

1988

Optimization model for long range planning in the chemical industry

Ignacio E. Grossmann
Carnegie Mellon University

Carnegie Mellon University. Engineering Design Research Center.

Follow this and additional works at: <http://repository.cmu.edu/cheme>

Published In

.

This Technical Report is brought to you for free and open access by the Carnegie Institute of Technology at Research Showcase @ CMU. It has been accepted for inclusion in Department of Chemical Engineering by an authorized administrator of Research Showcase @ CMU. For more information, please contact research-showcase@andrew.cmu.edu.

NOTICE WARNING CONCERNING COPYRIGHT RESTRICTIONS:

The copyright law of the United States (title 17, U.S. Code) governs the making of photocopies or other reproductions of copyrighted material. Any copying of this document without permission of its author may be prohibited by law.

**Optimization Model for Long Range Planning In
The Chemical Industry**

by

I.E.Grossmann, N.V.Sahinidis, R.E.Fomari and M.Chathrathi

EDRC-06-41-88

UNIVERSITY OF PITTSBURGH
CARNEGIE-ROBERTS LIBRARY
PITTSBURGH, PENNSYLVANIA 15261

OPTIMIZATION MODEL FOR LONG RANGE PLANNING IN THE CHEMICAL INDUSTRY

I.E. Grossmann,* N.V. Sahinidis, R.E. Fornari, and M. Chathrathi

*Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213*

March 1988

*Author to whom correspondence should be addressed.

Abstract

This paper presents a multiperiod MILP model for the optimal selection and expansion of processes given time varying forecasts for the demands and prices of chemicals. To reduce the computational expense of solving these long range planning problems, several strategies are investigated which include 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.

Chemical companies are increasingly concerned with acquiring and managing more efficiently the resources that they will need to survive and prosper in a very competitive environment. Therefore, they must evaluate their options from two perspectives. First, they must assess the potential benefits of new resources when these are used in conjunction with existing processes, but accounting for their effect over the long term. Second, companies must identify and assess the potential impact on their business of important uncertainties in the external environment. Included are uncertainties regarding demand, prices, technology, capital, markets, and competition. In selecting new resources, companies should seek to develop long term strategies for hedging against these uncertainties, and to provide contingency plans to be put into effect as the uncertainties are revealed. Therefore, due to increasing competition, changing economic environment and fluctuating 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 (see Hirshfeld, 1987).

Uncertainties in planning models are, however, difficult to handle. Random coefficients are often replaced by their expected values in the planning models which might lead to misleading solutions (Kallberg *et al* 1982). Using a single deterministic value other than the mean can also lead to large inaccuracies (Birge, 1982). In these cases, a stochastic optimization model for random coefficients should be ideally used for the planning model.

However, since stochastic programs are in general very difficult and expensive to solve, an alternative approach is to use a deterministic multiperiod optimization model. This model can be used to account for predicted changes over a given time horizon and also to account for a finite number of different scenarios which can be associated with discrete probabilities.

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 has been applied to chemical plant expansions (Roberts, 1964), 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 Jiménez and Rudd (1987). However, these approaches are often limited to 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 that can be used either in a strictly deterministic fashion or as an approximation to the stochastic optimization problem. Several solution strategies which include the use of integer cuts, strong cutting planes and Benders decomposition, are presented 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.

Problem Statement

The specific problem that is addressed in this paper assumes that a given network of processes and chemicals is given. This network includes an existing system as well as potential new processes and chemicals. Given are also 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 expansion capacity 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. As will be shown in the next section, 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 the other 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, as well as the purchases and sales from different markets.

Also, a finite number of NT time periods is considered where prices and demands of chemicals vary, as well as the investment and operating costs of the processes. 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 for the modelling that the material balances in each process can be expressed linearly in terms of the production rate of the 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 a process at time $t=0$. QE_{it} represents the capacity expansion of the plant of process i which is installed for starting its operation in period t . If y_{it} are the 0-1 binary variables which indicate the occurrence of the expansions at each time period and for each process, the constraints that apply are

$$\left. \begin{array}{l} y_{it}QE_{it}^L \leq QE_{it} \leq Q^U y_{it} \\ y_{it} = 0,1 \end{array} \right\} \quad i=1, NP, \quad t=1, NT \quad (1)$$

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

In equation (1), QE_{it}^L and QE_{it}^U are lower and upper bounds for the capacity expansions. It must be noted that a zero-value in 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 .

It should be noted that the above representation for expansions requires fewer continuous variables and constraints than the one presented by Grossmann and Santibanez (1980). Since these authors did not define the total capacity variables, production amounts and capacities had to be defined for each potential expansion. This problem can be avoided easily as shown below.

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

$$W_{frZO} \quad keL_i \quad i=1, \dots, P \quad t=1, \dots, NT \quad (3)$$

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

$$Q_u * W_{mf} \quad i=1, \dots, P \quad t=1, \dots, NT \quad (4)$$

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

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

$$W_{kt} = \sum_{i \in I} \alpha_{ik} W_{mf} \quad i=1, \dots, P \quad t=1, \dots, NT \quad (5)$$

where α_{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 in one of several markets, $l = 1, \dots, NM$. If the corresponding variables are represented, respectively, in each period by the variables $P_{jl}^t, S_{jl}^t, j=1, \dots, NC$, they must satisfy the inequalities

$$\left. \begin{aligned} d_{jl}^{L,t} \leq P_{jl}^t \leq d_{jl}^{U,t} \\ d_{jl}^{L,t} \leq S_{jl}^t \leq d_{jl}^{U,t} \end{aligned} \right\} \quad j=1, \dots, NC, \quad t=1, \dots, NT, \quad l=1, \dots, NM \quad (6)$$

where $d_{jl}^{L,t}, d_{jl}^{U,t}$ are the lower and upper bounds on the availabilities, and $d_{jl}^{L,t}, d_{jl}^{U,t}$ are lower and upper bounds on the demands.

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

$$\sum_{l=1}^{NM} P_{jl}^t + \sum_{k \in I(j)} W_{kt} = \sum_{l=1}^{NM} S_{jl}^t + \sum_{k \in O(j)} W_{kt} \quad j=1, \dots, NC \quad t=1, \dots, NT \quad (7)$$

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

$$\begin{aligned} & \sum_{i=1}^{NP} \sum_{t=1}^{NT} (\alpha_{it} QE_{it} + \beta_{it} y_{it}) - \sum_{m=1}^{NP} \sum_{t=1}^{NT} \delta_{m,t} W_{m,t} \\ & + \sum_{j=1}^{NM} \sum_{l=1}^{NC} \sum_{t=1}^{NT} (\gamma_{jt}^l S_{jt}^l - \lambda_{jt}^l P_{jt}^l) \end{aligned} \quad (8)$$

where the parameters α_{it} , β_{it} represent respectively the variable and fixed terms for the investment cost, $\delta_{m,t}$ is the unit operating cost, and γ_{jt}^l , λ_{jt}^l are the unit costs of sales and purchases of the chemical j in market l at $t = 1, \dots, NM$. 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 in 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 expansion

$$\sum_{i=1}^{NP} y_{it} \leq NEXP(i) \quad i=1, \dots, NP \quad (9)$$

- b) Limit on the capital available for investment at each time period

$$\sum_{i=1}^{NP} (\bar{\alpha}_{it} QE_{it} + \bar{\beta}_{it} y_{it}) \leq CI(t) \quad t=1, \dots, NT \quad (10)$$

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

Finally, for the case when shut-downs 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 (Garfinkel and Nemhauser, 1972) 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, 2 markets and 5 time periods would involve 200 0-1 variables, and approximately 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 at a greater variety of scenarios in 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 in 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:

- LB₁ - relaxed LP solution with non-zero binaries set to one
- LB₂ - relaxed LP solution with non-zero binaries of first active period set to one, and with maximum required capacity at that time period.

