

1986

Optimal retrofit design of multi-product batch plants

Jane A. Vaselenak
Carnegie Mellon University

Ignacio E. Grossmann

Arthur W. Westerberg

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.

Optimal Retrofit Design Of Multi-Product Batch Plants

by

J. F. Vaselenak, I. E. Grossmann, A. W. Westerberg

EDRC-06-05-86 ^

September 1986

OPTIMAL RETROFIT DESIGN OF MULTI-PRODUCT BATCH PLANTS

J.A. Vaselenak*, I.E. Grossmann*, and A.W. Westerberg

Department of Chemical Engineering

Carnegie-Mellon University

Pittsburgh, PA 15213

October, 1985

******Current address: Shell Development Co., Houston, TX 77001**

***Author to whom correspondence should be addressed.**

Abstract

The problem of retrofit design of multiproduct batch plants is considered in which the optimal addition of equipment to an existing plant must be determined in view of changes in the product demands. In order to circumvent the combinatorial problem of having to analyze many alternatives the problem is formulated as a mixed-integer nonlinear program (MINLP) and solved with the outer-approximation algorithm of Duran and Grossmann. By using suitable variable transformations and approximations, the global optimum solution is guaranteed. The proposed MINLP model is also extended to the case when time-varying forecasts for product demands are given. Numerical examples are presented.

Introduction

This paper will address the problem of optimal retrofit design of multiproduct batch plants. In this problem the sizes and types of equipment of an existing multiproduct batch plant are given. Due to the changing market conditions, it is assumed that new production targets and selling prices are specified for a given set of products. The problem then consists in finding those design modifications that involve purchase of new equipment for the existing plant to maximize the profit.

The production targets that are given for the retrofit problem could be fixed or be given as upper limits. In this work the production levels are treated as upper limits to account for the following possibility. If the cost of the new equipment to operate at these new production levels is more than the revenue from the increased production, then either no new equipment should be purchased or else limited additions of equipment should be made at lower production levels. Therefore, the production levels must be optimized as part of the retrofit design problem.

Other assumptions that will be used in the retrofit design problem of this paper correspond to the ones that are commonly used in the optimal design of multiproduct batch plants (e.g. see Sparrow et al, 1975, Grossmann and Sargent, 1978). These assumptions include the following: The recipes for all the products are given, while processing times are specified for each of the products in each type of equipment. The products are manufactured sequentially using an overlapping production schedule. Also, it is assumed that material can be held in its processing unit until the next stage is ready. That is, the processing vessels can act as their own storage tanks. In addition, a continuous range of equipment sizes is assumed to be available, and the number of batches is permitted to be non-integer since this is usually a large number. Finally no semi-continuous equipment is considered for the plant design, although in principle this aspect could be included in the problem formulation (see Knopf et al, 1982).

As will be shown in this paper the optimal retrofit design problem for multiproduct batch plants can be formulated as a mixed-integer nonlinear programming (MINLP) problem in which two possibilities for adding new equipment in each batch stage are included. The added equipment can be used to decrease cycle times or to increase the batch sizes of the different products. By using exponential transformations and piecewise linear approximations, it is shown that the outer-approximation method of Duran and Grossmann(1983) will converge to the global optimum solution of the MINLP problem. The extension to the multiperiod case where production forecasts are given for several time periods is also considered. Three examples are presented to show that the combinatorial problem in the retrofit design can be handled effectively.

Options for New Equipment

The design modifications that are considered in the retrofit design of a multiproduct batch plant will involve the addition of new equipment to the existing plant. Any new equipment can be utilized in two ways: (1) to ease bottleneck stages by operating in parallel but sequentially (option C), or (2) to increase the size of the present batches by operating in parallel and in phase with the current equipment (option B). Option C increases production by decreasing the cycle time of a product, the time needed to make one batch of a product. The new equipment used in this way operates out of phase with the existing equipment. The Gantt charts of Figure 1 demonstrate how production is increased with this design alternative. As can be seen option C decreases the idle time of a unit, thus allowing for more efficient utilization of the equipment. Option B on the other hand increases production by augmenting the batch size of a product. New equipment utilized in this fashion operates in parallel and in phase with the existing equipment, as shown in Figure 2. This option takes advantage of excess volume of a unit, allowing for better utilization of the capacity of the unit.

Since the two options cited above can be applied to each of the batch stages, all the alternatives for equipment addition in the retrofit of a multi-product batch plant can be embedded within a super-structure as shown in Figure 3. Although just one potential new unit per stage is shown in this figure, it is clearly possible to specify multiple units for each option at each stage. By using this superstructure representation, the retrofit problem can be formulated as a mixed-integer nonlinear program to determine the optimal design modification without having to examine all the possible alternatives.

Formulation

The goal of the retrofit design problem is to maximize the profit of the batch processing plant given new product demand and prices. Profit is defined here as the net income from selling the products minus the annualized investment cost. The expected net profit per unit of product P_i will be denoted as p_i . The cost of the equipment will be approximated by a fixed-charge cost model, where K_j is the annualized fixed charge of equipment type j , which includes the costs of piping, instrumentation, and some installation expenses, and c_j is the annualized proportionality constant of equipment type j , which accounts for the linear increase of cost with the size of the vessel.

