derived). Step 2 has been included, because in most examples solved, the optimum solution had only one nonzero z_i. It was found that the algorithm gave the optimum in all cases in the examples solved.