In other words LB₁ corresponds to a feasible solution where expansions are performed as determined by the relaxed LP solution. LB₂ 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

$$NVP \geq \max\{LB_1, LB_2\} \quad (11)$$

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 or equal to the maximum cost of any given expansion. This then leads to the following MILP problem for each process i:

$$\begin{aligned}
NEXP(i) &= \max_{t=1}^{NT} y_{it} \\
s.t. \quad & \sum_{t=1}^{NT} (O_{it} Q_{E_{it}} + \alpha_i) \leq a_{i \max} Q_{i \max} + \beta_{i \max} \\
& \sum_{t=1}^{NT} Q_{E_{it}} = Q_{i \max} \\
& Q_{E_{it}}^L y_{it} \leq Q_{E_{it}} \leq Q_{E_{it}}^U y_{it} \quad t=1, \dots, NT \\
& y_{it} = 0, 1, \quad Q_{E_{it}} \geq 0, \quad t=1, \dots, NT
\end{aligned} \tag{12}$$

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 can be determined from the upper bounds on capacity expansion, or else through an LP by maximizing Q_{it} in the network at the corresponding time period and by removing the 0-1 constraints in (1).

From the solution of the above small-scale MILP's 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, 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 lower bound of the relaxed LP problem when the investment constraints in (10) are present.

Strong Cutting Planes

Recently, a new approach to the solution of large scale ILP and MILP problems has started to emerge (Crowder *et al* 1983; Van Roy and Wolsey, 1984). The idea in 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 more economical.

At each iteration the procedure starts by finding (x^*, y^*) , the optimum 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 (typically 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 (1984), 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 $t, t=1, NT$:

$$S_t = \{ (x, y) : \sum_{i=1}^{NP} (\bar{\alpha}_i QE_{it} + \bar{\beta}_i y_{it}) \leq CI(t), \quad (13)$$

$$y_{it} QE_{it} \leq QE_{it} \leq y_{it} \quad y_{it} \in \{0,1\} \quad i=1, NP \}$$

To see the network structure we substitute

$$\left. \begin{aligned} x_{it} &= \bar{\alpha}_i QE_{it} + \bar{\beta}_i y_{it} \\ t_{it} &= \bar{\alpha}_i QE_{it} + \bar{\beta}_i y_{it} \\ u_{it} &= \bar{\alpha}_i QE_{it} + \bar{\beta}_i y_{it} \end{aligned} \right\} i=1, NP \quad (14)$$

and obtain

$$S_t = \{ (x, y) : \sum_{i=1}^{HP} x_{it} \leq CI(t), \quad (15)$$

$$t_{it} y_{it} \leq x_{it} \leq u_{it} \quad y_{it} \in \{0,1\} \quad \text{M.O.T.} \}$$

For this structure two families of valid inequalities have been derived (Van Roy and

Wolsey, 1983)). The Simple Generalized Flow Cover inequality

$$J [x_{it} + (u_{it} - X)^+ (1 - y_{it})] \leq CI(t) \quad (16)$$

and the Extended Generalized Flow Cover inequality:

$$\begin{aligned} \sum_{i \in C_t} [x_{it} + (u_{it} - \lambda_t)^+ (1 - y_{it})] \\ + \sum_{i \in L_t} [x_{it} - (\bar{u}_{it} - \lambda_t)^+ y_{it}] \leq CI(t) \end{aligned} \quad (17)$$

where $(C_t \subseteq \{1, 2, \dots, NP\})$ is a generalized cover, i.e.,

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

$$\text{and } L_t \subseteq \{X \gg NP\} \mid \bar{u}_{it} = \max_{i \in C_t} u_{it}$$

$$\bar{u}_{it} = \max(j_u, U_{it}) \quad ty^* = \max(0, X_t - \bar{u}_{it}) \quad \text{and } u_{it} > X_t > 0.$$

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 $\lambda, 1^\wedge$, (\wedge that maximize the violation of the relaxed binary solutions y_{it}^*). This can lead to the following Knapsack problem for each time period t :

$$\begin{aligned} \max J_t &= \sum_{i=1}^{NP} \{ -(1 - y_{it}^*) z_i \} \\ \text{s.t. } \sum_{i=1}^{NP} u_{it} z_i &> CI(0) \\ z_i &\in \{0, 1\} \quad i=1, NP \end{aligned} \quad (18)$$

where $z_i = 1$ if $i \in C_t$; $z_i = 0$ otherwise. The violated inequalities (16) and (17) are derived whenever $J_t > -1$. The indices i that are included in the set 1^\wedge for the inequality in (17) must satisfy the condition, $x_{it}^* - (1 - y_{it}^*) \leq 0$.

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 $NPV' - NPV > \text{tolerance}$, 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. Firstly, 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)]. 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 are 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:

$$u = [Q_{it}, QE_{it}, S_{jt}^s, P_{jt}^s, W_{kt}]$$

The basic steps in Benders decomposition method are then the following:

Algorithm I

- Step 1. Select y_{it} ; set $NPV^U = \infty$, $NPV^L = -\infty$, $K = 1$.
- Step 2. a) By fixing the variables y_{it} , solve the multiperiod MILP problem as an LP to determine NPV^K and u^K .
- b) Update the lower bound by setting $NPV^L = \max \{NPV^L, NPV^K\}$
- Step 3. To determine new values y_{it}^{k+1} for the 0-1 variables and an upper bound to NPV solve the pseudo-integer master problem

$$\begin{aligned}
 NPV^U = & \max_{y_{it}^k} \\
 \text{s.t.} & \quad L^k(y_{it}) \quad k=1, K \\
 & \quad \mathbf{HeR}^1, y_{it}=0,1
 \end{aligned} \tag{19}$$

where the lagrangian $L^k(y_{it}) = NPV(y_{it}, u^k) +$

$$\sum_{i=1}^{NPNT} \sum_{t=1}^{NT} [\lambda_{it}^k (QE_{it} - A_{it}) + W_{kt} (QE_{it} - QE_{it})] \tag{20}$$

and $NPV(y_{it}, u^k)$ is the NPV function with all continuous variables u^k fixed except the y_{it} and λ_{it}^k, W_{kt} are the Lagrange multipliers of constraint (1) in the LP solution of Step 2.

- Step 4. If $NPV^L = NPV^U$ stop. Otherwise set $K = K + 1$, and return to Step 2.

Although the above algorithm has the advantage of involving an integer programming problem with only one continuous variable $|i|$ in the master problem of Step 3, the disadvantage is that this problem is often too relaxed. This will then have the tendency of yielding initially very high values for the upper bound NPV^U , and hence require 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:

$$u = [S_{jr}^t, P_{jr}^t, W_{kt}]$$

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

- a) In Step 2.a y_j, Q_j, QE_j are fixed for solving the LP in which constraints (1) and (2) can be removed.
- b) In Step 3, the master problem corresponds to the following MILP problem

$$\begin{aligned}
 M^{\geq} V^t = & \max_i \\
 & y_{ib} Q_{it} QE_{it} \quad i \\
 \text{s.t. } & |i \in L^k(y_u, Q_u, QE_u, ifi) \quad k=1, K \\
 & \left. \begin{aligned}
 QE_{it}^L y_{it} \leq QE_{it} \leq QE_{it}^U y_{it} \\
 Q_{it} = Q_{i,t-1} + QE_{it}
 \end{aligned} \right\} \begin{aligned}
 & i=1, NP \\
 & t=1, NT
 \end{aligned} \\
 & Q_{it}, QE_{it} \in 0, \mu \in \mathbb{R}^1, y_{it} = 0, 1
 \end{aligned} \tag{21}$$

- c) where $L^k(y_{ib}, Q_{it}, QE_{it} \wedge \wedge NPV(y_u > Q_{it}, QE_{it} \wedge h + \% \% P_{it} (W_{m_{it}} - Qu) >$ and $NPV(y_{it}, Q_{it}, QE_{it}, u^K)$ is the NPV function with the variables u^K fixed, and p_{it} are the Lagrange multipliers of constraint (4).

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

Heuristic Procedure with Bounds

The procedures in the previous sections are aimed towards 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 asserted 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 in 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 will then simplify as follows for this upper bound:

$$\begin{aligned}
 UB_2 = \max & - \sum_{i=1}^{NP} (\alpha_{i \min} QE_i + \beta_{i \min} y_i) \\
 & - \sum_{i=1}^{NP} \sum_{t=1}^{NT} \delta_{m_{it}} W_{m_{it}} + \sum_{i=1}^{NM} \sum_{j=1}^{NC} \sum_{t=1}^{NT} (\gamma_{jt}^i S_{jt}^i - \lambda_{jt}^i P_{jt}^i) \\
 \text{s.t. } & Q_i = Q_o + QE_i \quad (22) \\
 & QE^L y_i \leq QE_i \leq QE^U y_i \quad i=1, NP \\
 & y_i = 0, 1 \\
 & Q_i \geq W_{m_{it}} \quad i=1, NP \quad t=1, NT
 \end{aligned}$$

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

Note that the above MILP only involves 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).

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

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

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

$$8 < 2P \frac{UB-NPV''}{UB} \quad (25)$$

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 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 with the branch and bound method. However, provisions are available in this program to use as alternate solution strategies the methods described previously in this paper. Also, a special version is available that can interface with any MILP solver through MPS files (e.g. MPSX, LINDO, ZOOM, APEX).

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

Examples

Example 1

In example 1, the network indicating all the alternatives is shown in Figure 1. Product 3 is to be produced by process 2 or 3 with the feedstock to process 2 and 3 either bought or manufactured in process 1. This problem spans over three periods with the lengths being 2, 3, and 5 years. Limits on investment are specified at each time period and process 2 has an existing capacity of 50 kton/yr.

Three scenarios of this example are considered and they differ from each other in the following way: Scenario 2 differs from scenario 1 by 20% reduction in sales prices of product 3; scenario 3 differs from scenario 2 by reducing the investment bound in period 2 to 0 and increasing by 20% the cost of chemical 1 and reducing by 20% the cost of chemical 2. 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 3 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 9 0-1 variables, 42 continuous variables and 58 rows.

Some of the results of the three scenarios obtained with MULPLAN are presented in Tables 1 to 4. The analysis of these results indicates that the optimal solution of scenario 1 involves shutting down process 2 in period 2 and 3 and installing process 3 in period 2 (see Figure 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. The net present value for scenario 1 is $\$1697.61 \times 10^5$. Though the results for scenario 2 are identical (see Figure 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 Figure 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 a larger production of chemical 3. Purchases and sales for the three scenarios are given in Table 4.

Example 2

Example 2 involves a larger chemical complex, which has 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 Figure 5. Product 6 is to be produced in 4 periods each with a length of 2 years and various constraints on the chemical demands and prices.

The alternatives presented in Figure 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 2 expansions per process was considered. The economic data and chemical prices, the constants for material balance equation, and the demand for chemicals are given in Chathrathi (1986). The corresponding MILP model involves 40 0-1 variables, 174 continuous

variables and 198 rows.

Some of the results of the problem that were obtained with MULPLAN are presented in Tables 5 to 8 for both scenarios. These results indicate that the optimum net present value of $\$51,027.1 \times 10^5$ 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; the capacity of process 7 and 8 is expanded in period 2. In this configuration process 6 operates below maximum capacity, in period 4; process 9 would be shut down in period 2 and 3, and reused in period 4. This optimal configuration is shown in Figure 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 is $\$45,244.50 \times 10^5$. This configuration does not use processes 2, 5, and 10. The details of the capacity expansions and production profiles are shown in Table 6 and Figure 7. Note that this second scenario features 3 processes with expansions versus the 2 for the first scenario.

Computational Results

The three scenarios of example 1 were solved with MULPLAN using the following techniques as seen in Table 9a: branch and bound, cutting planes followed by branch and bound, Benders decomposition (algorithms I and II), cutting planes followed by algorithm 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.

Firstly, cutting planes reduce the gap between the relaxed LP solution (Z_{LP}) and the optimal MILP solution (Z_{jp}) 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 MBLP model exhibits a more substantial reduction in these two items. Also note from Table 9b that the CPU time is slightly higher with the use of cutting planes.

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, here it is clear that the modified

formulation of algorithm II is much better than the one in algorithm 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, however, the use of cutting planes has only a small effect in speeding up the solution of algorithm II. It is also interesting to note that algorithm 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 seem to indicate that the use of strong cutting planes followed by branch and bound should be a more promising technique for solving larger multiperiod MILP problems than Benders decomposition. In the following section a larger example is presented to illustrate the heuristic techniques and the other bounds.

Example 3

The network of a proposed petrochemical complex is shown in Figure 8. Four time periods are considered each of 2 years. In this case processes 12, 13, 16 and 40 are assumed to exist with capacities 39.9, 25, 300 and 200×10^3 ton/year, 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 material balance equations are given in Fornari and Grossmann (1986). No bounds are specified for the investment cost at each time period. The problem has 148 integer variables, 768 continuous variables and 739 constraints.

Due to the large size of this MCLP an approximate solution was obtained. From the analysis of the solution of the relaxed problem lower bounds were obtained for the objective function. These lower bounds are $LB_1 = \$2408.1 \times 10^6$ (obtained by making 1 all the non-zero binary variables in the relaxed problem solution) and $LB_2 = \$2530.6 \times 10^6$ by installing only once the selected processes. Clearly the latter yields a better lower bound and can be regarded as a good suboptimal solution.

Results from the MILP problem (12) show that the maximum number of expansions for all processes is 1, except from processes 2 and 10, for which 2 is the maximum number of expansions. Adding constraints (9) and (11) after 2 hs of CPU time with branch and bound in

LINDO on a VAX 11/780 the optimal solution was not reached. In this case the best NPV value found was $\$2381.5 \times 10^6$.

The relaxed problem solution, however, gives a valid upper bound for the optimal solution of the problem ($UB_j = \$2761.3 \times 10^6$), and hence the gap with respect to the lower bound of $\$2530.6 \times 10^6$ is 8.4%. We can reduce this gap to obtain a tighter upper bound by solving the MDLP (22) assuming only initial expansions and with investment cost of last period of time. This yields a lower upper bound $UB_2 = \$2606.4 \times 10^6$. With this new upper bound the gap is reduced to 2.9%.

The solution corresponding to the lower bound $LB = \$2530.6 \times 10^6$ is as follows. The selected processes are: 1, 3,4, 5,6, 8,12, 13,14,16,20,23,26, 27,28, 33, 36 and 40. Note that since 12, 13, 16 and 40 are existing processes, these are the only ones whose capacity is expanded in period 2. All the other processes are installed in period 1 with an initial capacity that remains constant throughout the 4 periods. Since this solution has a gap of only 2.9%, it can be regarded as a good suboptimal solution.

It should be noted that the problem was also solved to optimality with the MPSX code on the IBM-3090 supercomputer at the Cornell Theory Center. The total CPU time required was 35 minutes. It was also found that the branch and bound requirements were reduced to only 9.5 minutes after addition of the limits on investment constraints (10) and that the application of the strong cutting plane algorithm along with the above mentioned constraints reduced even more the branch and bound requirements to only 8 minutes. This clearly shows that new developments in computer technology and optimization theory are making it computationally feasible to solve large-scale multiperiod MILP problems. On the other hand, since one is usually interested in the study of different scenarios there is still an incentive to develop methods that can greatly reduce the computational expense.

Conclusions

This paper has presented a multiperiod MILP model for long range planning of capacity expansions 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, it would seem that a combination of strong cutting plane generation and branch and bound is the most promising strategy for solving these problems to optimality. Benders decomposition in its various forms would seem to have little promise. Finally, the last example illustrated the usefulness of the heuristic procedure for which the quality of the solution can be predicted.

Acknowledgment

The authors would like to acknowledge financial support from the National Science Foundation under Grant CPE-8351237.

Appendix A: Modelling Shut-Downs

It is sometimes desirable to account for a penalty 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 d_{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 d_{it} are:

$$d_{it} \leq Q_{i,t-1} \quad i=1, NP, \quad t=1, NT+1 \quad (A1)$$

$$d_{it} \leq U_{it} \epsilon_{it} \quad i=1, NP, \quad t=1, NT+1 \quad (A2)$$

$$Q_{it} \leq d_{it} + U_{i,t-1} (1 - \epsilon_{it}) \quad (A3)$$

where $U_{it} = Q_{io} + \sum_{T=1}^{t-1} QE_i^U$. Equation (A2) will force d_{it} to zero for as long as $\epsilon_{it} = 0$. When $\epsilon_{it} = 1$, equations (A1) and (A3) enforce $d_{it} = Q_{i,t-1}$. Note that when a process is selected and not shut down at anytime $\epsilon_{i,NT+1} = 1$, 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

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

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

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

$$W_{m,t} \geq x_{it} Q_{it} \quad i=1, NP, \quad t=1, NT \quad (A6)$$

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 L_{it} units of the main product,

$$W_{m,t} \geq L_{it} (1 - \epsilon_{it}) \quad i=1, NP, \quad t=1, NT, \text{ for } Q_{to} = X \quad (A7)$$

$$W_{m,t} \geq L_{it} (y_{iT} - \sum_{i=1}^t \epsilon_{it}) \quad i=1, NP, \quad t=1, NT, T \leq t, \text{ for } Q_{io} = 0 \quad (A8)$$

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:

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

where α'_i and β'_i are discounted cost coefficients. In the case of profit then $\alpha'_i > 0$ and $\beta'_i > 0$ 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:

$$\sum_{i=1}^{NP} \sum_{t=1}^{NT} pen_{it} QP_{it}$$

along with the following constraint

$$QP_{it} \geq -U_{it} W_{m,t} + Q_{it} - \sum_{t=1}^i d_{it} \quad i=1, NP, \quad t=1, NT \quad (A9)$$

that will force QP_{it} to be equal to the installed capacity of the process. Here pen_{it} are again discounted coefficients. Finally, the decision to shut down a process is applied exactly once for each process, and therefore

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

which gives rise to Special Ordered Sets of type 1. 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:

$$\max \sum_{i=1}^{NP} (r_i - \lambda C_i) z_i \quad (B1a)$$

$$\text{s.t. } \sum_{i=1}^{NP} u_i z_i > CI(t) \quad (B1b)$$

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

where $Z_j = 1$ if $i \in C_j$, $Z_j = 0$ otherwise. Here y_u^* 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 takes advantage of the fact that we are interested only in solutions for which $J_t > -1$ (because only in this case a violated inequality is derived).

The algorithm is as follows:

- Step 1. Set $Z_j = 1$ for i such that $y_u^* = 1$. Set $Z_j = 0$ for i such that $y^* = 0$. If constraint (B1b) is satisfied, Exit.
- Step 2. Examine if by setting to 1 only one of the remaining z^* s, constraint (B1b) is satisfied. If so, set this to 1 and Exit. Ties are broken by choosing the i for which $-(1 - y_u^*)$ 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 $(1 - y_u^*)$.
 - ii) Select $z_j = 1$ one at a time in the order found in (i) until (B1b) is satisfied.

In Step 1 the variables Z_j are assigned to avoid -1 terms in the objective J_t . 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.

REFERENCES

- Benders, J.F., "Partitioning Procedures for Solving Mixed-Variables Programming Problems," *Numerische Mathematik*, 4, 238-252 (1962).
- Birge, J.R., "The Value of the Stochastic Solution in Stochastic Linear Programs with Fixed Recourse," *Math. Program.*, 24, 314-325 (1982).
- Chathrathi, M., "Computer System for Long Range Planning in the Chemical Industry," M.S. Thesis, Carnegie Mellon University (1986).
- Crowder, H., E.L. Johnson, M. Padberg, "Solving Large-Scale Zero-One Linear Programming Problems," *Operations Research*, 31, 803 (1983).
- Fornari, R.E.J.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., G.L. Nemhauser, "Integer Programming," Wiley, New York (1972).
- Geoffrion, A.M., "Generalized Benders Decomposition," *JOTA*, 10, 4 (1972).
- Grossmann, I.E., J. Santibanez, "Application of Mixed-Integer Linear Programming in Process Synthesis," *Computers and Chem. Engng.*, 4, 205 (1980).
- Himmelblau, D.M., T.C. Bickel, "Optimal Expansion of a Hydrodesulfurization Process," *Computers and Chem. Engng.*, 4, 101 (1980).
- Hirshfeld, D.S., "Mathematical Programming and the Planning, Scheduling and Control of Process Operations," paper presented at the FOCAPO Conference, Park City (1987).
- Jiménez, A.G., D.F. Rudd, "Use of a Recursive Mixed-Integer Programming Model to Detect an Optimal Integration Sequence for the Mexican Petrochemical Industry," *Computers and Chem. Engng.*, 3, 291 (1987).
- Kallberg, J.G., R.W. White, W.T. Ziemba, "Short Term Financial Planning Under Uncertainty," *Mgmt. Sci.*, 28, 670-682 (1982).
- Kendrick, D., A. Meeraus, "GAMS - An Introduction, User's Manual for GAMS," Development and Research Dept. of the World Bank (1985).
- Luss, H., "Operations Research and Capacity Expansion Problems: A Survey," *Operations Research*, 30, 907 (1982).
- Padberg, M.W., T.J. Van Roy, L.A. Wolsey, "Valid Linear Inequalities for Fixed Charge Problems," *Operations Research*, 33, 842 (1985).
- Roberts, S.M., "Dynamic Programming in Chemical Engineering and Process Control," Academic Press, New York (1964).

Shimizu, Y., T. Takamatsu, "Application of Mixed-Integer Linear Programming in Multiterm Expansion Planning Under Multiobjectives," *Computers and Chem. Engng.*, 9, 367 (1985).

Van Roy, T.J., L.A. Wolsey, "Valid Inequalities for Mixed 0-1 Programs," CORE Discussion Paper 8316, Université Catholique de Louvain, Louvain-A-Neuve (1983).

Van Roy, T.J., L.A. Wolsey, "Solving Mixed Integer Programs by Automatic Reformulation," CORE Discussion Paper 8432, Université Catholique de Louvain, Louvain-A-Neuve (1984).

Table 1* Example i . scenario 1

Selected Process and Production Prof11**

Process	Period (Kton/Year)			
	1	2	3	
1	Capacity	7.76	7.76	7.76
	Production	6.41	9.79	7.76
2	Capacity	60.00 •	60.00 •	60.00 •
	Production	20.92	0	0
3	Capacity	0	36.96	36.96
	Production	0	30.72	36.96

Table 2. Example I - Scanarlo 2

Selected Process and Production Profiles

Process	Period (Kton/Year)			
	1	2	3	
1	Capaeity	7.76	7.76	7.76
	Production	6.41	9.79	7.76
2	Capacity	60.00 •	•60.00 •	60.00 •
	Production	20.92	0	0
3	Capacity	0	36.96	36.96
	Production	0	30.72	36.96

Table 3. Example 1 - Scenario 3

Selected Process and Production Profiles

Process	Period (Kton/Year)			
	1	2	3	
1	Capaolty	0	0	7.76
	Production	0	0	7.76
2	Capaeity	60.00 •	60.00 •	60.00 •
	Production	0	0	11.62
3	Capaolty	61.14	61.14	61.14
	Production	39.10	49.67	61.14

• Existing Capacity

Table 4. Example i - Purchases and Sales

Chemical	Period (Kton/year)		
	1	2	3
Scenario 1 - Purchases			
1	6.00	7.60	8.60
2	20.00	25.60	30.00
Sales			
3	20.82	30.72	35.95
Scenario 2 - Purchases			
1	6.00	7.60	8.60
2	20.00	25.50	30.00
Sales			
3	20.82	30.72	35.95
Scenario 3 - Purchases			
1	0	0	8.6d
2	40.00	61.00	60.00
Sales			
3	38.10	48.64	62.66

Table 5. Example 2 - Scenario 1

Selected Process and Production Profiles

Process		Period (Kton/yr)			
		1	2	3	4
1	Capacity	99.10	99.10	99.10	99.10
	Production	40.54	67.57	89.19	99.10
2	Capacity	0	0	0	0
	Production	0	0	0	0
3	Capacity	0	0	0	0
	Production	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
	Production	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	100.00	128.72	128.72	128.72
	Production	81.47	121.15	126.00	128.72
8	Capacity	100.00	200.00	200.00	200.00
	Production	81.47	175.00	199.00	200.00
9	Capacity	45.00	45.00	45.00	45.00
	Production	45.00	0	0	10.00
10	Capacity	0	0	0	0
	Production	0	0	0	0

Table 6. Example 2 - Scenario 1

Purchases and Sales

Chemical	Period (Kton/yr)			
	1	2	3	4
Purchases				
1	45.00	76.00	99.00	110.00
2	37.67	0	0	0
3	0	0	0	0
4	45.00	75.00	75.00	27.92
6	45.00	69.64	64.73	110.00
Sales				
6	145.00	176.00	199.00	210.00

Table 7.

Example 2 - Scenario 2

Selected Process and Production Profiles

Process	Period (Kton/yr)				
	1	2	3	4	
1	Capacity	0	67.67	99.10	99.10
	Production	0	67.57	89.19	99.10
2	Capacity	0	0	0	0
	Production	0	0	0	0
3	Capacity	0	63.20	63.20	63.20
	Production	0	63.20	42.08	51.62
4	Capacity	42.86	42.86	42.86	42.86
	Production	42.86	42.66	42.86	42.86
5	Capacity	0	0	0	0
	Production	0	0	0	0
6	Capacity	0	0	34.66	34.66
	Production	0	0	34.66	26.47
7	Capacity	54.63	64.63	129.97	129.97
	Production	42.86	64.63	127.20	129.97
8	Capacity	100.00	176.00	176.00	176.00
	Production	100.00	175.00	176.00	176.00
9	Capacity	0	0	35.00	35.00
	Production	0	0	24.00	35.00
10	Capacity	0	0	0	0
	Production	0	0	0	0

Table 8. Example 2 - Scenario 2

Purchases and Sales

Chemical	Period (Kton/yr)			
	1	2	3	4
Purchases				
1	0	75.00	99.00	110.00
2	45.00	33.29	0	0
3	20.29	34.82	0	0
4	0	0	38.36	29.38
6	45.00	67.36	99.00	110.00
Sales				
6	100.00	175.00	199.00	210.00

Table 9. CPU times^{*} for examples 1 and 2

a) Example 1

	Scenario 1	Scenario 2	Scenario 3
Branch and bound	2.62	3.00	2.55
Branch and bound/cuts	4.39	4.43	4.37
Benders decomposition I	68.20	76.79	49.81
Benders decomposition II	43.32	48.70	35.33
Benders decomposition II/cuts	39.15	43.81	31.82

b) Example 2

	Scenario 1	Scenario 2
Branch and bound	7.81	11.99
Branch and bound cuts	—	16.34

* CPU-seconds on IBM-3083. MILP and LP solver: MPSX.

Table 10. Effect of addition of cuts on branch and bound*

	z_{IP} (no ⁵)	Branch and Bound			Branch and Bound/Cuts		
		z_{LP} (\$10 ⁵)	No. Branches	No. Pivots	z_{LP} (\$10 ⁵)	No. Branches	No. Pivots
<u>Example 1</u>							
Scenario 1	1,697	1,898	11	145	1,874	11	160
Scenario 2	1,063	1,246	13	142	1,223	12	159
Scenario 3	2,236	2,540	7	151	2,472	6	96
<u>Example 2</u>							
Scenario 2	45,248	46,540	183	8580	46,236	140	5182

* LINDO computer code.

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

	Benders I	Benders II	Benders II/Cuts	Z_{LP} (\$10 ⁵)	Z_{IP}
Scenario 1	17	11	10	1,898	1,697
Scenario 2	19	12	10	1,246	1,063
Scenario 3	12	9	9	2,540	2,235

Table 12, Iterations for alternative Benders decomposition schemes in example 1, scenario 2

Iteration #	Benders decomposition I			Bende ¹ 's decomposition II			Benders decomposition II/cuts		
	Z ^L	Z ^U	Selected y's	Z ^L	Z ^U	Selected y's	Z ^L	Z ^U	Selected y's
0	-∞	+∞		.00	+∞		.00	+∞	
1	684.5	1246.5	y ₁₁	684.5	1246.5	y ₁₃	684.5	1223.2	y _n
2	899.7	1246.5	y ₃₂	746.8	1246.5	y ₃₁ y ₃₂	892.	1223..2	y _n .7 ₃₂
3	899.7	1246.5	y ₁₃ .7 ₃₃	746.8	1246.5	y ₁₁ .7 ₃₃	892.	1223..2	y _n y ₁₃ y ₃₁ *y ₃₂
4	899.7	1246.5	y ₁₂ y ₃₂	914.3	1246.5	y ₁₂ .7 ₃₁	892.	1223..2	y _n 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 .7 ₂₁ y ₃₁	1033.8	1075.5	y ₁₁	1033.	1071,4	y ₁₂ >y ₃₁
7	1057.	1246.5	y ₁₁ .7 ₃₁	1033.8	1069.5	y ₁₂ »7 ₃₁	1033.	1067.2	y ₁₁ >y ₃₂
8	1057.	1246.5	y ₁₁ .7 ₃₁ .7 ₃₂	1033.8	1067.3	y ₁₁ >y ₃₂	1040.9	1065.5	y ₁₁ .7 ₃₂
9	1057.	1246.5	y ₁₁ »y ₁₃ y ₃₁	1039.5	1065.5	y ₁₁ .7 ₃₂	1054.4	1063.	y ₁₁ »7 ₃₂
10	1057.	1246.5	y ₁₁ y ₁₃ y ₃₁ .7 ₃₂	1054.4	1063.8	y ₁₃ .7 ₃₁	1063.		
11	1057.	1246.5	y ₁₁ .7 ₁₂ y ₃₁	1054.4	1063.	y ₁₁ >y ₃₂			
12	1057.	1246.5	y ₁₁ .7 ₁₂ y ₃₁ y ₃₂	1063.					
13	1057.	1246.5	y ₁₁ .7 ₁₂ y ₃₁ >y ₃₃						
14	1057.	1246.5	y ₁₁ .7 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 .7 ₃₁						
19	1063 [^]	1063.							

* Optimum Z = 1063. , y₁₁ = y₃₂ = 1

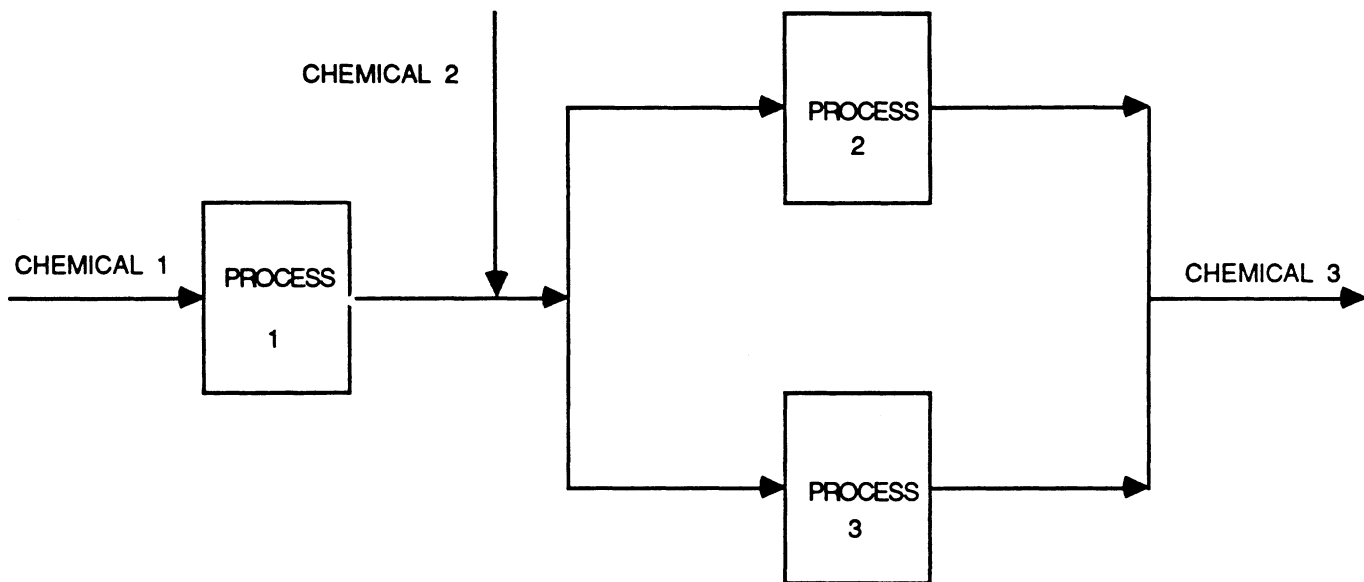


Fig. 1: Flow Diagram for Example 1

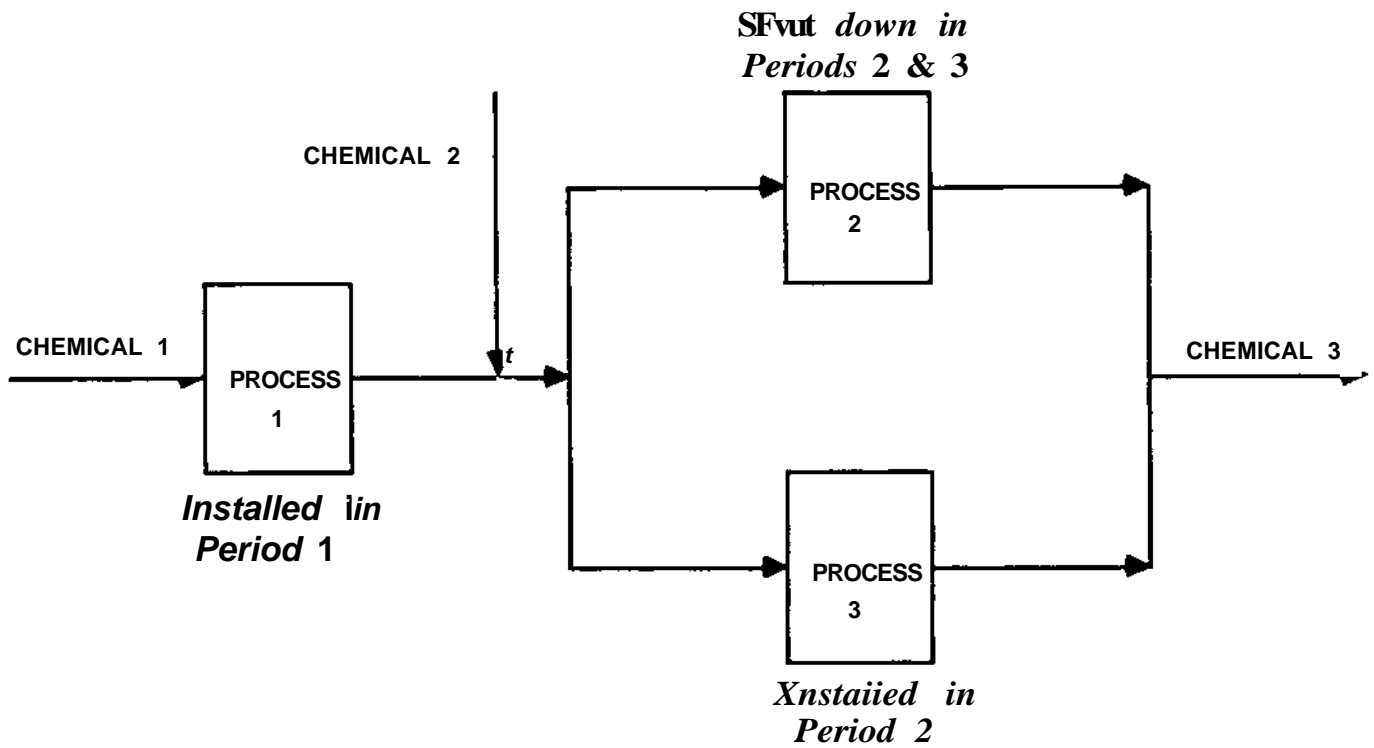


Fig. 2: Example 1: Optimum for Scenario 1. Net Present Value: \$ 1697.6 x 10⁵

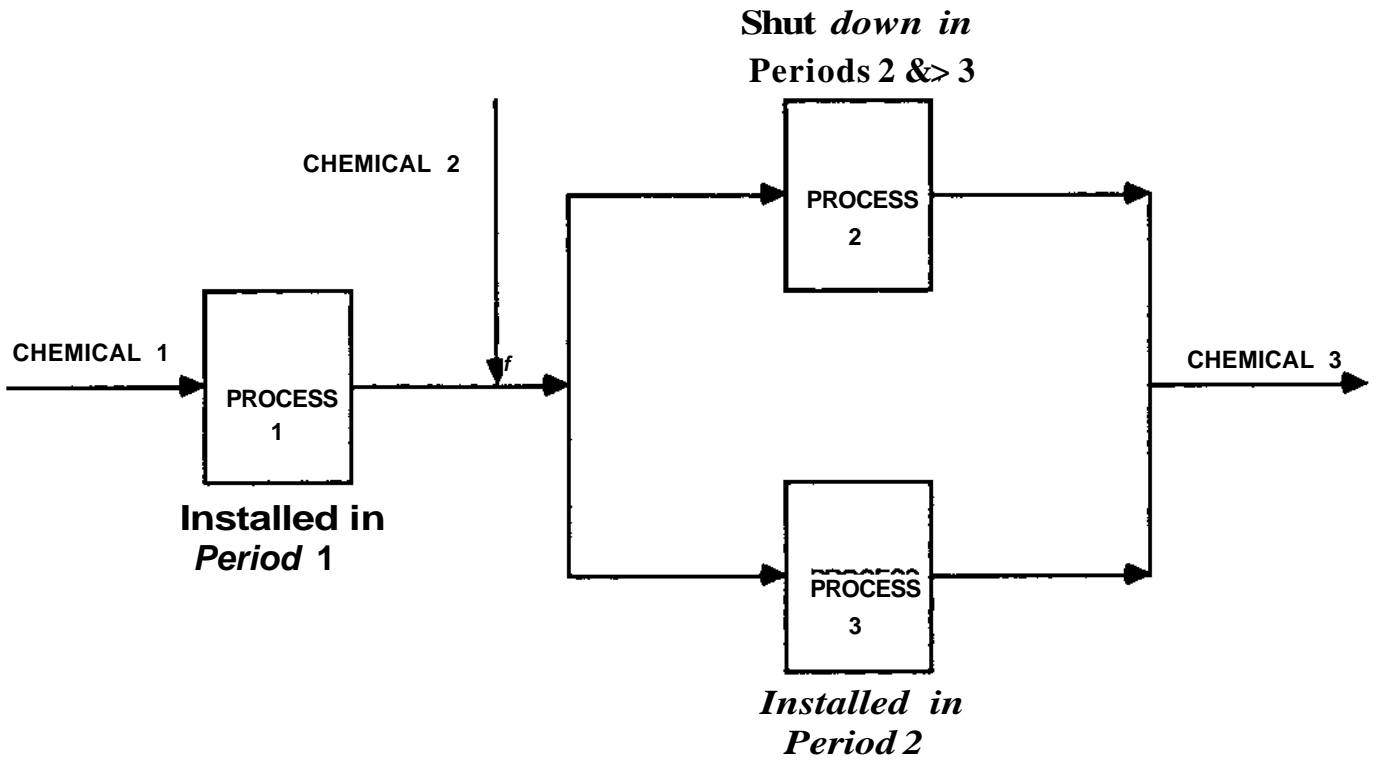


Fig. 3: Example 1: Optimum for Scenario 2. Net Present Value: \$ 1063. x 10⁵

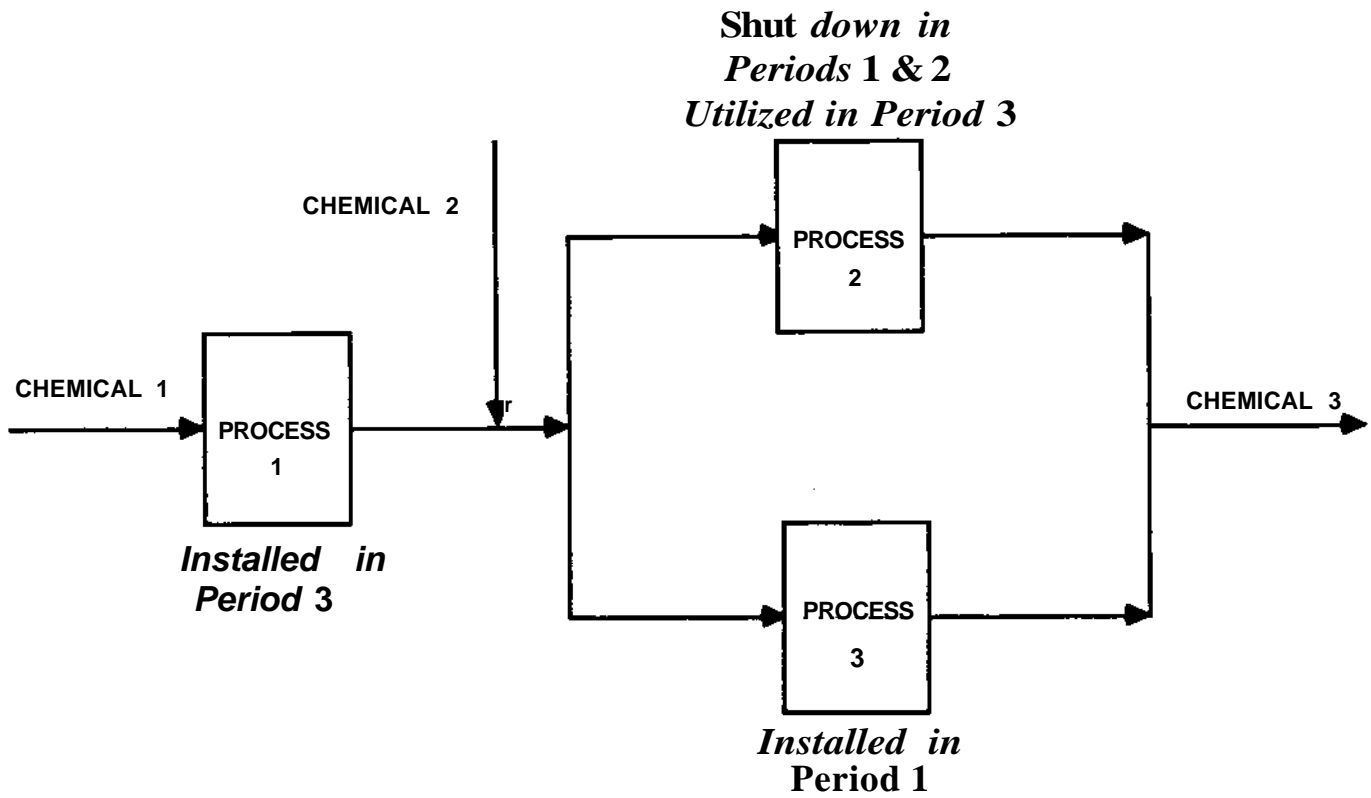


Fig. 4: Example 1: Optimum for Scenario 3. Net Present Value: \$ 2236.4 x 10⁵

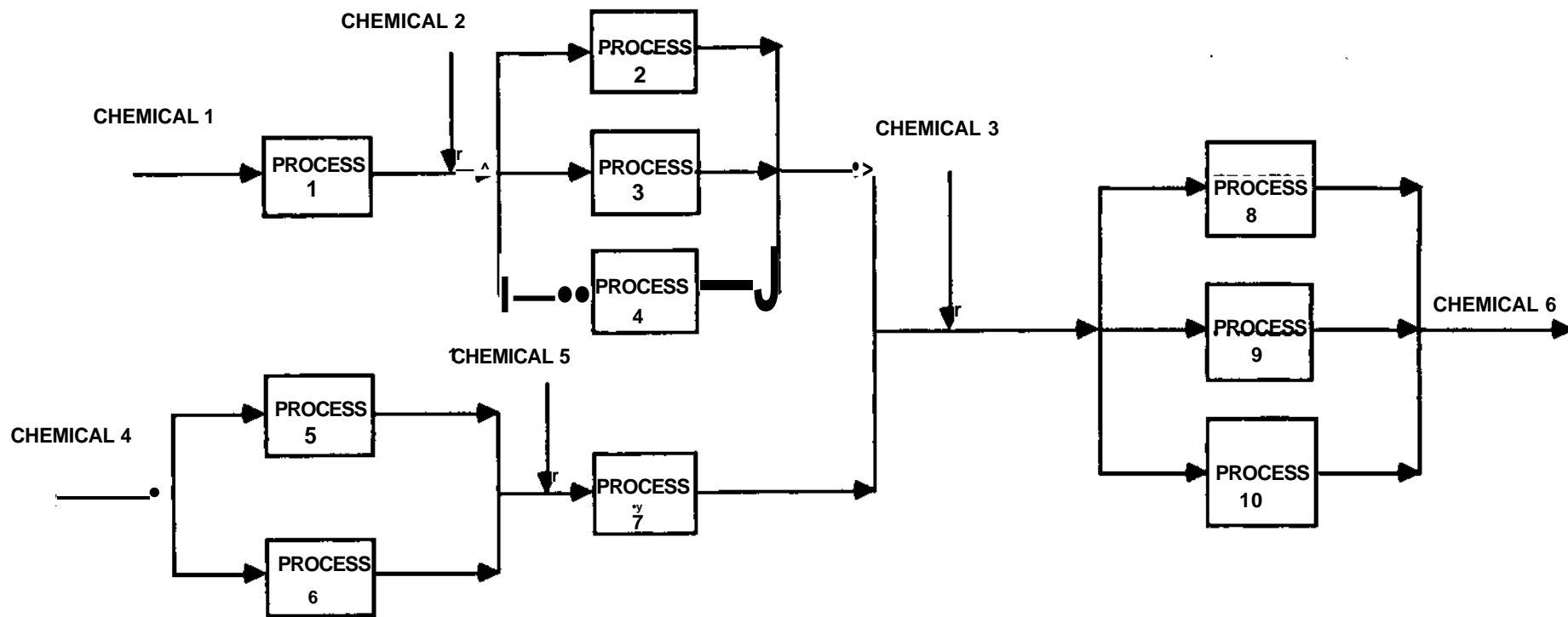


Fig. 5: Flow Diagram for Example 2

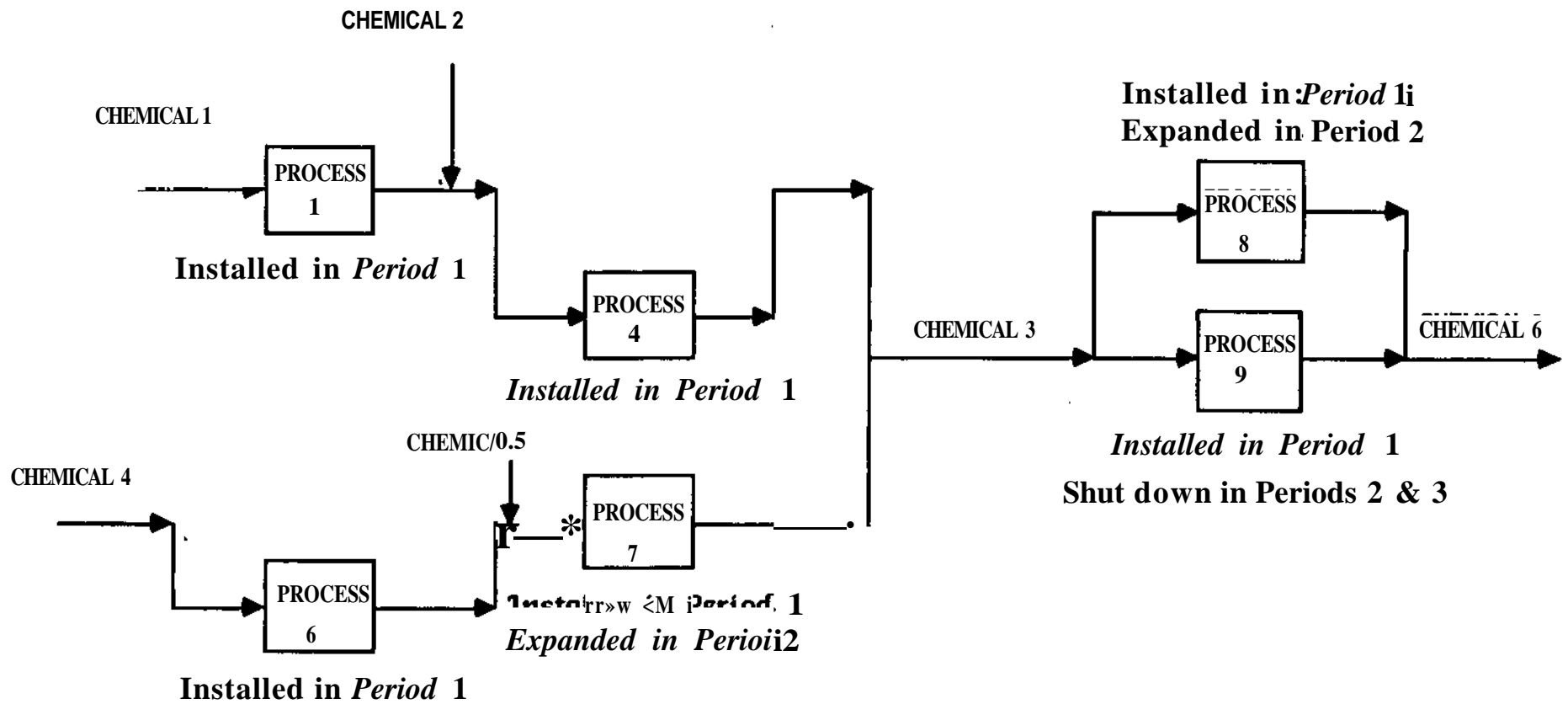


Fig. 6: Example 2 - Optimum for Scenario 1. Net Present Value \$ 51027.1 x 10⁵

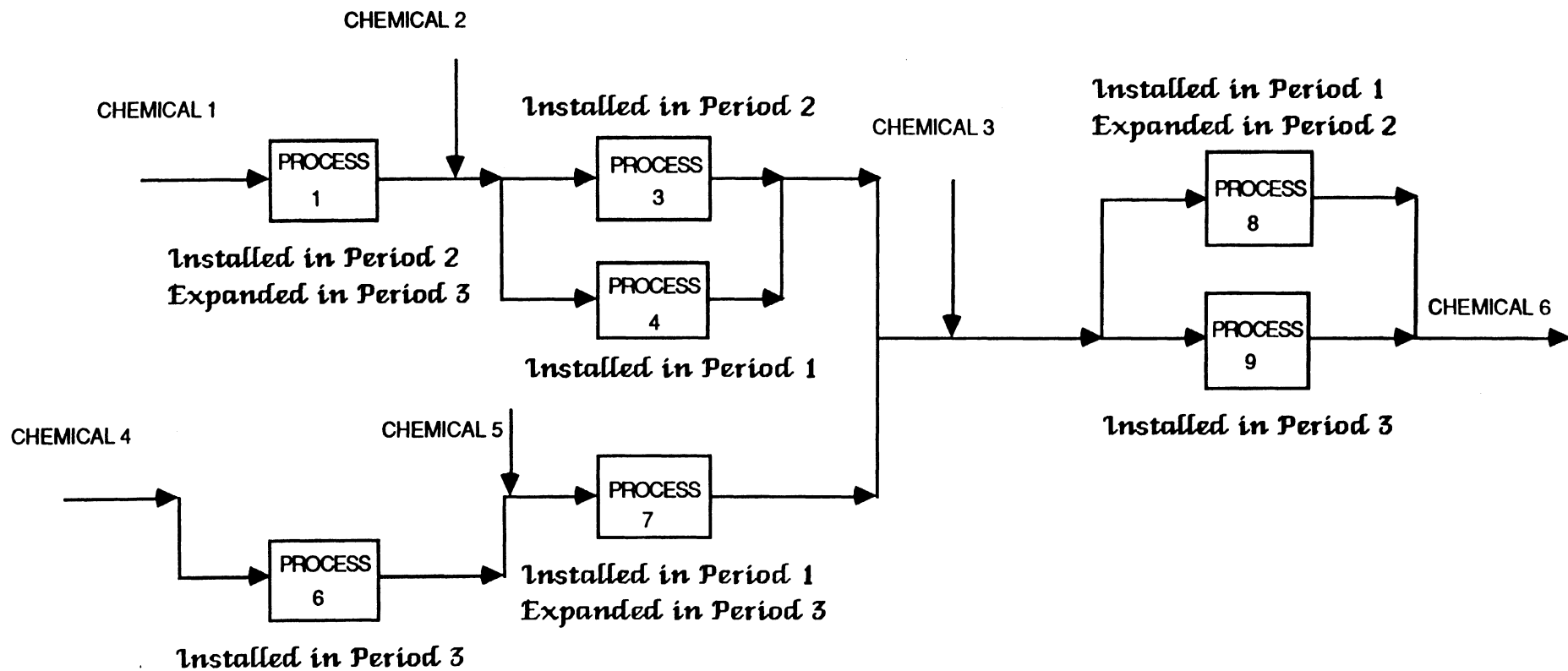


Fig. 7: Example 2 - Optimum for Scenario 2. Net Present Value $\$ 45244.5 \times 10^5$