The objective function for the retrofit problem can then be formulated as:

$$\max \sum_{i=1}^I p_i n_i - \sum_{j=1}^M Y_j \left(\sum_{k=1}^{Z_j^B} \sum_{m=1}^{N_j^{old}} K_j (y_{jk}^B)_m + \sum_{k=1}^{Z_j^C} K_j y_{jk}^C \right) - \sum_{k=1}^{Z_j^C} T_k c_j V^C \quad (n)$$

where n_i = number of batches of product i

B_i = batch size of product i

$(y_{jk}^B)_m$ = binary variable for the k th new unit used to expand batch size of the m th old unit of stage j

y_{jk}^C = binary variable for the decrease cycle time option for the k th unit of stage j

$(V_{jk}^B)_m$ = volume of the k th new unit of stage j used for option B (increase batch size) of existing unit m stage j

V_{jk}^C = volume of the k th unit of stage j used for option C (decrease cycle time)

i = index for products, $i = 1, 2, \dots, N$

j = index for stages, $j = 1, 2, \dots, M$

k = index for number of possible new units for stage j ;

$k = 1, 2, \dots, Z_j^B$ for option B; $k = 1, 2, \dots, Z_j^C$ for option C

m = index for existing parallel units of stage j , $m = 1, 2, \dots, N_j^{\text{old}}$

Note that new vessels used for option C are denoted by y_{jk}^C (binary variable for the existence of a unit) and V_{jk}^C (volume); new items used for option B are symbolized by y_{jk}^B (binary variable for the existence of a unit) and V_{jk}^B (volume). The binary variables, y_{jk}^C and y_{jk}^B represent the existence of a particular unit ($y_{jk} = 1$) or the absence of a particular unit ($y_{jk} = 0$) in the superstructure. Also, this definition of variables allows different equipment items to have unequal sizes; for example stage s can have the volumes V_s^{old} , V_{s1}^C and V_{s2}^C

Upper bounds on the production of each product, as given by the predicted demand, are expressed in the following way.

$$n_i B_i \leq Q_i \quad i = 1, 2, \dots, N \quad (2)$$

where Q_i = the upper limit on production of product P_i

The total number of units N_j used in determining the cycle time for each stage j is

the sum of the number of old and new units, omitting the "expand batch size" (option B) type units since they operate in phase with the old, existing units. That is,

$$N_j^{old} + N_j^{new} * \frac{z_j^C}{\sum_{k=1}^M y_k^C} \quad i \ll 1, 2, \dots, M \quad (3)$$

The limiting cycle time of product P_i is given by,

$$T_{Li} \geq (t_{ij} / N_i) \quad i = 1, 2, \dots, N; \quad j \ll 1, 2, \dots, M \quad (4)$$

where t_{ij} is the processing time of product i in stage j .

Combining constraints (3) and (4) leads then to the inequality

$$(N_j^{old} + \sum_{k=1}^M y_k^C) * (T_{Li} / N_i) \leq \sum_{j=1}^M t_{ij} \quad i = 1, 2, \dots, N; \quad j = 1, 2, \dots, M \quad (5)$$

The cycle time T_{Li} and the number of batches n_i , $i = 1, 2, \dots, N$, define the total processing time that is required for each product. These processing times must not exceed the total time available, H , as stated by the following constraint:

$$\sum_{i=1}^N n_i T_{Li} \leq H \quad (6)$$

The total number of new units for each stage must lie between a lower bound, 0, and a specified upper bound, N_j^u :

$$0 \leq \sum_{k=1}^{Z_j^0} y_{jk}^B \leq \sum_{k=1}^{Z_j^C} V_{jk}^C \quad j = 1, 2, \dots, M \quad (7)$$

Also, to ensure that the equipment can accommodate the required production levels, constraints are written such that the size of the equipment must be greater than the batch volume needed by each product using that stage. For the case of expanding the batch size (option B), the constraint is given by:

$$\sum_{k=1}^{Z_j^B} (V_{jk}^B)_m + (V_j^{\text{old}})_m \geq S_{ij} B_i \quad i = 1, 2, \dots, N; \quad j = 1, 2, \dots, M \quad (8)$$

$$V_j^{\text{old}} = 1, 2, \dots, N_j^{\text{old}}$$

where S_{ij} is the size factor for product P_i in stage j , and V_j^{old} is the size of the existing piece of equipment.

For the case of the option for reducing the cycle time (option C), the capacity constraint is:

$$U [1 - y^C] \leq v^C \sum_{k=1}^{Z_j^C} S_{ij} B_i \quad i = 1, 2, \dots, N; \quad j = 1, 2, \dots, M; \quad (9)$$

$$k = 1, 2, \dots, Z_j^C$$

where U is a large number that makes this constraint redundant when this option is not selected (i.e. $y^C = 0$).

Additional bounds and integrality constraints for the above cases are:

$$0 \leq (V_{jk}^A)_m \leq (V_j^A)^U \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, Z_j^A; \quad a_i = 1, 2, \dots, N_j^{\text{old}} \quad (10)$$

$$0 \leq V_j \leq (V_j^A)^U \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, Z_j^A \quad (11)$$

$$(V_{jk}^A)_m \leq U \sum_{i=1}^M a_i \quad i = 1, 2, \dots, M; \quad k = 1, 2, \dots, Z_j^A; \quad j = 1, 2, \dots, N_j^{\text{old}} \quad (12)$$

$$V_{jk}^A \leq U \sum_{i=1}^M a_i \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, Z_j^A \quad (13)$$

where $(V_j^B)^u$ is the maximum size of a new unit for stage j , option B

$(V_j^C)^u$ is the maximum size of a new unit for stage j , option C

Finally, constraints that assign a priority selection for the postulated units in each stage, are included to eliminate redundant combinations of the binary variables.

$$\left(y_{jk}^B \right) \cdot \left(\sum_{m=1}^{N_j^{old}} z_{jm}^B - 1 \right); \quad (14)$$

$$y_{jk}^B \leq y_{j,k+1}^B \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, (Z_j - 1) \quad (15)$$

The problem defined by Equations (1M2), (5H15) corresponds to a mixed-integer non-linear program (MINLP). In this MINLP formulation the goals for retrofit design of multiproduct batch facilities are mathematically expressed, and all of the alternatives that are postulated for the new addition of equipment are embedded in this formulation.

In order to appreciate the combinatorial nature of this formulation it will be useful to consider first a simple **example problem**.

Example

To illustrate the use of the MINLP formulation presented in the previous section, consider the case of two products, A and B, that are currently manufactured in a multi-product plant consisting of two stages. Each stage has one unit with volumes $V_1 = 4000$ liters and $V_2 = 3000$ liters. The size factors and processing times are given in Tables 1 and 2.

The existing equipment is used to produce one million kg/yr of product A and 800,000 kg/yr of product B. From market research data, it is established that production can be increased to 1.2 million kg/yr for product A, and to one million kg/yr for product B. These goals represent upper limits on production. The net profit

is \$1/kg for A and \$2/kg for B. Thus, if product A and product B are manufactured at the upper limits, the maximum revenue is 3200 (10^3 \$/yr.). The cost of installing a new unit in the plant is given by the correlation $32.54 (V/1000) + 30.56 (10^3$ \$/yr.). Based on this information, it is desired to determine what new equipment, if any, should be purchased to maximize profit for a given horizon of one year (6000 working hours).

Figure 4 shows the super-structure for this problem, where two possible additions for the two options is considered in each stage. The corresponding MINLP formulation, which can be found in Vaselenak (1985), involves 8 binary variables, 6 continuous nonlinear variables (number batches, cycle times, batch sizes), 8 continuous linear variables (volumes new vessels), and 31 inequality constraints.

One simple method to solve this MINLP is to enumerate all of the possible alternative plant configurations by solving the corresponding **NLP** problems that result from fixing different combinations for the binary variables. As shown in the Appendix, these NLP subproblems have a unique optimum solution provided the production amounts for each product are strictly greater than zero.

Fifteen different alternatives can be considered for the purchase of two or fewer pieces of equipment, as shown in Table 3. For each alternative, MINOS/Augmented (Murtagh and Saunders, 1980) was used to solve the resulting NLP, requiring about 2.5 CPU-seconds on a DEC-20 computer for each case. Thus, the total CPU-time required to analyze the fifteen cases was about 38 CPU-seconds.

In Table 3 the production levels for the existing plant are optimized first to obtain a lower bound on profit, as seen in case 1. The next four cases show the maximum profit that is obtained when one new piece of equipment is added in the plant. The remaining cases show the profits for the addition of two units. The optimal solution is case 5, the use of one unit to expand the capacity of stage 2 which leads to a

profit of 3,115 (10^3 \$/yr). This represents a 13% increase of the profit with respect to the case when no new new equipment is added to the existing plant.

The following reasoning allows the search in this example to be terminated at two units for each stage. The maximum profit that can be attained from using three units or more is the difference between the maximum revenue and the fixed-charge cost of three units, $3200 - 3(30.56) = 3108(10^3$ \$/yr). Since this maximum profit is less than the profit of case 5, combinations involving three or more units can be eliminated.

This small example problem examined fifteen different plant configurations and solved fifteen NLP problems. Since larger and more realistic problems would require analyzing a much larger number of possibilities, an efficient solution procedure for solving the MINLP is required.

Solution Procedure

The primary methods used to solve general MINLP problems include generalized Benders decomposition (Geoffrion, 1972), the alternative dual approach (Balas, 1971), and branch and bound search with solution of a NLP subproblem at each node of the enumeration tree (see Garfinkel and Nemhauser, 1972, for example). The solution approach used here is the outer-approximation algorithm (Duran and Grossmann, 1983), which has been developed for solving the class of mixed-integer nonlinear programs that are linear in the binary variables and nonlinear in the continuous variables. This is precisely the structure of the MINLP formulation of this paper.

The outer-approximation method consists of solving an alternating sequence of NLP and MILP master problems to optimize the continuous and the binary variables, respectively. Specifically, this method involves first fixing the binary variables and finding an optimal solution of the resulting NLP subproblem. For the case of minimization of the objective function, this solution provides an upper bound. The original MINLP is then approximated with a master problem by linearizing the

nonlinear functions at the solution of NLP. For nonlinear convex functions these linearizations will underestimate the objective function and overestimate the feasible region. By including an integer cut to exclude the binary combination that was analyzed, the resulting MILP master problem is solved to obtain a new set of binary variables and a lower bound on the objective function (minimization case).

The new binary values are then substituted in the NLP subproblem, and the alternating sequence is repeated by accumulating in the MILP master problem all the successive linear approximations, as well as integer cuts to exclude alternatives previously analyzed. In this way, as iterations proceed in the sequence, the lower bounds predicted by the MILP master problem will increase monotonically since an increasingly tighter approximation of the original MINLP is obtained. The upper bounds predicted by the NLP subproblems will not necessarily decrease monotonically. The search procedure is stopped when the MILP master problem has no feasible solution because it cannot locate a new binary combination whose lower bound lies below the best upper bound obtained from the NLP subproblems. The global optimal solution will then correspond to the combination of binary variables that produced the best upper bound. This method can be shown to require fewer iterations than generalized Benders decomposition (Duran and Grossmann, 1984) and details of this algorithm are given in Duran and Grossmann (1983).

In order to guarantee a global optimum solution in the outer-approximation algorithm of Duran and Grossmann, the MINLP formulation for the retrofit problem must be transformed to a convex form to ensure that feasible solutions that might correspond to the global optimum are not excluded by the master problem. For example, Figure 5a shows a bilinear constraint that is typical of this formulation. Linearization of this constraint excludes the shaded regions from analysis. To avoid elimination of potential solutions, an exponential transformation of the variables results in a convex constraint. In the two variable example, the constraint becomes linear as shown in Figure 5b. The required transformations for the retrofit design

problem are detailed in the following section.

Exponential Transformation of Variables

From the section on problem formulation the objective function in terms of minimization can be expressed as:

$$\begin{aligned} \min \quad & - \sum_{i=1}^N p_i n_i B_i + \sum_{j=1}^M \left\{ \sum_{k=1}^{Z_j^B} \sum_{m=1}^{N_j^{\text{old}}} c_j (V_{jk}^B)_m + \sum_{k=1}^{Z_j^C} c_j V_{jk}^C \right\} \\ & + \sum_{j=1}^M \left\{ \sum_{k=1}^{Z_j^B} \sum_{m=1}^{N_j^{\text{old}}} K_j (y_{jk}^B)_m + \sum_{k=1}^{Z_j^C} K_j y_{jk}^C \right\} \end{aligned} \quad (1)$$

Since bilinear terms are involved in the final summation term, the following variables are defined and substituted into the objective function.

$$n_i = \exp(u_{1i}) \quad i = 1, 2, \dots, N \quad (16)$$

$$B_i = \exp(u_{2i}) \quad i = 1, 2, \dots, N \quad (17)$$

$$\min \quad - \sum_{i=1}^N p_i \exp(u_{1i} + u_{2i}) + \sum_{j=1}^M \left\{ \sum_{k=1}^{Z_j^B} \sum_{m=1}^{N_j^{\text{old}}} c_j (V_{jk}^B)_m + \sum_{k=1}^{Z_j^C} c_j V_{jk}^C \right\} \quad (18)$$

$$+ \sum_{j=1}^M \left\{ \sum_{k=1}^{Z_j^B} \sum_{m=1}^{N_j^{\text{old}}} K_j (y_{jk}^B)_m + \sum_{k=1}^{Z_j^C} K_j y_{jk}^C \right\}$$

Using Equations (16) and (17), the production goals:

$$n_i B_i \leq Q_i \quad i = 1, 2, \dots, N \quad (2)$$

become the following linear constraints.

$$u^i \cdot u_{2j} \leq \ln Q_i \quad i = 1, 2, \dots, N \quad (19)$$

The constraint (5) defining cycle times can be rearranged as:

$$- \sum_{k=1}^{z_j^c} y_{f_k} \cdot \frac{-\Lambda}{T_{Li}} \cdot N_j^d \quad (20)$$

Note that the term (t_{ij} / T_{Li}) is convex. However, T_u appears in the horizon constraint (6) in the bilinear term $n_i T_{Li}$, which is nonconvex along some directions.

Therefore, it is convenient to define:

$$T_u = \exp(u_{3i}) \quad i = 1, 2, \dots, N \quad (21)$$

with which (20) becomes,

$$- \sum_{k=1}^{z_i^c} y_{JK}^c \cdot t_{ij} \exp(-u_{oi}) \cdot N_j^{old} \quad (22)$$

which is also a convex constraint.

Finally, using Equations (16) and (21), the horizon constraint in (6) can be expressed as a convex constraint:

$$\sum_{i=1}^N \exp(u_{oi} \cdot u_{oi}) \cdot H \quad (23)$$

The constraints defining the volumes of the new vessels are shown below.

$$\sum_{k=1}^Z (V_{jk}^B L_{jk} + V_{jk}^{old} L_{jk} \cdot S_{ij} B_i) \quad i = 1, 2, \dots, N; j = 1, 2, \dots, M; \quad (24)$$

$$m \ll 1, 2, \dots, N_j^{\text{old}}$$

$$U [1 - y_j^C] \cdot V_j^C \leq S_i \cdot B_i \quad i \ll 1, 2, \dots, N; j \ll 1, 2, \dots, M; \quad (25)$$

$$k = 1, 2, \dots, Z_f$$

$$0 \leq (V_j^B)^U \leq (V_j^B)^U \quad j = 1, 2, \dots, M; k = 1, 2, \dots, Z_f; m = 1, 2, \dots, N_j^{\text{old}} \quad (26)$$

$$0 \leq V_j^C \leq (V_j^C)^U \quad j = 1, 2, \dots, M; k = 1, 2, \dots, Z_f \quad (27)$$

$$(V_{jk}^B)_m \leq (V_{jk}^B)_m \quad j = 1, 2, \dots, M; k = 1, 2, \dots, Z_f; m \ll 1, 2, \dots, N^A \quad (28)$$

$$V_{jk}^C \leq (V_{jk}^C)^U \quad j = 1, 2, \dots, M; k = 1, 2, \dots, Z_f. \quad (29)$$

If B_i is transformed as in (17), the above linear constraints for capacity become nonlinear. Since the number of nonlinear constraints should be kept at a minimum to facilitate the solution procedure, it is convenient to keep the variable B_i for the constraints (24) and (25). The following convex inequalities can be used for this purpose:

$$\exp(u_{2j}) - B_i \leq 0 \quad i = 1, 2, \dots, N \quad (30)$$

Because u_{2j} is maximized in the objective function (18), this variable will take its largest possible value. However, since B_i will be limited by at least one constraint in (24) or (25), and increasing B_i increases the required volumes constraint (30) will actually hold as an equality. Finally, the constraints used previously to eliminate redundant combinations of binary variables are included here also.

$$(y_j^B)_m \geq (y_{i,k+1}^B)_m \quad j = 1, 2, \dots, M; k = 1, 2, \dots, (Z_j^B - 1); \quad (3D)$$

$$m = 1, 2, \dots, N_j^{\text{old}}$$

$$y_{jk}^C \leq y_{j^*-M}^C \quad j = 1, 2, \dots, M; k = 1, 2, \dots, (Z_j^C - 1) \quad (32)$$

Piece-Wise Linear Approximation of Objective Function

All the nonlinear terms in the transformed MINLP defined by Equations (18) to (20) and (22) to (32) are convex except for the negative exponentials of the income term in the objective function. Despite the fact that these terms are concave, for fixed values of the binary variables, the corresponding NLP has a unique optimum solution as shown in the Appendix. However, since the linearization of the negative exponential terms in (18) will overestimate the objective function, the MILP master problem may eliminate some valid solutions, possibly the global optimum. To remedy this situation, a piece-wise, linear underestimator must be constructed to approximate the negative exponentials in the objective function, as shown in Figure 6.

The scheme that will be used to underestimate the objective function with a piece-wise linear approximation consists of selecting as base points those that result from the solution of successive NLP subproblems. Lower and upper bounds of the function are selected for the initial iteration. The following constraints can then be written for the selected points of the piece-wise linear approximation (see Garfinkel and Nemhauser, 1972):

$$x = \sum_{i=1}^N X_i s_i \quad (33)$$

$$y^* = 3^{\sum_{i=1}^N X_i} \quad (34)$$

$$\sum_{i=1}^N X_i = 1 \quad (35)$$

$$X_i \leq 3, \quad (36)$$

$$X_i < h_i * 5^{-x_i} \quad i = 2; 3, \dots, (N-1) \quad (37)$$

$$X < d \quad (38)$$

$$N^s \quad N-1$$

$$\sum_{i=1}^{N-1} S_i = 1 \quad (39)$$

where s_i, f_i are given variable and function values

x, X_i are continuous variables

y^* is the approximation of the function

S_i are 0*1 binary variables

Each binary variable S_i is associated to a line segment. A value of S_i equal to one indicates that x lies within the interval (s_i, s_{i+1}) , whose function is approximated by the line segment containing function values f_i and f_{i+1} . Constraint (39) forces only one S_i to be non-zero. Using Inequalities (36), (37), and (38), at most two consecutive X_i can be non-zero. Equation (33) defines then the point at which the approximation y^* is obtained as a linear combination of the two function values contained in the line segment as given by Equation (34).

The underestimation of the negative exponential terms of the objective function assures the global solution of the MINLP because valid linearizations that preserve the bounding properties are used in the MILP master problem. Note also that the solution of the NLP problems is unique.

Example 1

The example problem presented previously in the paper will be solved with the outer-approximation method of Duran and Grossmann (1983) using the exponential transformations and the piece-wise linear approximations for the master problem. The existing plant (all integer variables set equal to zero) was selected as the initial point. MINOS/Augmented was used to solve the NLP, and the MILP was solved using LINDO (Schrage, 1981). Two iterations were necessary to find the optimal solution, 3,115 (10^3 \$/yr), as listed in Table 4. It should be noted that since maximization of the objective function has been used, the NLP provides for this case a lower bound, while the MILP provides an upper bound. Each iteration (MILP and NLP solutions) required about six CPU-seconds on a DEC-20 computer. Thus, this method only required 12 CPU-seconds versus the 38 CPU-seconds of the enumeration of the fifteen cases in Table 3. For larger problems greater savings with the outer-approximation method can be expected as will be shown with the next example.

Example 2

Tables 5 through 8 present the data for example 2, a multi-product facility involving four products and four stages. The super-structure embedding all of the alternatives for new equipment are shown in Figure 7. The thick lines represent the existing structure. The use of one item for each option (cycle or batch) has been considered in each stage. The resulting MINLP formulation requires 9 binary variables to represent the potential new units, 25 continuous variables, 26 nonlinear constraints, and 52 linear constraints. The cost coefficients (in 10^3 \$/yr) for this model are shown in Tables 7 and 8; the total operating time considered is 6000 hours/year.

Using the outer-approximation algorithm, the three iterations (one NLP and one MILP for an iteration) shown in Table 9 required 1.7 minutes of CPU-time on a DEC-20 computer. As seen in Table 10, the optimal solution is to buy one unit ($V_4^B = 2547$ L) to expand the capacity of stage 4. This solution was found at the second iteration

and has a profit of \$513,300/year, compared to the profit of \$460,900/year when no additional equipment is purchased for the existing plant. Thus, an 11% increase in the profit is achieved with the optimal retrofit design. The production levels of the products were at their upper bounds in the optimal solution.

This example problem has 2^9 or 512 possible different combinations for additions of new equipment. Since the NLP for each iteration requires an average of 6.5 CPU-seconds, 55 CPU-minutes would have been required to enumerate all of the possibilities. Since the outer-approximation method only required 1.7 CPU-minutes, it is clear that significant computational savings have been achieved.

Extension to Multi-Period Problems

The MINLP formulation presented for the optimal retrofit design of a multi-product plant can be extended to multi-period forecasts. For instance, different production levels of a product may be specified for different time periods due to the seasonal nature of the product, such as the case for pesticides, fertilizers, soups, etc., or due to expected changes in the marketplace. This scenario is shown in Figure 8. Given a demand forecast for a set of products over several time periods, the retrofit design must then determine when new equipment should be purchased, as well as what size and what option (B or C), and also what operating levels for each product in each period. The time value of money must be taken into account here.

The MINLP formulation for NT periods of operation is a direct extension of Equations (1M2), (5M15). The objective function that reflects maximization of profit of NT periods is given by:

$$\begin{aligned} \max \left\{ \sum_{t=1}^{NT} \sum_{i=1}^N p_i^t n_i^t B_i^t - \sum_{t=1}^{NT} \sum_{j=1}^M K_j^t \left(\sum_{k=1}^{Z_j^B} \sum_{m=1}^{N_j^{\text{old}}} (y_{jk}^{Bt})_m + \sum_{k=1}^{Z_j^C} y_{jk}^{Ct} \right) \right. \\ \left. - \sum_{t=1}^{NT} \sum_{j=1}^M c_j^t \left(\sum_{k=1}^{Z_j^B} \sum_{m=1}^{N_j^{\text{old}}} (v_{jk}^{Bt})_m + \sum_{k=1}^{Z_j^C} v_{jk}^{Ct} \right) \right\} \end{aligned} \quad (40)$$

where K_j^t and c_j^t are discounted costs of equipment

NT is the number of time periods

t is the index for time periods, $t = 1, 2, \dots, NT$

The production goals and horizon constraints are expressed as a function of the periods.

$$n_i^t B_i^t \leq Q_i^t \quad i = 1, 2, \dots, N; t = 1, 2, \dots, NT \quad (41)$$

$$\sum_{i=1}^N n_i^t T_{Li}^t \leq H^t \quad t=1, 2, \dots, NT \quad (42)$$

H^t is the length of each period t, $t = 1, 2, \dots, NT$

Units purchased in previous time periods as well as the current period must be counted in the total number of units.

$$- \sum_{l=1}^t \sum_{k=1}^{Z_j^C} y_{jk}^{cl} + \frac{t_{ij}}{T_{Li}^t} \leq N_j^{\text{old}} \quad (43)$$

$$i = 1, 2, \dots, N; \quad j = 1, 2, \dots, M; \quad t = 1, 2, \dots, NT$$

The capacity constraints also depend on the time periods:

$$S_{ij} B_i^t \leq (V^{\text{old}}) \cdot \frac{t}{X} \sum_{k=1}^{Z_j^B} (V_{jk}^{\text{B}^\ell})_m \quad (44)$$

$$i = 1, 2, \dots, N; \quad j = 1, 2, \dots, M; \quad \ell = 1, 2, \dots, N_j^{\text{old}}; \quad t = 1, 2, \dots, NT$$

$$S_{ij} B_i^t \leq U [1 - y^A] \cdot V_j^A \quad (45)$$

$$i = 1, 2, \dots, N; \quad j = 1, 2, \dots, M; \quad t = 1, 2, \dots, NT$$

$$l = 1, 2, \dots, t$$

where ℓ is an index for time periods; $\ell = 1, 2, \dots, t$

Finally, bounds on equipment size and logical constraints are included.

$$(V_{jk}^{\text{B}^\ell})_m \leq U (Y_j^A X_j^S)^{\wedge 2} \dots^M; \quad k = 1, 2, \dots, Z_j^B; \quad m = 1, 2, \dots, N_j^{\text{old}}; \quad t = 1, 2, \dots, NT \quad (46)$$

$$V_{jk}^{\text{C}^t} \leq U Y_{jk}^{\text{C}^t} \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, Z_j^{\text{C}^t}; \quad t = 1, 2, \dots, NT \quad (47)$$

$$(Y_{jk}^{\text{B}^t})_m \geq (Y_{j,k+1}^{\text{B}^t})_{m^0} \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, (Z_j^B - 1); \quad \ell = 1, 2, \dots, N_j^{\text{old}}; \quad t = 1, 2, \dots, NT \quad (48)$$

$$Y_{jk}^{\text{C}^t} \wedge Y_{S+i}^S \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, (Z_j^A - 1); \quad t = 1, 2, \dots, NT \quad (49)$$

$$0 \leq (V_{jk}^{\text{B}^\ell})_m \wedge (V_j^A)^U \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, Z_j^B; \quad m = 1, 2, \dots, N_j^{\text{old}}; \quad t = 1, 2, \dots, NT \quad (50)$$

$$0 \leq V_j^A \wedge (V_{jk}^{\text{B}^\ell})_m \quad j = 1, 2, \dots, M; \quad k = 1, 2, \dots, Z_j^A; \quad t = 1, 2, \dots, NT \quad (51)$$

This MINLP formulation can also be convexified using the transformations in (16) and (17). Thus, by using the piece-wise linear approximation scheme for the MILP master problem, the global optimum can be found by solving the MINLP given by (40M51) with the outer-approximation method.

Example 3

In this example, the same plant used in example 1 is considered, but with new production goals for two years as shown in Table 11. The prices listed in period 2 of Table 12 and the cost of the equipment in period 2 of Table 13 are discounted to take into account the time value of money. The use of two items for each option for each stage per time period has been considered in this retrofit study, as shown by the super-structure of Figure 9. The MINLP formulation involves 16 binary variables, y_{ij} , to represent these new units, 28 continuous variables, 6 nonlinear constraints, and 56 linear constraints. Applying the outer-approximation algorithm, four iterations have been required, using a total of approximately 4.5 CPU-minutes (see Table 14).

As shown in Table 15, the optimal solution consists of expanding the volume of stages 1 and 2 in period 1. In this way 75% of the capacity of vessel V^1 and 72% of that of vessel $V_{2,1}^1$ is used in period 1, with full utilization of both vessels occurring in period 2. As seen in Table 14, which reports the results for the maximization case (i.e., lower bounds from the NLP, upper bounds from the MILP), the optimal profit is \$6,079,000/year which is a 20% increase over the case when no equipment is added to the plant. The production levels of the two products were at their upper bounds in the two periods.

Discussion

The retrofit design of multiproduct batch plants has been formulated as an MINLP problem which provides a systematic approach for solving this problem. As has been shown, by using exponential transformations and piece-wise linear approximations the global optimum solution is guaranteed with the outer-approximation method. Furthermore, this method circumvents the combinatorial problem of having to analyze all possible alternatives for the addition of equipment. In the three examples only 2 to 4 alternatives had to be analyzed with very modest computer time to determine the global optimum solution.

Also it has been shown that the MINLP model can be extended to account for multiperiod forecasts of the demands. This allows to determine the optimal expansion policy of a multiproduct batch plant over several periods of time. Further work may be required, however, to decompose the MINLP for problems involving many time periods.

Finally, it is interesting to note that the solution of the three examples had their production limits at the upper bounds, and that the equipment selected was for increasing the batch sizes. In general, however, one cannot expect that the optimal solutions will always exhibit this characteristic (see Vaselenak, 1985).

Acknowledgement

The authors gratefully acknowledge financial support from the National Science Foundation under Grants CPE-8210971 and CPE-8315237.

References

1. Avriel, M., *Nonlinear Programming: Analysis and Methods*, Prentice Hall, 1976.
2. Balas, E. A Duality Theorem and an Algorithm for (Mixed-) Integer Nonlinear Programming. *Linear Algebra and its Applications*, 1971, 4, 341-352.
3. Duran, M. A., and I. E. Grossmann. An Outer-Approximation Algorithm for a Class of Mixed-Integer Nonlinear Programs; Part I: The Algorithm and its Properties. Technical Report DRC 06-58-83, Carnegie-Mellon University Design Research Center, 1983.
4. Duran, M. A., and I. E. Grossmann. An Outer-Approximation Algorithm for a Class of Mixed-Integer Nonlinear Programs; Part II: The Relation With Generalized Benders Decomposition. Technical Report DRC 06-68-84, Carnegie-Mellon University Design Research Center, 1984.
5. Garfinkel, R. S. , and G. L. Nemhauser. *Integer Programming*. New York, NY: John Wiley and Sons 1972.
6. Geoffrion, A. M. Generalized Benders Decomposition. *Journal of Optimization Theory and Applications*, 1972, 10, 237-260.
7. Greenberg, H. J. and W. P. Pierskalla, A Review of Quasi-Convex Functions, *Operations Research*, 1971, 19, 1553-1570.
8. Grossmann, I.E., and Sargent, R.W.H. Optimum Design of Multipurpose Chemical Plants. *Ind. Eng. Chem. Proc. Des. Dev.*, 1979, 18(2), 343-348.
9. Knopf, F.C., M.R. Okos and G.V. Reklaitis. Optimal Design of Batch/Semicontinuous Processes. *Ind. Eng. Chem. Proc. Des. Dev.*, 1982, 21(1), 79-86.
10. Murtagh, Bruce A., and Saunders, Michael A. *MINOS/AUGMENTED User's Manual*. Technical Report SOL 80-14, Stanford University Systems Optimization Laboratory, June 1980.
11. Schrage, L. *User's Manual for UNDO*. Palo Alto, California: The Scientific Press 1981.
12. Sparrow, R.E., G.J. Forder and D.W.T. Rippin. The Choice of Equipment Sizes for Multiproduct Batch Plants: Heuristics vs. Branch and Bound. *Ind. Eng. Chem. Proc. Des. Dev.*, 1975, 14(3), 197-203.
13. Vaselenak, J., "Studies in the Optimal Design and Scheduling of Batch Processing Plants", Ph.D. Thesis, Carnegie-Mellon University, Pittsburgh, 1985.

Appendix

On the uniqueness of the solution of the NLP subproblems

For fixed values of the binary variables the MINLP defined by Equations (1-2), (5-15) can be written in compact form as

$$\max \sum_{i=1}^N p_i n_i B_i - \Phi(V_1, V_2, \dots, V_M) \quad (\text{A1})$$

$$\text{s.t.} \quad n_i B_i \leq Q_i \quad i = 1, 2, \dots, N \quad (\text{A2})$$

$$T_{Li} \geq t_{ij} / N_j \quad i = 1, 2, \dots, N, \quad j = 1, 2, \dots, M \quad (\text{A3})$$

$$V_j \geq S_{ij} B_i - a_j \quad i = 1, 2, \dots, N, \quad j = 1, 2, \dots, M \quad (\text{A4})$$

$$\sum_{i=1}^N n_i T_{Li} \leq H \quad (\text{A5})$$

where the cycle and batch volumes have been merged in the vector variables V_1, V_2, \dots, V_M which have zero components for the volumes not selected by the binary variables; Φ is the linear investment cost function. In constraint (A3) the number of units N_j is a constant for fixed binary variables as implied by Equation (3); constraint (A4) represents constraints (8) and (9) with a_j being the corresponding non-negative constant terms. Finally, (A5) is identical to Equation (6).

Since the variables N_j are constant, as well as the processing times t_{ij} , the cycle times T_{Li} in (A3) can be set to

$$T_{Li} = \max \{ t_{ij} / N_j \} \quad i=1, 2, \dots, N \quad j=1, 2, \dots, M \quad (\text{A6})$$

Furthermore, by defining the actual production amounts q_i as

$$q_i \leq n_i B_i \quad i = 1, 2, \dots, N \quad (\text{A7})$$

the formulation given by equations (A1MA5) can be written as

$$\begin{aligned} \max \quad & \sum_{i=1}^N P_i q_i - 4(V_1 V_2 \dots V_J) \\ \text{s.t.} \quad & q_i \leq n_i B_i \quad i = 1, 2, \dots, N \\ & q_j \in Q_j \quad i = 1, 2, \dots, N \\ & V_j \leq \sum_{i=1}^N B_i - a_j \quad i = 1, 2, \dots, N \quad j = 1, 2, \dots, M \\ & \sum_{i=1}^N n_i T_{Li} \leq H \end{aligned} \tag{A8}$$

since n_i , B_i are bounded by the last two constraints, and q_i has a positive incremental profit in the objective function. Note that the variables for the optimization are q_i , V_j , B_i , n_i . Also, the objective function and all the constraints are linear, except the first one which can be rewritten as

$$q_i/n_i B_i \geq 1 \quad i = 1, 2, \dots, N \tag{A9}$$

If $n_i B_i > 0$, this constraint is quasi-convex since in general the ratio function $f(x)/g(x)$, where $f(x)$ is convex and $g(x) > 0$, can be shown to be quasi-convex (see Greenberg and Pierskalla, 1971). