Reformulation of the Multiperiod MILP Model for Capacity Expansion of Chemical Process

by

N. V. Sahinidis, I. E. Grossmann

EDRC 06-71-89 5

REFORMULATION OF THE MULTIPERIOD MILP MODEL FOR CAPACITY EXPANSION OF CHEMICAL PROCESSES

N.V. Sahinidis and I.E. Grossmann*

Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213

July 1989 / Revised October 1989

*Author to whom correspondence should be addressed.

ABSTRACT

The problem of selecting processes and capacity expansion policies for a chemical complex consisting of continuous chemical processes can be formulated as a multiperiod mixed integer linear programming problem. Based on a variable disaggregation technique that exploits lot sizing substructures, we propose two reformulations of the conventional MILP model. The first one is an NLP reformulation that yields very quickly good suboptimal solutions. The second is an MILP reformulation for exact solutions that leads to up to an order of magnitude faster computational results for large problems due to its tighter linear programming relaxation.

Chemical companies are increasingly concerned with the development of planning techniques for their process operations. The incentive for doing so is a result of 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 of important changes in the external environment on their business. 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.

This paper addresses the following long range planning problem for chemical processes. It is assumed that a network of continuous 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. As stated, this is a multi-product, multi-facility, dynamic, location-allocation problem.

A rather large number of papers and books has been published in the operations research literature on capacity expansion in applications which are closely related to the problem discussed in this paper. The synthesis and capacity expansion models in communications networks (and other dynamic networks) have a long history and have recently been surveyed by Minoux (1987). Planning the expansion of electric power generation networks is discussed by Noonan and Giglio (1977), who used Benders decomposition coupled with a successive linearization procedure to solve a nonlinear multiperiod mixed integer model. In manufacturing, Merges and Mutlu (1988) developed a multiperiod mixed integer linear programming model for the acquisition and allocation of computing systems. In the public sector, Bergendahl (1969) developed a combined linear and dynamic programming model for the expansion of road networks, and Armstrong and Willis (1977) used the Generalized Benders decomposition to solve a mixed integer nonlinear (quadratic) program for the planning of water resources.

In the chemical process industries, perhaps the best known applications are those described by Manne for several heavy processes in India (Manne, 1967) and Mexico (Goreux and Manne, 1973). More recently, Himmelblau and Bickel (1980) presented a nonlinear programming formulation for a hydrodesulfurization process, and Grossmann and Santibanez (1980) developed a multiperiod mixed integer linear programming formulation applicable to the chemical process industries. Fong and Srinivasan (1981a, 1981b) developed a heuristic solution strategy for the multifacility dynamic expansion problem. Shimizu and Takamatsu (1985) discussed a goal programming approach where in addition to cost minimization, minimizing the number of expansions is also suggested. Jimenez and Rudd (1987) presented a recursive mixed integer linear programming technique and applied it to the Mexican petrochemical industry. Recently, Sahinidis *et al.* (1989) presented a multiperiod MILP formulation for long range planning in the chemical process industries and extensive computational results to evaluate the performance of several solution procedures for this model.

With respect to the computational complexity of the problem, it has been shown that even though some important special cases can be solved in polynomial time, the more general planning problems are NP-hard (Florian, Lenstra and Rinnooy Kan, 1980; Akileswaran, Hazen and Morin, 1983). It is therefore not surprising that most previous approaches address simplified versions of the problem, or else they involve integer programs which are limited in the size of problems that they can handle.

However, it is well known that for integer programs some formulations are more efficient than others, even though they may contain more constraints and/or variables. For instance, Rardin and Choe (1979) described how variable disaggregation can be used to reformulate fixed charge network problems and yield tighter formulations. Jeroslow and Lowe (1984 and 1985) have shown how certain ("sharp") mixed integer formulations can give rise to stronger linear programming relaxations by introducing more variables than the common formulation. Closely related is the work of Balas (1985), who used disjunctive programming to develop a framework for the description of a hierarchy of relaxations for discrete optimization programs. Martin (1987a) developed a theory of variable redefinition and once again showed that the new formulations provide a more accurate linear programming relaxation, which is an important property at least within the context of linear programming based branch and bound.

The purpose of this paper is to show that formulations based on variable disaggregation are possible for the long range planning problem of chemical processes. These formulations are different from a conventional mixed integer programming model in that they utilize more constraints and variables. The development is based on the observation that, for fixed production levels, the remaining capacity expansion problem can be recast as a lot sizing problem. For the lot sizing part of the problem, the formulations of Krarup and Bilde (1977) and Martin (1987b), which can be solved as linear programs, are utilized. The former is used within an NLP reformulation of the conventional MILP model and yields very quickly good suboptimal solutions. The latter is used within an MILP reformulation for exact solutions that leads to up to one order of magnitude faster computational results for large problems due to its tighter linear programming relaxation.

The paper is organized as follows. In Section 1, a straightforward multiperiod MILP formulation of the problem is presented. Section 2 is a description of different formulations for the lot sizing problem which constitute the basis of our reformulation for the planning problem. Section 3 presents our main observation: the link between the long range planning problem and the lot sizing problem. Sections 4 and 5 present the main results: an NLP and an MILP reformulation of the model presented in Section 1. Theoretical properties of the reformulations are also given in these sections while, at the same time, computational procedures are derived for their solution. Computational results with the new models are presented in Section 6 where the practical significance of the MILP reformulation becomes apparent. The conclusions of this work and some recommendations for future research are presented in Section 7.

1. Multiperiod MILP Model for Long Range Planning

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. The processes will be interconnected by a total of NS streams to represent the different alternatives that are possible for the processing and the purchases and sales from NM different markets. 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.

The objective function to be maximized is the net present value of the project over a long range horizon consisting of a finite number of NT time periods during which prices and demands of chemicals, and investment and operating costs of the processes can vary. The operating cost of a plant will be assumed to be proportional to the flow of its main product. 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 description of the model, the following notation will be used:

Indices:

i	process (i = 1, NP)
t	time period (t = 1, NT)
j	chemical (j = 1, NC)
k	stream in the network (k = 1, NS)
l	market (l = 1, NM)

Parameters:

NP	number of processes in the network
NT	number of time periods considered
NM	number of markets
NC	number of chemicals in the network
NS	number of streams in the network
$I(j)$	the index set of streams of chemical j which are produced in the complex
$O(j)$	the index set of streams of chemical j which are consumed in the complex
L_i	the index set of the subset of the NS streams corresponding to inputs and outputs of process i, and $\cup_{i=1}^{NP} L_i = \{1,2,...,NS\}$
m_i	stream corresponding to the main product of process i ($m_i \in L_i$)
Q_{i0}	existing capacity of process i at time $t = 0$
QE_{it}^L	lower bounds for the capacity expansions
QE_{it}^U	upper bounds for the capacity expansions
μ_{ik}	material balance coefficients characteristic of each process i and stream k
α_{it}	variable term of investment cost [$ / unit of capacity installed]
β_{it}	fixed term for the investment cost [$]
$\delta_{m_i t}$	unit operating cost[$ / unit of production amount of the main product]

$1j_t^l$ prices of sales of the chemical / in market / during time period *t* [$ / unit sold]

I\$_{j*}$ prices of purchases of the chemical *j* in market / during time period *t* [$ / unit purchased]

NEXP(z') the maximum allowable number of expansions for process *i*

CI(r) the capital investment limitation corresponding to period *t*

Variables:

y_{zr} decision variable which is 1 whenever there is an expansion for process / at the beginning of time period r, and 0 otherwise

Q_{it} total capacity of the plant of process *i* that is available in period *t*

QE_ZY capacity expansion of the plant of process *i* which is installed in period *t*

P_{jt}^l amount of product *j* purchased from market / at the beginning of period *t*

S_{jt}^l amount of product; sold to market / at the beginning of period *t*

W^$_r$ amount of flow of stream *k* during time period r.

A multiperiod MILP model for the long range planning problem is as follows:

Model PI:

$$\max \; NPV = -\sum_{i=1}^{NP}\sum_{r=1}^{NT} ("/,<£;,+M*,) - \sum_{i=1}^{NP}\sum_{r=1}^{NT} 5_{Wi}W_{m*} + \sum_{l=1}^{NM}\sum_{j=1}^{NC}\sum_{t=1}^{NT} \left(\gamma_{jt}^l S_{jt}^l - \Gamma_{jt}^l P_{jt}^l\right) \qquad (1.1)$$

s.t.

y_{it} QEf, ≤ QE,; ≤ QE,? y,-, j=l,NP f=l,NT (1.2)

j=l,NP r=l,NT (1.3)

Q_{it} ^ $W_{OT_t f}$ j=l,NP r=l,NT (1.4)

$W_{kt} = \mu_{ik} W_{m_i t}$ $k \in L_i \setminus \{m_i\}$ a* = 1,NP t = 1.NT (1.5)

$\sum_{/ = !}^{NM}$ P/i+ $X_{kel(j)}$ $W_{4|}$ = $I_{/ = 1}^{NM}$ s j , + $X_{keO(j)}$ W*, y=l,NC f-l,NT (1.6)

$$\left.\begin{array}{l} a_{jt}^{l,L} \le P_{jt}^{l} \le a_{jt}^{l,U} \\ d_{jt}^{l,L} \le S_{jt}^{l} \le d_{jt}^{l,U} \end{array}\right\}$$

;=1,NC t = l.NT / = 1,NM (1.7)

$X_{t=1}^{NT}$ y/, <NEXP(/) I'e I'C {1,2,... NP} (1.8)

$\sum_{i=1}^{NP} (\alpha_{it}\, QE_{it} + \beta_{it}\, y_{it}) \le$ CI(r) reT c{1,2,...NT} (1.9)

y_{it} = 0 or 1 j=l,NP r=l,NT (1.10)

QE_{it}, W_{kt}, P/,,sj$_f \ge 0$ (1.11)

In equation (1.1), the net present value is defined as the sum of the investment cost, the operating cost, the sales revenue and the cost for purchasing the raw materials. All the coefficients are discounted at a specified interest rate and include the effect of taxes in the net present value. Constraint (1.2) is a variable lower and upper bounding constraint for the capacity expansions. A zero-value of the binary variables y_{it} forces the capacity expansion of process i at period t to zero, *i.e.* $QE_{it} = 0$. If the binary variable is equal to one, a capacity expansion between the specified bounds is performed. Equation (1.3) simply defines the total capacity, Q_{it}, that is available for process i at each time period t, while Q_{i0} is the initial capacity (zero for nonexisting processes). Constraint (1.4) expresses the condition that the operating level of a process – expressed in terms of the flow of its main product – cannot exceed the installed capacity. The material balances in each plant are given by the linear relations (1.5): the flow of each product is proportional to the flow of the main product of the process, where μ_{ik} are positive constants characteristic of each process. The material balances for each chemical in the entire network are given in (1.6) according to which the total amount of a chemical's purchases from the various markets plus the amounts produced within the network must be equal to the sum of sales and the total consumption within the network. Constraints (1.7) express the lower and upper bounds for the availability of raw materials and the demand of the products. Finally, constraints (1.8) and (1.9), which are optional, express limits on the number of expansions of some processes and on the capital available for investment during some time periods, respectively.

The MILP model given above can typically be solved directly with branch and bound enumeration procedures (see Nemhauser and Wolsey, 1988) such as the ones that are implemented in standard computer packages (e.g. MPSX, SCICONIC, ZOOM). Consider, as an example, a chemical complex involving 10 processes and 6 chemicals. None of these processes is assumed to have an existing capacity. The network showing all the alternatives for this complex is shown in Fig. 1. Chemical 6 is to be produced in 4 periods, each having a length of 2 years and various constraints on the chemical demands and prices. The corresponding MILP model involves 40 binary variables, 174 continuous variables and 198 rows. The optimum configuration for an instance of this problem considered by Sahinidis *et aL* (1989) is shown in Fig. 2 and was obtained by solving model (PI) using MPSX-MIP/370 (IBM, 1979). The computational requirements were only 2 seconds on an IBM-3090.

For large process 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 binary 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 nodes must usually be examined in a branch and bound search. Therefore, there is a clear incentive to develop efficient computational strategies since this allows the examination of a greater variety of scenarios with the planning model. Sahinidis *et aL* (1989) have compared the performance of several computational strategies including branch and bound, strong cutting planes followed by branch and bound, Benders decomposition and strong cutting planes followed by Benders decomposition. For the test problems that were considered, the combination of integer cuts, strong cutting plane generation and branch and bound was found to be the most efficient strategy for solving large-scale problems to optimality.

In order to obtain further significant reductions in the computational effort, we take a different approach in this paper by developing alternative formulations for the problem. In particular, we propose to disaggregate the capacity expansion variables and describe two alternative reformulations. The following section provides the necessary background by describing the lot sizing problem. This not only serves as an example to illustrate the variable disaggregation ideas, but it also plays an essential role in the development of the reformulations of the long range planning model.

2. Reformulation and Lot Sizing

Consider the production planning problem where the objective is to minimize the sum of the costs of production, storage, and set-up, given that demand must be satisfied in each of NT time periods and backlogging is not allowed. For t = 1, NT, let dj be the demand in period r, and let Cj, pj, and h_t be the set-up, unit production, and unit storage cost, respectively, in period t.

A common formulation for this problem is obtained (see Nemhauser and Wolsey, 1988) by defining x_t and s_t as the production and storage amounts in period t and by defining a binary variable y^, indicating whether $x_t > 0$ or not. This leads to the model:

Model LS:

$$\min \sum_{r=1}^{NT} (p_r x_r + h_r s_r + c_r y_r) \qquad (2.1)$$

St.

$$s_{t-1} + x_t = d_t + s_t \qquad r=1,NT \qquad (2.2)$$

$$x_r \leq co\ y, \qquad r=1,NT \qquad (2.3)$$

$$s_O = O \qquad (2.4)$$

$$s_r,\ x_t \geq 0, \quad y_r \in \{0,1) \qquad r=1,NT \qquad (2.5)$$

where $\omega = \sum_{t=1}^{NT} d_t$ is an upper bound on x_t for all t.

Theorem 1. (Wagner and Whitin, 1958). For the lot sizing problem, there always exists a minimal cost policy with the property that x_t has one of the following values:

$$0, \quad d_t, \quad d_t + d_{t+1}, \quad d_t + d_{t+1} + d_{t+2}, \quad \dots, \quad \sum_{T=t}^{NT} d_T.$$

Based on this result, Wagner and Whitin (1958) developed an efficient dynamic programming algorithm to search over the above discrete set of solutions to find the optimum solution of the lot sizing problem. Another alternative is to directly solve the integer program (LS). In order to efficiently solve this problem, Krarup and Bilde (1977) presented the formulation that we describe next.

By defining $q_{t\tau}$ as the quantity produced in period t to satisfy the demand in period $\tau \geq t$, and y_t as above, we have:

$$x_t = \sum_{\tau=t}^{NT} q_{t\tau} \qquad t = 1,NT \qquad (2.6)$$

Problem (LS) can then be reformulated as follows:

<u>**Model RLS1:**</u>

$$\min \quad \sum_{t=1}^{NT} \sum_{\tau=t}^{NT} (p_t + h_t + h_{t+1} + \dots + h_{\tau-1}) \, q_{t\tau} + \sum_{t=1}^{NT} c_t y_t \qquad (2.7)$$

St.

$$\sum_{\tau=1}^{r} q_{\tau r} = d_r \qquad r=1,NT \tag{2.8}$$

$$q_{r\tau} \leq d_\tau y_r \qquad r=1,NT \quad \tau=r,NT \tag{2.9}$$

$$q \in \Re_+^{NT(NT+1)/2}, \quad y \in \{0,1\}^{NT} \tag{2.10}$$

As mentioned, the extra variables $q_{r\tau}$ introduced in this reformulation of model (LS) can be seen as amounts produced in period t in order to satisfy demand *for* period $\tau \geq t$. This is depicted in Fig. 3, where we show the problem representation before (a) and after the reformulation (b). It is clear that in (a) we have a fixed charge network. Therefore, the reformulation in (b) can be derived from the suggestions of Rardin and Choe (1979) for obtaining tighter relaxations of network flow problems with fixed charges: each variable x_t of the original formulation is now disaggregated into NT-t-1 new variables $q_{t\tau}$ ($\tau = t$, NT). The variable disaggregation in this case gives not just a tighter formulation but the absolute tightest one:

Theorem 2 (see Nemhauser and Wolsey, 1988). The solution to the linear programming relaxation of (RLS1) yields 0-1 values for the y-variables. In addition, the image in the (x, s, y)-space under the transformation (2.6) of all the points (q, y) feasible in the linear programming relaxation of model (RLS1) produces the convex hull of model (LS).

It follows from the theorem that, one only needs to solve (RLSl) as a linear program where the y-variables are relaxed to take values in the interval [0,1] and obtain the solution to the integer program (LS). It is interesting to note that model (RLSl) is not the only possible formulation exhibiting this property. Based on the work of Barany, Van Roy and Wolsey (1984), Martin (1987b) used separation algorithms and derived for the lot sizing problem another alternative formulation for which Theorem 2 holds. His reformulation is the following:

Model RLS2:

$$\min \sum_{t=1}^{NT} \left(P_r^x r^{+h} r^s r^{+c} r^v_r \right) \qquad (2.1)$$

St.

$$s_{t-1} + x_t = d_r + s_r \qquad r=1,NT \qquad (2.2)$$

$$x, \leq C_{r>NT} y_f \qquad r=1,NT \qquad (2.11)$$

$$x, \geq X_n \qquad r=1,NT \qquad T=r,NT \qquad (2.12)$$

$$\lambda_{t\tau} \leq C_{t\tau} \; y, \qquad r=1,NT \qquad r=r,NT \qquad (2.13)$$

$$\sum_{T=1} l_{Tt}* \quad C_{1r} \qquad f\text{-}1.NT \qquad (2.14)$$

$$s_0 = 0 \qquad (2.4)$$

$$s_t,\ x_t \geq 0, \quad y_t \in \{0,1\} \qquad t = 1, NT \qquad (2.5)$$

where $C_{t\tau} = \sum_{T=t}^{\tau} d_T$ are upper bounds for the disaggregated production variables $\lambda_{t\tau}$ which can now be interpreted as amounts produced in period t in order to satisfy demand *up to* period $\tau \geq t$.

In addition to models (RLS1) and (RLS2), based on the work of Barany, Van Roy and Wolsey (1984), Pochet and Wolsey (1988) used the theory of strong cutting planes to derive yet another formulation for which Theorem 2 is valid. These three, slightly different representations, differ in the number of constraints and variables they include, and therefore in their computational efficiency. Of course, efficient dynamic programming techniques are available to solve the lot sizing problem (Wagner and Whitin, 1958; Zangwill, 1969). However, the above reformulations are very important when the lot sizing problem is part of a more complex planning model. For example, based on the variable redefinition theory of Martin (1987a), Eppen and Martin (1987) developed a formulation that gave very encouraging computational results to the solution of some multiproduct capacitated lot sizing problems. The importance of reformulations (RLS1) and (RLS2) will also be shown in the development of Models (R1) and (R2) of this paper. This development is based on the observation described in the next section.

3. The Main Observation

Let us assume that, for the long range planning problem, there are zero lower bounds and infinite upper bounds for the capacity expansions (1.2), no limits for the expansions (1.8) and no constraints on the investment (1.9) – this assumption will be removed later in the paper.

Refer now to Fig. 1 and imagine for a moment that all flows of chemicals (W&, $Pj_{r>}$ SJ,) in the network have been fixed in such a way that material balances (constraints (1.5) to (1.7)) are satisfied for all time periods. Then every process can be isolated from the rest of the network and the design problem for each process /becomes: "Find the cheapest capacity expansion sequence ($QE_{;r,}$ t = 1,NT) that will allow production of the prespecified flows of chemicals (W_{kt}, P^j_{jh} S^j_{jt})". Mathematically the problem reduces to:

<u>Model P2-i:</u>

$$\min \sum_{t=1}^{NT} (<*;,Q^E z7+Pz,y;/) \qquad (3.1)$$

s.t.

$$QE_{Z}, \leq U \; y_{it} \qquad r=1,NT \qquad (3.2)$$

$$Q_{i,t-1} + QE_{it} = Q_{ir} \qquad r=1,NT \qquad (3.3)$$

$$Q_{/r} \geq W_{m \cdot r} \qquad r=1,NT \qquad (3.4)$$

$$QE_{/r}\ f\ Q_{/r} \geq 0, \quad y_{it} = 0 \text{ or } 1 \qquad r = 1,NT \qquad (3.5)$$

where U is a large positive quantity.

The objective in (3.1) is to minimize the investment cost of process *i* for the given flows of the main product in the right hand side of (3.4). Assume, for a moment only, that these flows are such that:

$$Q/0 * {}^{W}m,1 * {}^{w}m,2 * \cdots * {}^{w}m,,NT \qquad (3.6)$$

By letting:

$$SQ;, = Q_{/r} - W_{m/f} \qquad /=1,NT \qquad (3.7)$$

$$d_{it} = W_{m_it} - W_{m_i,}M \qquad r= 1.NT \qquad (3.8)$$

and using the convention that W_{mj}-0 = Q,o» then $SQ_{,-f}$ ^ 0 implies (3.4) and (P2-i) can be transformed into the following equivalent lot sizing problem:

Model P3-i:

$$\min \sum_{*=1}^{NT} (<*«<\&«+V>«yit) \qquad (3.1)$$

s.t.

$$QEi_{,} \leq Uy_{j(} \qquad r=1,NT \qquad (3.2)$$

$$SQ_{J>;} + QE_{/r} = d_{|7} + SQ_{/r} \qquad /= 1.NT \qquad (3.9)$$

$$SQ_{i0} = 0 \qquad (3.10)$$

$$QE_{j7}\ ,\ SQ_{;r} \geq 0, \quad y_{it} = 0 \text{ or } 1 \qquad r= 1,NT \qquad (3.5)$$

In the lot sizing terminology, we can view $SQ_{;f}$ as the "inventory" of capacity, *i.e.* excess of capacity installed at early times in order to serve demand during subsequent time periods. At the same time, the QE_{it}'s can be regarded as "production" of capacity in order to satisfy some "demand" for capacity as determined by the flows of the main products ($W_{m_i t}$) in (3.8). For example, if there is no capacity initially installed and if $W_{m_i t}$ = (10, 15, 18, 20), then the demand for capacity is: d_{it} = (10,.5, 3, 2). In the general case – when (3.6) may not hold – this demand for capacity can be obtained as follows:

1) Subtract any existing capacity (Q_{i0}) from $W_{m_i t}$. If positive, let this difference be called additional required capacity, m_{it}, then:

$$m_{it} = \max(0, W_{m_i t} - Q_{i0}) \qquad t = 1,NT \qquad (3.11)$$

2) For each time period t, find the maximum additional required capacity during all previous time periods; this maximum is:

$$M_{it} = \max_{T \le t-1} m_{iT} = \max(M_{i,t-1}, m_{i,t-1}) \qquad t = 1,NT \qquad (3.12)$$

where $m_{i0} = M_{i0} = 0$.

3) The demand, d_{it}, for capacity during time period t is the difference between the current additional capacity requirements (m_{it}) and the maximum additional capacity requirements up to the previous time period (M_{it}), provided this difference is positive:

$$d_{it} = \max(0, m_{it} - M_{it}) \qquad t = 1,NT \qquad (3.13)$$

As an example, consider the case where the installed capacity is 3 units and $W_{m_i t}$ = (10, 8, 9, 12). Then it follows from the above equations that the demand for capacity is d_{it} = (7, 0, 0, 2). The equivalence of problems (P2-i) and (P3-i) – with the demands d_{it} obtained through (3.11) to (3.13) – for values of the flows not necessarily satisfying (3.6) is established by the following theorem:

Theorem 3. Problems (P2-i) and (P3-i) have the same optimal solution.

Proof: We shall show that (P2-i) and (P3-i) have the same set of feasible solutions. Note first of all, that by summing the equality constraints in (3.3), one can solve for Q_{zr}. Then the result can be substituted into (3.4) therefore eliminating the variables Q_{zr} and the equality constraints (3.3) from model (P2-i). In this case, (3.4) becomes:

$$Q_{i0} + \sum_{T=1}^{t} \qquad (3.14)$$

Similarly, in model (P3-i), one can solve (3.9) for SQ_{zr} and substitute the result into the nonnegativity constraint SQ_{zr} (3.5). Then (3.9) and SQ^*_{zr} can be eliminated by rewriting the nonnegativity constraint as follows:

$$\sum_{T=1}^{t} QE_{iT} \geq \sum_{T=1}^{t} d* \qquad r=1,NT \qquad (3.15)$$

We need to prove that feasibility in (3.14) implies feasibility in (3.15) and *vice versa.* In the following, we drop the indices / and *m^* for simplicity; so consider any process /. The case where none of the flows W_r (r=1, NT) exceeds the installed capacity is trivial since no expansions are required for both problems. Consider the case of arbitrary flows where expansions are required and let p_1 be the earliest time period for which $Wp_1 > QQ$. Also let $p_2 > p_1$ be the earliest time period for which $Wp_2 > Wp_1$. Continue in this way to define the set of time periods Np = {pp ^ *Vy* => P_n) for which pj < pj < p^ <...< p_n and

$$QO < W_{P_1} < W_{P_2} < \cdots < W_{P_{n-1}} < W_{P_n} \qquad (3.16a)$$

Because of the way Np is constructed, we also have:

$W_p \leq W_{p_x}$ if $p_x < p < p_{x+1}$, with $p_x, p_{x+1} \in N_p$, $p \notin N_p$ **(3.16b)**

From the definitions (3.11) to (3.13):

$d_{p_1} = W_{p_1} - Q_0$, $d_{p_2} = W_{p_2} - W_{p_1}$, $d_{p_3} = W_{p_3} - W_{p_2}$,

$\ldots,\ d_{p_n} = W_{p_n} - W_{p_{n-1}}$ while $d_p = 0$ for $p \notin N_p$ (3.17)

For any time period p ($1 \leq p \leq NT$), we have:

$$\sum^{p} d_i = d_{p_1} + d_{p_2} + \ldots + d_{p_k} \qquad (3.18)$$

where k is the largest element of N_p not exceeding p. Substituting (3.17) into (3.18) yields:

$$\sum_{r=1}^{p} d_i = W_{p_k} - Q_0 \qquad (3.19)$$

Then for any point feasible in (P2-i) we have

$$\sum^{p} QE_t \geq W_{p_k} - Q_0 = \sum_{t=1}^{p} d_t \qquad (3.20)$$

where the inequality follows from (3.14) and the equality from (3.19). Since constraint (3.20) implies (3.15), it follows that for any capacity expansion sequence which is feasible in problem (P2-i), the demand of problem (P3-i) will be satisfied for any period p (p=l, NT).

Inversely, for any capacity expansion sequence satisfying the demand of problem (P3-i) and for any time period p (p=l, NT), we have:

$$\sum_{t=1}^{p} QE_t \geq \sum_{r=1}^{p} d_r = W_{pk} - Q_0 \geq W_p - Q_0 \qquad (3.21)$$

where the first inequality follows from the feasibility of problem (P3-i) (constraint (3-15)), the equality from (3.19) and the second inequality from (3.16) and the definition of k in (3.18). Since (3.21) implies (3.14), it follows that any feasible point in (P3-i) corresponds to a feasible point in (P2-i).

Since the problems (P2-i) and (P3-i) have the same set of feasible solutions and they have the same objective function, they also have the same optimal solution. •

4. NLP Reformulation (Model Rl)

Theorem 3 indicates that if an algorithm is devised that decomposes the problem by first fixing the values of the flows (Wfo, $P_{t,}^{l}$, S_{y}^{l},) in such a way that all material balances (constraints (1.5) to (1.7)) are satisfied, then the rest of the problem can be solved as a sequence of independent lot sizing problems (P3-i), one for each process. In this case, the Krarup-Bilde reformulation (RLS1) can be used for each problem (P3-i) in order to solve it as a linear program. As indicated in the previous section in the description of problem (P3-i), the variables QE_{tr} denote "capacity production" and therefore correspond to the production variables x_t of model (LS). Then, in order to apply the reformulation, let us proceed as in (2.6) and disaggregate the capacity expansions by defining the variable $O/_{rT}$ as capacity expansion of process / in time period *t* in order to serve "capacity demand" *during* period *x* (T ^ *t)*. These variables correspond to the variables q^of model (RLS1); thus, similarly to (2.6) we have:

$$QE/r = \underset{x \geq t}{X} \; ®in \qquad /=1,NP \quad r=l,NT \qquad (4.1)$$

Moreover, similarly to (2.8) and (2.9), we now have the following constraints:

$$\sum_{\tau \leq t} \Phi_{i\tau t} = d_{it} \qquad z=l,NP \quad r=l,NT \qquad (4.2)$$

$$®in \;\wedge\; {}^{d}/x \;\; yit \qquad J'=1,NP \quad r=l,NT \quad \%\geq t \qquad (4.3)$$

Rather than using the above constraints in order to solve the lot sizing subproblems and then try to adjust the values of the flows within an iterative procedure, one can try to "build" this algorithm into the MRP model (PI) by including constraints (4.1) to (4.3) into this model. In this case, since the capacity demands d_{zr} are defined in terms of $m_{z\varsigma}$ and M_{zr} these must also be included as variables in the model while the definitions (3.11), (3.12) and (3.13) must be included as constraints. However, the *max* operators in these equations involve nondifferentiabilities. Therefore, we prefer to translate the equations (3.11), (3.12) and (3.13) into constraints that involve continuous and differentiate functions so as to be able to use the effective commercially available codes for smooth optimization. For this, we substitute the nondifferentiable constraint:

$$u = \max_{n=1,N} f_n \qquad (4.4)$$

where $f_n = f_n(x)$ are continuous and differentiable functions and $x \in \Re^K$, by the following set of differentiable constraints:

$$u \geq f_n(x) \qquad n = 1, N \qquad (4.5)$$

$$u \leq \sum_{n=1}^{N} \delta_n f_n(x) \qquad (4.6)$$

$$\sum_{n=1}^{N} \delta_n = 1 \qquad \text{with all } \delta_n \geq 0 \qquad (4.7)$$

According to (4.5), u must be at least equal to the *max* of f_n (n = 1,N). According to (4.6), u can be at most equal to the *max* of f_n (n = 1,N), if the corresponding multiplier (δ) is set to 1. Therefore, the only feasible solution of (4.5) - (4.7) is (4.4).

By incorporating the lot sizing constraints (4.1) to (4.3) into problem (PI) (where (1.8) and (1.9) are ignored) and by applying the transformation (4.5) to (4.7) to the equations (3.11) to (3.13), the first reformulation of the long range planning model corresponds to the following MINLP problem:

Reformulated Model R1

$$\max \quad NPV = -\sum_{i=1}^{NP}\sum_{t=1}^{NT}(a_{it}QP_{it} + p_{it}y_{it}) - \sum_{i=1}^{NP}\sum_{t=1}^{NT}\delta_{m_i t}W_{m_i t} \tag{1.1}$$

$$\bullet \sum_{l=1}^{NM}\sum_{j=1}^{NC}\sum_{t=1}^{NT}(V,!-\wedge,!)$$

s.t.

$$W_{kt} = \mu_{ik} W_{m_i t} \qquad ike L,-Mm/\} \qquad i = 1,NP \qquad t = 1,NT \tag{1.5}$$

$$\sum_{l=1}^{NM} P;!+ \sum_{k \in I(j)} {}^{TM}kt = \sum_{l=1}^{NN1} SJ, + \sum_{k \in O(j)} {}^{W}*/ \qquad j = 1,NC \qquad t=1,NT \tag{1.6}$$

$$\left.\begin{array}{l} a_{jt}^{l,L} \le P_{jt}^{l} \le a_{jt}^{l,U} \\ d_{jt}^{l,L} \le \xi_{jt}^{l} \le d_{jt}^{l,U} \end{array}\right\} \qquad j=1,NC \qquad t=1,NT \qquad l = 1,NM \tag{1.7}$$

$$QE_{it} = \sum_{\tau \ge t} \wedge rx \qquad i = 1,NP \qquad t=1,NT \tag{4.1}$$

$$\sum_{\tau \le t} \Phi_{i\tau t} = d_{it} \qquad i = 1,NP \qquad t=1,NT \tag{4.2}$$

$$\Phi_{it\tau} \leq d_{i\tau} \; y_{it} \qquad i = 1,NP \quad t = 1,NT \quad \tau \geq t \qquad (4.3)$$

$$\left.\begin{array}{r} m_{it} \geq W_{m_i t} - Q_{i,0} \\ m_{it} \leq v_{it} \, (W_{m_i t} - Q_{i,0}) \end{array}\right\} \qquad i = 1,NP \quad t = 1,NT \qquad (4.8)$$

$$\left.\begin{array}{l} M_{it} \geq M_{i,t-1} \, , \qquad M_{it} \geq m_{i,t-1} \\ M_{it} \leq \pi_{it} \, M_{i,t-1} + (1 - \pi_{it}) \, m_{i,t-1} \end{array}\right\} \qquad i = 1,NP \quad t = 1,NT \qquad (4.9)$$

$$\left.\begin{array}{r} d_{it} \geq m_{it} - M_{it} \\ d_{it} \leq \rho_{it} \, (m_{it} - M_{it}) \end{array}\right\} \qquad i = 1,NP \quad t = 1,NT \qquad (4.10)$$

$$y_{it} = 0 \text{ or } 1 \qquad i = 1,NP \quad t = 1,NT \qquad (1.10)$$

$$QE_{it}, \; W_{kt}, \; P_{jt}^{l}, \; S_{jt}^{l} \geq 0 \qquad (1.11)$$

$$m_{it}, \; M_{it}, \; d_{it}, \; \Phi_{it\tau} \geq 0 \, , \qquad m_{i0} = M_{i0} = 0 \, , \qquad 0 \leq v_{it}, \; \pi_{it}, \; \rho_{it} \leq 1 \qquad (4.11)$$

In the above formulation, constraints (4.8), (4.9) and (4.10) are nonlinear and they serve to explicitly evaluate the demands for the capacity expansions as a function of the flows (W_{kt}); they are expressing relations (3.11), (3.12) and (3.13), respectively. Notice that constraints (4.8), (4.9) and (4.10) are nonconvex since their second corresponding inequalities involve bilinear terms. Therefore, model (R1) corresponds to a nonconvex MINLP problem. However, this nonconvex problem has the following interesting properties:

Theorem 4: For any fixed value of flows (Wfo, P^{l}_{jt}, S^{l}_{jt}), the solution of the rest of model (Rl) yields integer values for the variables y_{it} when these are relaxed in the interval [0,1].

Proof: When the flows are fixed, constraints (4.8) - (4.10) become linear and they uniquely determine the demands $d_{i\tau}$. Then, the problem decomposes into as many subproblems as processes. By relaxing the integrality conditions, each subproblem is as follows:

$$\max \quad - \sum_{t=1}^{NT} (\alpha_{it} QE_{it} + \beta_{it} y_{it})$$

s.t.

$$QE_{it} = \sum_{\tau \geq t} \Phi_{it\tau} \qquad t = 1,NT$$

$$\sum_{\tau \leq t} \Phi_{i\tau t} = d_{it} \qquad \tau = 1,NT \qquad \textbf{(Model P4-I)}$$

$$\Phi_{it\tau} \leq d_{i\tau} y_{it} \qquad \tau = 1,NT \quad \tau \geq t$$

$$\Phi_{it\tau} \geq 0, \qquad 0 \leq y_{it} \leq 1$$

Each subproblem (P4-i), corresponds to the Krarup-Bilde formulation (RLSl) of the lot sizing problem (P2-i). Hence, from Theorem 2, (P4-i) will give natural 0-1 solutions. •

Theorem 5: Solving model (Rl) with the variables y_{it} being relaxed in the interval [0, 1], yields integral values for the y-variables.

Proof: From Theorem 4, for any fixed value of the flows (Wfo, Py„ Sy,) and with the integrality requirements of the variables y^ being relaxed, the rest of model (Rl) yields 0 or 1 values for the y-variables. Therefore, this is also true for the optimal value of (Wfo, Py„ Sj$_r$).

●

It follows from Theorem 5 that the integrality requirements (1.10) of model (Rl) can be relaxed to $0 \le y_{it} \le 1$ (/ = 1,NP t = 1,NT). Therefore, model (Rl) can be solved as an NLP. The next corollary is an immediate consequence of Theorem 4 and the role of the complicating variables in generalized Benders decomposition (Geoffrion, 1972).

Corollary 5.1: If the generalized Benders decomposition method is applied to model (Rl), with the flows (Wfo, Py„ Sy,) being the complicating variables, the subproblems (P4-i) have natural 0-1 solutions when solved as linear programs.

An algorithm using Generalized Benders Decomposition

In order to take advantage of the special properties discussed in the previous paragraph, the variables of the multiperiod MINLP model (Rl) are partitioned as follows:

a) Complicating variables for the master problem:

$$\mathbf{v} = [\mathbf{W}_{4|},\ \mathbf{S},!,\ \mathbf{P_y J}]$$

b) Remaining variables for the MINLP subproblem:

$$\mathbf{u} = [\ y_{it},\ \mathbf{QE}_{/r},\ O_{in}\ ,\ m_{it},\ M_{it},\ d_{it},\ v_{it},\ p_{it},\ n_{in}\ ]$$

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

Algorithm:

Step 1. Select a value (v*) for the complicating variables so that mass balances of model (Rl) are satisfied (this can be done by finding a feasible solution to the set of equations (1.5),(1.6) and (1.7)); set NPV^ = +~, NPV^ = -«,/? = 1.

Step 2. a) By fixing the variables v^, problem (Rl) becomes a nonlinear program (NLP-u) in terms of the variables u. However, since equations (4.8) to (4.10) can be *a priori* solved for m/f, M/f, d/f, v/f, rc/j, and p/j, the solution to the multiperiod MINLP problem (Rl) can be obtained through the LP subproblems (P4-i) that determine the remaining variables u^ and NPV^. In addition, once these LP's are solved, the primal solution to (NLP-u) is known and can be used to produce the dual solution either by using an NLP code or by analytically solving the Kuhn-Tucker optimality conditions for problem (Rl).

b) Update the lower bound by setting NPV^ = max {NPV^, NPV^}

Step 3. To determine new values v^+1 for the complicating variables and an upper bound to NPV, solve the *linear programming* master problem:

$$NPV^U = \max \ \mu, \qquad (4.12)$$

s.t.

$$\mu \leq L^r(v) \qquad r = 1,R \qquad (4.13)$$

$$W_{kt} = \mu_{ik} W_{m_i t} \qquad k \in L_i \ Mm/\} \qquad i = 1,NP \quad t = 1,NT \qquad (1.5)$$

$$\sum_{l=1}^{NM} P_{jt}^{l} + \sum_{k \in I(j)} W_{kt} = \sum_{l=1}^{NM} S_{jt}^{l} + \sum_{k \in O(j)} W_{kt} \quad j = 1,NC \quad t = 1,NT \qquad (1.6)$$

$$\left.\begin{array}{l} a_{jt}^{l,L} \leq P_{jt}^{l} \leq a_{jt}^{l,U} \\ d_{jt}^{l,L} \leq S_{jt}^{l} \leq d_{jt}^{l,U} \end{array}\right\} \quad j=1,NC \quad t = 1,NT \quad l = 1,NM \qquad (1.7)$$

$$\mu \in \Re^{1} \qquad (4.14)$$

where the Lagrangian

$$L^{r}(v) = NPV(v, u^{r}) \qquad (4.15)$$

$$+ \sum_{i=1}^{NP} \sum_{t=1}^{NT} \left[\sigma_{it}^{1,r} \left(m_{it}^{r} - v_{it} \left(W_{m_i t}^{r} - Q_{i,0} \right) \right) + \sigma_{it}^{2,r} \left(W_{m_i t}^{r} - Q_{i,0} - m_{it}^{r} \right) \right]$$

and NPV(v, u^r) is the NPV function with all variables u^r fixed and $\sigma_{it}^{1,r}$, $\sigma_{it}^{2,r}$ are the Lagrange multipliers of the first and second constraints of (4.8) in the solution of (NLP-u) in Step 2.

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

As mentioned, in Step 2, the equations (4.8), (4.9) and (4.10) can be solved *a priori* by simply using expressions (3.11) to (3.13). This leads to an LP which can be decomposed into a sequence of independent LP's (one lot sizing problem (P4-i) for each process *i*). Therefore, the global optimum will always be attained for the Benders subproblems. However, the nonconvexities in the NLP model (Rl) (constraints (4.3) and (4.8) to (4.10)) do not guarantee rigorous lower bounds in the master problem which may therefore lead to local optima. We are interested in finding the *exact* solution of the problem and, for that reason, we will present a different reformulation which can be solved to global optimality. Furthermore, in this reformulation it will also be possible to specify limits on the number of expansions and the capital investment (constraints (1.8) and (1.9)), as well as finite bounds for the capacity expansions in constraints (1.2) which were ignored in model (Rl). This is described in the next section.

5. Second Reformulation of the Long Range Planning model

In the reformulation of the planning model presented in the previous section, we expressed the demands for the capacity expansions as functions of the flows in the network (equations (3.11), (3.12) and (3.13)). Since this has led to nonconvexities (constraints (4.3) and (4.8) to (4.10)), the alternative suggested here is to *a priori* (over)estimate bounds for the capacity expansions and to use a linear model. It is easy to find upper bounds for the expansions themselves as it will be shown later. However, we cannot simply use these bounds to overestimate the demands for the capacity expansions (d/f in (4.3)) in the Krarup-Bilde reformulation of the lot sizing problem (model (RLS1)), as this would force the expansions to be equal to the overestimated upper bounds (because of (4.3)). For that reason, we will make use of Martin's reformulation (model (RLS2)) although it contains more variables and constraints. First, we will introduce extra variables, $(p\wedge$ in the original planning model to denote capacity expansion of plant i made in period *t* in order to serve production requirements *up to* period x $(x \geq i)$. These variables correspond to the variables $\backslash_n$ of model (RLS2) and therefore they have to satisfy the following constraints:

$$QE_{it} \geq \varphi_{i\tau t} \qquad i = 1,NP \quad \tau = 1,NT \quad t \geq \tau \qquad (5.1)$$

$$\varphi_{i\tau t} \leq C_{i\tau} \; y_{i\tau} \qquad i = 1,NP \quad \tau = 1,NT \quad t \geq \tau \qquad (5.2)$$

which are completely analogous to (2.12) **and** (2.13), respectively. Furthermore, from the definition: $C_{i\tau} = \sum_{t=1}^{\tau}$ [illegible] in conjunction to (3.21), it follows that **a** valid relaxation of **(2.14)** is the following constraint:

$$\sum_{\tau=1}^{t} \varphi_{i\tau t} \ast W_{m,\tau} - Q$$ [illegible] $$\qquad i = 1,NP \quad t = 1,NT \qquad (5.3)$$

By including constraints (5.1), (5.2) and (5.3) in model (PI), the second reformulation of the long range planning model is then the following multiperiod MILP model:

Reformulated Model R2

$$\max \quad NPV = -\sum_{i=1}^{NP}\sum_{t=1}^{NT} (\alpha_{it} QE_{it} + \beta_{it} y_{it}) - \sum_{i=1}^{NP}\sum_{t=1}^{NT} \delta_{Wit} W_{mt} + \sum_{l=1}^{NM}\sum_{j=1}^{NC}\sum_{t=1}^{NT} (\gamma_{jt}^{l} S_{jt}^{l} - \Gamma_{jt}^{l} P_{jt}^{l}) \qquad (1.1)$$

s.t.

$$y_{it}\, QE_{it}^{L} \leq QE_{it} \leq QE_{it}^{U}\, y_{it} \qquad i = 1,NP, \quad t = 1,NT \qquad (1.2)$$

^{w}/tr = N*^{w}/»|* teL/Mm,} / = 1,NP t = 1,NT (1.5)

NM NM
Z ^{p} 7 7 $^{l+}$ X w*, = X ^{s} ; / $^{l+}$ Z ^{w}*/ ; = i,NC r=i,NT (1.6)
/ = 1 ***k€l(j)*** ***1=1*** ***keO{j)***

$a_{[jt}^{l,L}$ < P >' _ a >' ^{l} < ^{l,U} \ ;=1,NC r, = 1,NT / = 1,NM (1.7)
d$_{jt}$ – –$_{jt}$ – –$_{jt}$

NT
X y$_{if}$ ≤NEXP(O 16 I'C {1,2, ... NP} (1.8)
t = 1

$$\sum_{i=1}^{NP} (a,-, QE;,+ P;, y,-,) \le CI(r)$$ *te TQ* {1,2, ... NT} (1.9)

QE/$_{r}$ ≥ <p/$_{n}$ i=1,NP r=1,NT $z \ge t$ (5.1)

φ$_{irt}$ ^ Qri y« /=1,NP r=1,NT %>t (5.2)

r
X q>$_{Jtr}$ ≥ W$_{mt f}$ - Q$_{j0}$ i = **1,NP** r = 1,NT (5.3)
t=1

y_{it} = 0 or 1 i = **1.NP** t= 1,NT (1.10)

$$QE_{it},\ W_{kt},\ P_{jt}^{l},\ S_{jt}^{l} \geq 0 \qquad (1.11)$$

$$\varphi_{it\tau} \geq 0 \qquad i = 1,NP \quad t = 1,NT \quad \tau \geq t \qquad (5.4)$$

The model contains the definition of the net present value (equation (1.1)), the variable lower and upper bounds on the capacity expansions (constraints (1.2)) and the material balances (constraints (1.5) to (1.7)). In contrast to model (R1), the constraints on the number of expansions (1.8) and the budget constraints (1.9) can now be included. Constraint (5.1) expresses the obvious fact that the capacity expansion $\varphi_{it\tau}$ in period t to satisfy demand up to period τ cannot exceed the capacity expansion QE_{it} during period t. Constraint (5.3) is now used instead of constraint (1.4) and it implies that capacity cannot be devoted to production during time period t unless it was previously acquired for this purpose.

The upper bounds $C_{it\tau}$ for the capacity expansions in (5.2) must be postulated *a priori* and they are not known. However, valid upper bounds for the capacity expansions can be evaluated by maximizing the individual production rate of each process i (i = 1, NP) for each time period t (t = 1, NT) by solving the following linear program:

$$\omega_{it} = \max\ W_{m_i t} \qquad (5.5)$$

st.

$$W_{kt} = \mu_{ik} W_{m_i t} \qquad k \in L_i \backslash \{m_i\} \qquad (1.5)$$

$$\left.\begin{array}{l} a_{jt}^{l,L} \leq P_{jt}^{l} \leq a_{jt}^{l,U} \\ d_{jt}^{l,L} \leq S_{jt}^{l} \leq d_{jt}^{l,U} \end{array}\right\} \qquad j = 1,NC \quad l = 1,NM \qquad (1.6)$$

$$\sum_{l=1}^{NM} P_{jt}^{l} + \sum_{k \in I(j)} W_{kt} = \sum_{l=1}^{NM} S_{jt}^{l} + \sum_{k \in O(j)} W_{kt} \qquad j=1,NC \qquad (1.?)$$

$$W_{kt},\ P_{jt}^{l},\ S_{jt}^{l} \geq 0 \qquad (1.11)$$

In this LP model the flow of the main product of a process is maximized subject to mass balances around the entire network. If finite bounds are specified for the inequalities (1.6), the solution will always be bounded. In addition, this LP has special structure. It is a "processing network" for which special solution algorithms are available (Koene, 1983; McBride, 1985; Chen and Enguist, 1988).

Then the upper bounds for the capacity expansions are:

$$C_{in} = \max \{ 0, \min \{ QE_{i}^{U}, \max_{\tau = t,\ldots T} co^{\wedge} \} - Q_{io} \} \qquad (5.6)$$

The *algorithm* to solve the reformulated planning model (R2) is then as follows:

Step 1: Solve (NP)(NT) processing network problems of the form (5.5).

Step 2: Calculate capacity expansion upper bounds through (5.6).

Step 3: Solve the reformulated MILP model (R2).

The following theorem can be established for the tightness of the LP relaxation in Step 3:

Theorem 6. The optimal cost of the linear programming relaxation of model (R2) is not greater than the optimal cost of the linear programming relaxation of model (PI), and it may be strictly less.

Proof: First we observe that constraints (1.3) can be used to solve for the variables Q_{ir} of model (PI) and then both these variables and constraints can be eliminated with the provision that (1.4) is changed to:

$$Q_{i0} + \sum_{t=1}^{t} CP_{ft} * W_{m,f} \qquad (1.4')$$

Now with the exception of (1.4') the rest of the constraints of model (PI) also appear in model (R2). But from (5.1):

$$Q_{i0} + \sum_{1=1}^{t} OP_{ix} * Q_{i0} + \sum_{T=1}^{t} P_{i\tau}$$

This means that (1.4') is implied by (5.3). It follows that every solution to the linear programming relaxation of model (R2) gives rise to a feasible solution of the linear programming relaxation of model (PI). This shows that the optimal net present value of the linear programming relaxation of (R2) cannot be greater than that of the linear programming relaxation of (PI). The examples of Section 6 show that the linear programming relaxation of (R2) can yield a strictly smaller upper bound, thus completing the proof. •

The theorem indicates that the new formulation of model (R2) is at least as accurate as that of model (PI), but nothing is said about the degree of its accuracy. Note, however, that, if the overestimated capacity expansion upper bounds (the ones from (5.6)) are equal to the

optimal values of the capacity expansions, the relaxation will yield an integral solution since the formulation of the lot sizing substructures that has been used satisfies Theorem 2. We can then expect that the closer the overestimated values to the optimal solutions, the more accurate the relaxation will be. Moreover, we anticipate that, for those processes that are profitable, the optimum will be to run them at the highest possible operating level, and therefore the upper bounds from (5.6) will be equal to the optimal values for the capacity expansions in which case the relaxation of model (R2) will be close to an integer solution.

It should be mentioned here that, while the relaxation becomes more accurate, the number of continuous variables and constraints of the model is at the same time increased, but at least this increase is polynomial in the number of time periods (NT) and the number of processes (NP). In fact, we are adding (NP)(NT)2(NT+l)/2 new variables and $(NP)(NT)^2(NT+1)-(NP)(NT)$ new constraints in the original model (PI).

Relation to Strong Cutting Plane Methods and to the Disaggregation of Fixed Charge Network Problems

The idea of the strong cutting plane approach to integer programming 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 (Crowder, Johnson and Padberg, 1983; Van Roy and Wolsey, 1987). 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.

Martin (1987b) suggested that for some problems the separation problem can be incorporated into the original problem by adding more constraints and variables. In this way, the separation problem is dynamically being solved and no iteration is needed. What we have done, by using Martin's reformulation for the lot sizing problem, is essentially equivalent to including in the model an approximate – due to the overestimation of the demands – solution to the separation problem for the lot sizing substructures. Then, the reformulation can be regarded as an application of strong cutting plane techniques based on Martin's results for the solution of the separation problem of the lot sizing.

Also related to our approach is the work of Rardin and Choe (1979) who described alternative formulations for fixed charge network flow problems and showed that a multicommodity formulation of a single commodity flow problem can yield tighter linear programming relaxations. In this formulation, a flow (f) along an arc associated with a fixed charge is disaggregated into new variables which are as many as the different destinations in the network which are satisfied by the flow (f). Fig. 4 is a representation of constraints (1.3) of model (P1). Since the capacity expansions are associated with fixed charges in the objective function, we have a fixed charge network substructure in the model. Therefore the disaggregation of variables in models (R1) and (R2) is in the spirit of the recommendations of Rardin and Choe although the complication that arises here is that the demands for the nodes of the fixed charge network are not explicitly given.

6. Computational Results

Three planning examples will be considered as shown in Table I. These three examples will be considered in four, three and three different scenarios, respectively; a total of 10 test problems. The different scenarios differ in the numerical values of the parameters, and in the presence or not of constraints on the number of expansions (1.8) and budget limitations (1.9). The examples are from Sahinidis *et al.* (1989) with the only exception of examples 1/1 (a) and 2/l(a) which have been derived from 1/1 and 2/1, respectively, by excluding constraints (1.8) and (1.9). All the test problems were solved through the modelling system GAMS (Brooke, Kendrick and Meeraus, 1988).

Computational results with the NLP reformulation (Rl)

Theorem 5 sugges:> that the reformulated model can be solved as an NLP. However, constraints (4.3) and tht cond constraints of (4.8), (4.9), and (4.10) are nonconvex and in the examples solved, the NLP code used (MINOS, see Murtagh and Saunders, 1986) was trapped in suboptimal (still integer, of course) solutions. This is shown in Table II for all of our test problems that do not involve constraints on the number of expansions (1.8) and budget limitations (1.9) and can be therefore solved using model (Rl). Moreover, notice that these solutions were usually far from the optimum. Clearly, the performance of this procedure depends on the starting point used.

When Benders decomposition was applied, convergence was achieved in a relatively small number of iterations as shown in the summary of the results in Table II. It is interesting to note that the solution obtained was usually quite close to the global optimum independently of the starting point used. Since only few iterations are required - each iteration consisting of solving small LP's - the proposed procedure using Benders decomposition seems to be a very effective approach to obtain feasible (sub)optimal solutions to the long range planning problem. The reason for which Benders decomposition does not converge to the global optimum - even though the subproblems and the master problems are linear problems - is because, due to the nonconvexities of model (Rl), the lagrangian constraints (4.13) of the master problem cut off part of the feasible space of the original problem. The performance of Benders decomposition in the case of nonconvexities is analyzed by Sahinidis and Grossmann (1989).

Computational Results with the MILP Reformulation (R2)

Computational results using branch and bound to solve the MILP reformulation (R2) of our 10 test problems are shown in Tables **in** through VII.

Table **in** shows the effect of the reformulation on th6 linear programming relaxation of the problem. The relaxation is tighter in the sense that the gap between the integer solution and the relaxation is considerably reduced.

Table IV shows the effect of the reformulation on the computational requirements of the solution. Branch and bound has now to examine a much smaller number of nodes. Although this has no effect to the CPU requirements for the small problems, note that the CPU times for the larger examples are up to ont order of magnitude lower than those with the conventional model (PI). We can also see that the reformulation makes possible the solution of one problem which could not be solved before.

The CPU times in Table IV include the time needed to solve the linear programs to evaluate the upper bounds for the reformulation variables. However, this time is small when compared to the total. For example, for the largest problem (Example 3) this is less than 10 seconds for all the 156 LP's (using MINOS and *not* any specialized algorithm). For the rest of the problems, this time is almost zero. Some statistics for these LP's are shown in Table V.

'•The effect of the reformulation on the problem size is shown in Table VI. The number of continuous variables and constraints is increased, but as pointed out in Section 5 this increase is polynomial in size.

Finally, it is interesting to compare the proposed reformulation (R2) with the case where improved upper bounds (the ones obtained by solving (5.5)) are used for the expansions in the original model (PI). McKeown and Ragsdale (1988) have actually shown that using improved upper bounds can have dramatic effects on the solution of some integer programs. What will happen if instead of using the reformulated model (R2), we simply use the originally proposed (Model (PI)) but with improved upper bounds:

$$\widehat{QE}^{\wedge} = \max \{ 0, \min \{ QE_{i-r}, \max_{T \geq} {}^{\wedge} co_{jT} \} - \dot{Q}_{i0} \} \tag{6.1}$$

in the variable upper bound constraints (1.2) ? The answer is shown in Table VII, from which it is clear that this approach may or may not lead to improvements in the solution time of our problem. In fact, it led to an even worse (!) performance for some of our larger examples. This should not lead to the false conclusion that it is not worth to improve the bounds for the long range planning problem. It only means that the bounds used for solving the e · ginal model (PI) were already tight enough and that small changes in them may affect the solution requirements of branch and bound slightly positively or negatively - depending on the effect on the branching procedure and on the iterations of the Simplex method. In fact, when computational experiments were performed with Model (PI) using very large numbers for these bounds, the solution requirements were one and two orders of magnitude more than those reported in Table VII.

1. Conclusions

The results of this paper have been based on the observation that the long range planning problem for capacity expansion of a chemical complex can be solved as a series of independent lot sizing problems when the flows in the network (production, purchases and sales) are fixed. To take advantage of this property, a variable disaggregation technique has

been proposed that led to two different ways of reformulating the conventional MILP model. The first reformulation led to an MINLP that can be solved as an NLP and an efficient way to take advantage of its special properties was proposed in order to quickly find a good suboptimal solution. However, due to the presence of nonconvexities in this model, there is no guarantee that its global optimum will always be found. Furthermore, limits on expansions and capital investment cannot be considered with this formulation. To overcome all these difficulties, a second reformulation was proposed which led to an MILP with tighter linear programming relaxation which for large problems led to solution time reductions of up to one order of magnitude, when compared to the solution requirements of the conventional formulation of the planning problem. Regarding the implications of this work on future research, we should point out that the planning problems mentioned in the introduction of this paper have much in common with the problem we have been looking at. We therefore anticipate that similar reformulations will be beneficial for solving these problems more efficiently.

Acknowledgments

The authors would like to acknowledge partial financial support from the National Science Foundation under Grant CPE-8351237. Access to the IBM-3090 computer at the Cornell Theory Center is also gratefully acknowledged.

REFERENCES

Akileswaran, V., G.B. Hazen, and T.L. Morin. 1983. "Complexity of the Project Sequencing Problem", *Operations Research,* 31(4), 772-778.

Armstrong, R.D., and C.E. Willis. 1977. "Simultaneous Investment and Allocation Decisions Applied to Water Planning", *Management Science,* 23(10), 1080-1088.

Balas, E. 1985. "Disjunctive Programming and a Hierarchy of Relaxations for Discrete Optimization Problems", *SIAMJ. Alg. Disc. Math.,* 6(3), 466-486.

Barany, L, TJ. Van Roy, and L.A. Wolsey. 1984. "Strong Formulations for Multi-item Capacitated Lot Sizing", *Management Science,* 30(10), 1255-1261.

Bergendahl, G. 1969. "A Combined Linear and Dynamic Programming Model for Interdependent Road Investment Planning", *Transportation Research,* 2, 211-228.

Brooke, A., D. Kendrick and A. Meeraus. 1988. *"GAMS - A User's Guide",* The Scientific Press, Redwood City.

Chen, C.J., and M. Enguist. 1988. "A Primal Simplex Approach to Pure Processing Networks", *Management Science,* 32(12), 1582-1598.

Crowder, H., E.L. Johnson, and M. Padberg. 1983. "Solving Large-Scale Zero-One Linear Programming Problems," *Operations Research,* 31, 803.

Eppen, G.D., and R.K. Martin. 1987. "Solving Multi-Item Capacitated Lot-Sizing Problems Using Variable Redefinition", *Operations Research,* 35(6), 832-848.

Florian, M_M J.K. Lenstra, and A.H.G. Rinnooy Kan. 1980. "Deterministic Production Planning: Algorithms and Complexity", *Management Science,* 26(7), 669-679.

Fong, "C.O., and V. Srinivasan. 1981a. "The Multiregion Dynamic Capacity Expansion Problem", Pan I, *Operations Research,* 29(4), 787-799.

Fong, CO., and V. Srinivasan. 1981b. "The Multiregion Dynamic Capacity Expansion Problem[1]', Part II, *Operations Research*, 29(4), 800-816.

Geoffrion, A.M. 1972. "Generalized Benders Decomposition," *JOTA*, 10,4.

Goreux, L.M., and A.S. Manne (eds.). 1973. *"Multi-level Planning: Case Studies in Mexico"*, North-Holland, Amsterdam.

Grossmann, I.E., and J. Santibanez. 1980. " Application of Mixed-Integer Linear Programming in Process Synthesis," *Computers and Chemical Engineering*, 4,205.

Himmelblau, D.M., and T.C. Bickel. 1980. "Optimal Expansion of a Hydrodesulfurization Process," *Computers and Chemical Engineering*, 4, 101.

IBM, Mathematical Programming System Extended / 370 (MPSX / 370). 1979. Basic Reference Manual. Technical Report, IBM, White Plains, New York .

Jeroslow, R.G., and J.K. Lowe. 1984. "Modelling with Integer Variables", *Mathematical Programming Study*, 22, 167-184.

Jeroslow, R.G., and J.K. Lowe. 1985. "Experimental Results on the New Techniques for Integer Programming Formulations", 7. *OpL Res. Soc.f* 36(5), 393-403.

Jimenez, A.G., and D.F. Rudd. 1987. "Use of a Recursive Mixed-Integer Programming Model to Detect an Optimal Integration Sequence for the Mexican Petrochemical Industry," *Computers and Chemical Engineering*, 3, 291.

Koene, J. 1983. *"Minimal cost flow in processing networks: a primal approach"*, Centrum voor Wiskunde en Informatica, Amsterdam.

Krarup, J., and O. Bilde. 1977. "Plant Location, Set Covering and Economic Lot Size: An O(mn) Algorithm for Structured Problems", in L. Collatz et al. (eds.), *"Optimierung bei graphentheoretischen und ganzzahligen Problemen"*, International Series of Numerical Mathematics, 36,155-180, Birkhäuser Verlag, Basel.

Manne, A.S. (ed.). 1967. *"Investments for Capacity Expansion"*, The MIT Press, Cambridge, MA .

Martin, R.K. 1987a. "Generating Alternative Mixed-Integer Programming Models Using Variable Redefinition", *Operations Research*, 35(6), 820-831.

Martin, R.K. 1987b. "Using Separation Algorithms to Generate Mixed Integer Model Reformulations", Paper presented at the *TIMS/ORSA meeting*, (April 1987).

McBride, R.D. 1985. "Solving Embedded Generalized Network Problems", *European Journal of Operational Research*, **21, 82-92.**

McKeown, P.G., and C.T. Ragsdale. 1988. "Using Preprocessing and Stronger Formulations to Solve Large Linear Fixed Charge Problems", Paper presented at the *TIMS/ORSA meeting*, Washington, D.C. (April 1988).

Merges, M.J., and H.B. Mutlu. 1988. "A Linear Programming Model for Determining the Optimum Multi-Period Strategy for the Acquisition and Allocation of Computing Systems", Paper presented at the *TIMS/ORSA meeting*, Washington, D.C. (April 1988).

Minoux, M. 1987. "Network Synthesis and Dynamic Network Optimization", *Annals of Discrete Mathematics*, **31, 283-324.**

Murtagh, B.A., and M.A. Saunders. 1986. *"MINOS 5.0 User's Guide"*, Technical Report SOL 83-20, Systems Optimization Laboratory, Dept. of Operations Research, Stanford University, CA.

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

Noonan, F., and R.J. Giglio. 1977. "Planning Electric Power Generation: A Nonlinear * Mixed Integer Model Employing Benders Decomposition", *Management Science*, 23(9), 946-956.

Pochet, Y., and L.A. Wolsey. 1988. "Lot-Size Models with Backlogging: Strong Reformulations and Cutting Planes", *Mathematical Programming*, **40**(3), 317-335.

Rardin, R.L., and U. Choe. 1979. *"Tighter Relaxations of Fixed Charge Network Flow Problems"*, Georgia Institute of Technology, Industrial and Systems Engineering Report Series #J-79-18, Atlanta.

Sahinidis, N.V., and I.E. Grossmann. 1989. "Some Theoretical and Computational Issues in Generalized Benders Decomposition", *in preparation*.

Sahinidis, N.V., I.E. Grossmann, R. Fornari and M. Chathrathi. 1989. "Long Range Planning Model for the Chemical Process Industries", *Computers and Chemical Engineering*, accepted for publication.

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

Van Roy, T.J., and L.A. Wolsey. 1987. "Solving Mixed Integer Programs by Automatic Reformulation," *Operations Research*, **35**(1), 45-57.

Wagner, H.M., and T.M. Whitin. 1958. "Dynamic Version of the Economic Lot Size Model", *Management Science*, **5**, 89-96.

Zangwill, W. I. 1968. "Minimum Concave Cost Flows in Certain Networks", *Management Science*, **14**(7), 429-450.

LIST OF TABLES

Table I. The example problems.

Table EL Results with the Nonlinear reformulation.

Table IIL Effect of the MTTP reformulation on the Linear Programming Relaxation.

Table IV. Effect of the MILP reformulation on the solution of the MILP([a]).

Table V. Size and number of linear programs solved to obtain upper bounds.

Table VI. Effect of the MILP reformulation on the problem size.

Table VII. Effect of improved bounds on MILP solution([a]) (no reformulation).

Table I. The example problems.

Example / Scenario	Processes	Time Periods	Chemicals
1/1, l/l(a), 1/2,1/3	3	3	3
2/l,2/l(a),2/2	10	* 4	6
3/l(a),3/l(b),3/2	38	4	25

Table II. Results with the Nonlinear reformulation.

Example / Scenario	Global optimum^	Minos 5.2		Generalized Benders Decomposition		
		Solution found	Time (sec)(b)	Solution found	Iterations	Time(sec)<b>'<c>
1/Ka)	1,775	1,118	0.3	1,775	1	0.2
2/l(a)	51,450	0	3.6	51,450	3	0.9
3/l(a)	529.8	113	29.8	442	8	8.7

(a) Found by solving model (PI).

(b) IBM-3090.

(c) Minos 5.2 was used for solving the LP master problems and the subproblems.

Table III. Effect of the MILP reformulation on the Linear Programming Relaxation.

Example / Scenario	Integer optimum Z_{IP}	Initial Model: Relaxation optimum Z_R	Initial Model: Gap $\frac{Z_R}{Z_{IP}} \times 100$	Reformulation: Relaxation optimum Z_R^R	Reformulation: Gap $\frac{Z_R^R}{Z_{IP}} \times 100$	Reformulation: Gap reduction $\frac{Z_R - Z_R^R}{Z_R - Z_{IP}} \times 100$
1/1	1,697	1,898	111.8	1,744	102.8	77
1/1(a)	1,775	1,932	108.8	1,775	100.0	100
1/2	1,063	1,246	117.3	1,099	103.4	80
1/3	2,235	2,540	113.7	2,305	103.1	77
2/1	51,031	51,207	100.3	51,117	100.2	51
2/1(a)	51,450	51,837	100.8	51,481	100.1	92
2/2	45,248	46,540	102.9	46,370	102.5	13
3/1	529.8	648.6	122.5	621	117.2	23
3/2	529.8	631	119.1	598	112.9	33

Table IV. Effect of the MILP reformulation on the solution of the MILP([a]).

Example / Scenario	Initial Model #nodes	Initial Model iterations	Initial Model time (sec)	Reformulation #nodes	Reformulation iterations	Reformulation **timeO[5])(sec)**
1/1	10	93	0.6	3	113	0.6
1/Ka)	14	93	0.6	1	96	0.6
1/2	11	85	0.6	3	104	0.6
1/3	11	86	0.6	5	120	0.6
2/1	37	439	1.7	14	590	1.9
2/l(a)	1,064	2,862	10.7	17	544	2
2/2	1,272	6,305	21.8	23	916	2.7
3/l(a)	NA<[C]>	>356,609<[c]>	>5,520<[c])	1,516	14,323	222
3/l(b)	28,696	134,440	2,100	1,037	12,329	192
3/2	4,530	32,713	540	1,164	20,503	324

(a) MPSX-MIP/370 computer code used on IBM-3090.

(b) Includes LP computations for upper bounds of capacities using MINOS 5.1.

([c]) Procedure terminated with a lower bound of 529.8 and an upper bound of 561.

Table V. Size and number of linear programs solved to obtain upper bounds.

Example	Rows	Variables	Nonzeroes	# problems solved
1	7	9	17	9
2	17	40	48	40
3	83	127	236	152

Table VI. Effect of the MILP reformulation on the problem size.

Example / Scenario	Initial Model: Constraints	Initial Model: Variables Total	Initial Model: Variables Integer	Initial Model: Nonzeroes	Reformulation: Constraints	Reformulation: Variables Total	Reformulation: Variables Integer	Reformulation: Nonzeroes
1/1,1/2,1/3	49	55	9	160	76	64	9	217
l/l(a)	46	55	9	142	73	64	9	199
2/1	195	225	40	639	355	285	40	989
2/l(a)	185	225	40	599	345	285	40	949
2/2	199	225	40	719	359	285	40	1,069
3/l(a)	785	961	152	2,551	1,431	1,189	152	4,033
3/Kb)	823	961	152	2,703	1,469	1,189	152	4,185
3/2	827	961	152	3,007	1,473	1,189	152	4,489

Table VII. Effect of improved bounds on MILP solution[(a)] (no reformulation).

Example / Scenario	Relaxation optimum	# nodes	# iterations	time (sec)
1/1	1,786.	7	72	0.6
1/1(a)	1,786	5	66	0.6
1/2	1,134	8	74	0.6
1/3	2,373	9	80	0.6
2/1	51,206	37	471	1.6
2/2(a)	51,837	1,064	2,789	10.5
2/2	46,537	1,273	6,035	24.5
3/1(a)	629.5	44,005	318,479	3,780
3/1(b)	629.5	28,443	246,210	3,120
3/2	608.03	4,094	39,830	450

(a) MPSX-MIP/370 computer code, used on IBM-3090.

List of Figures

Fig. 1 Flow Diagram of a Chemical Complex

Fig. 2 Optimum Network Configuration

Fig. 3 Lot Sizing Model Representation:
(a) prior to reformulation
(b) after reformulation

Fig. 4 Fixed charge network
for capacity expansion

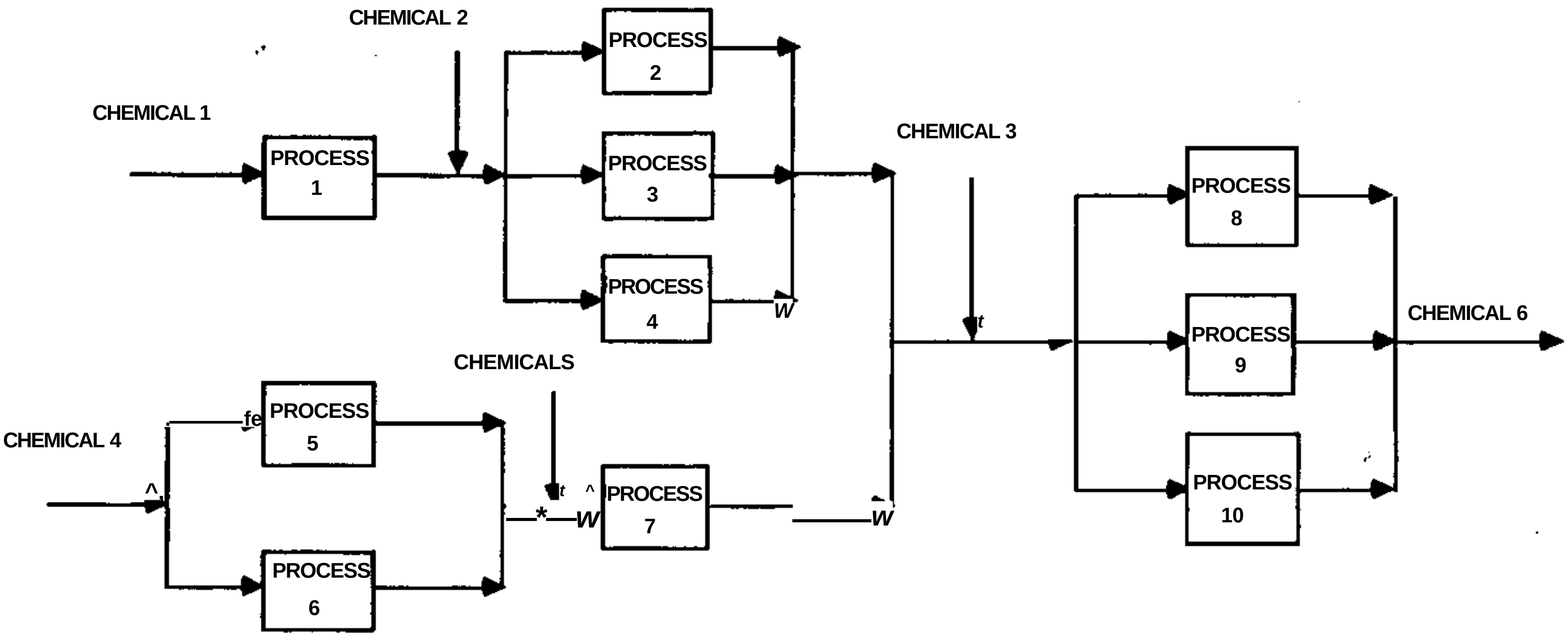

Fig. 1 Flow Diagram of a Chemical Complex

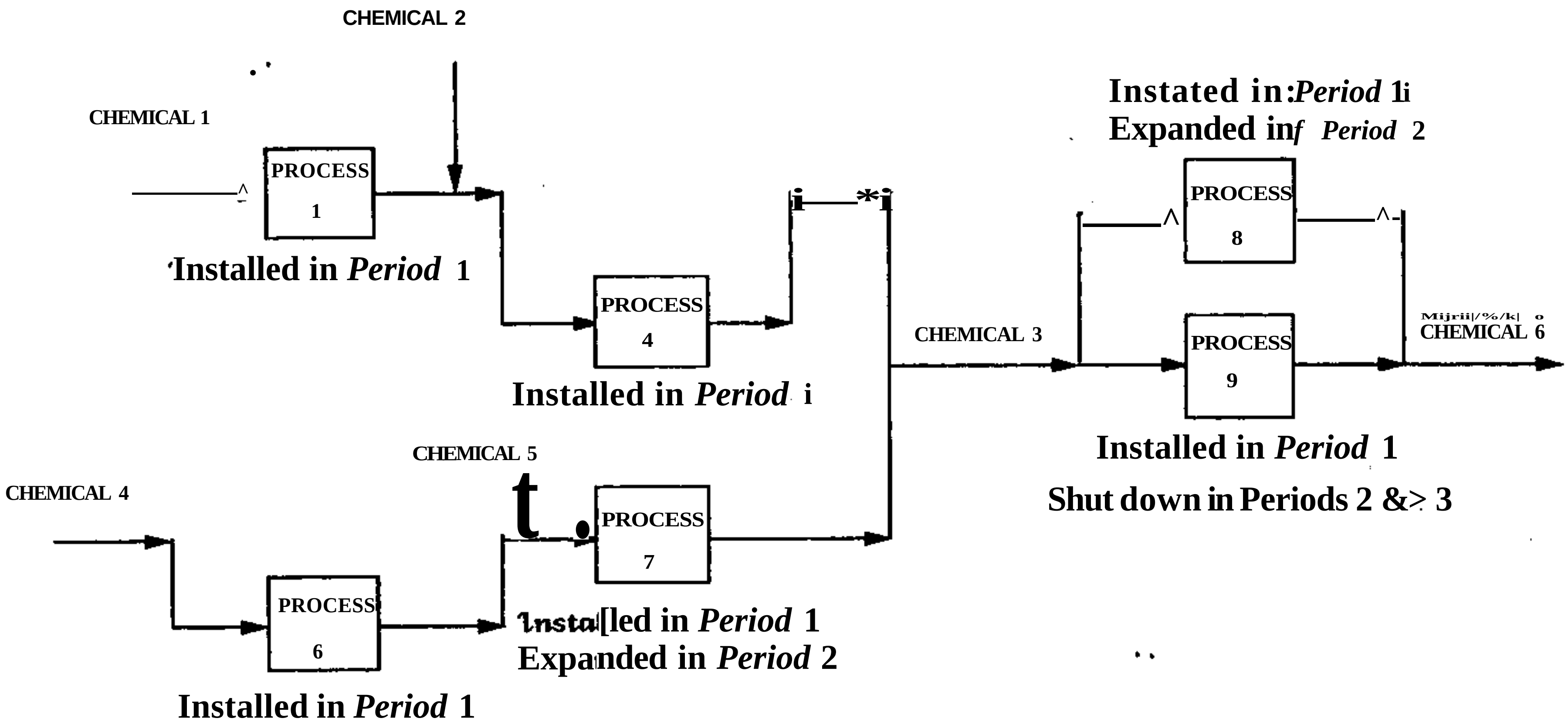

Fig. 2 Optimum Network Configuration

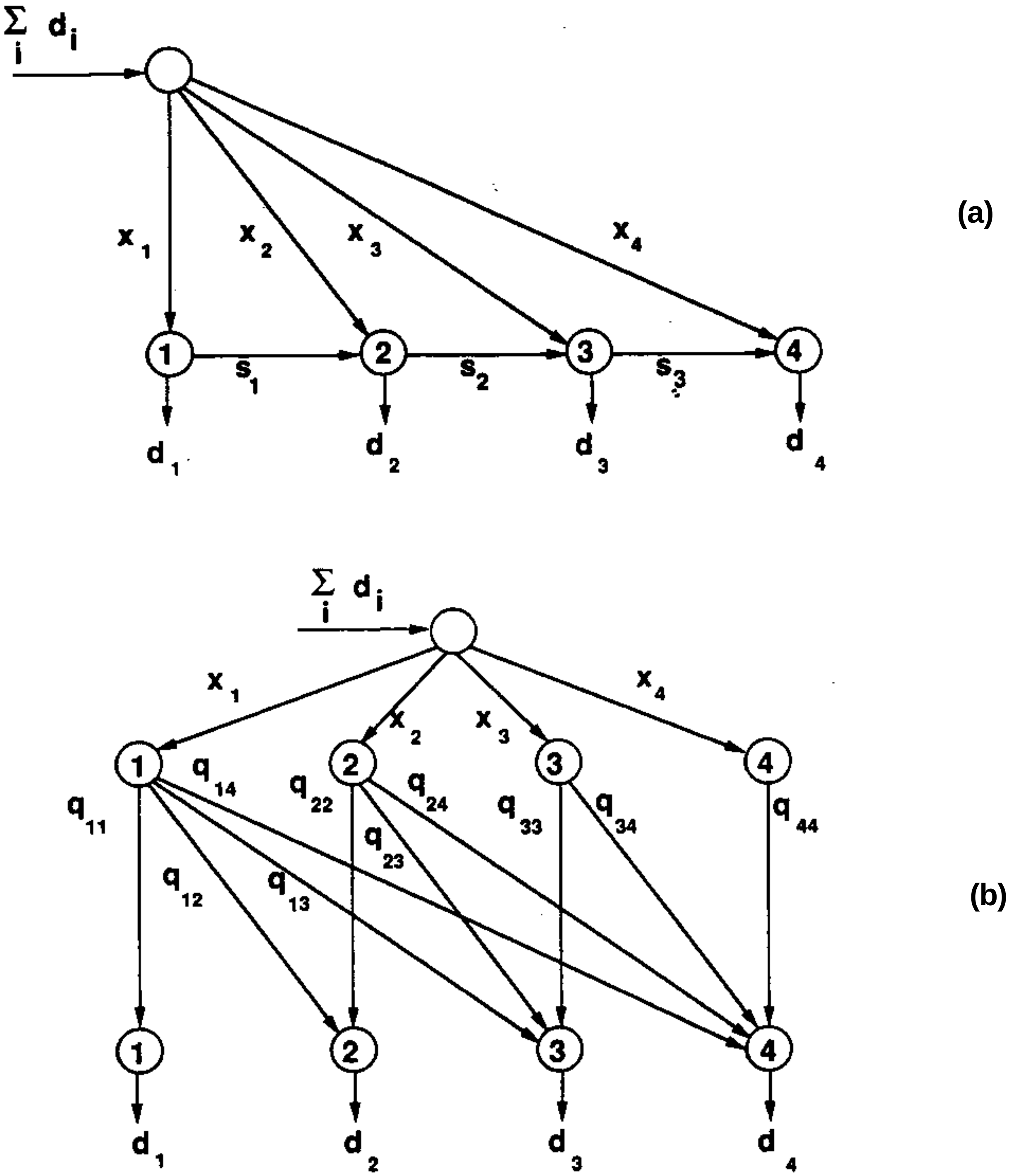

Fig. 3 Lot Sizing Model Representation:
(a) prior to reformulation
(b) after reformulation

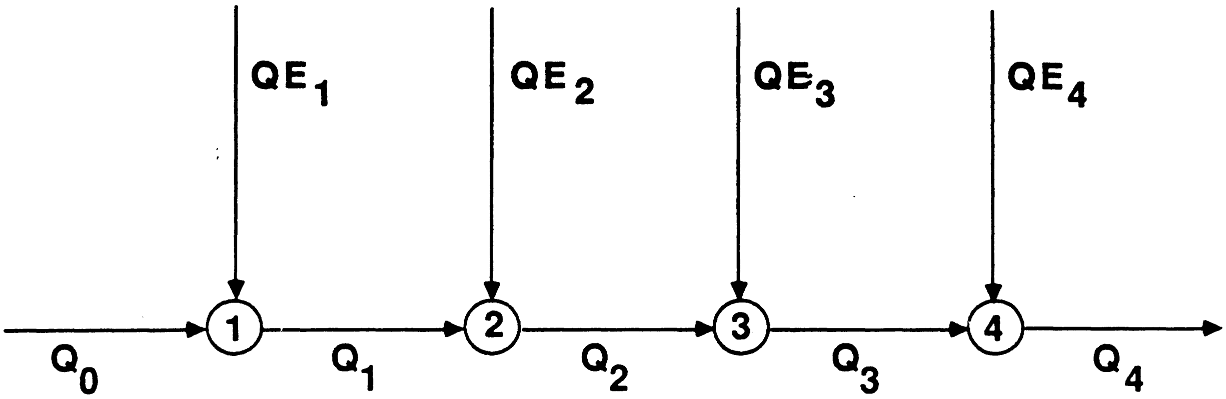

Fig. 4 Fixed charge network for capacity expansion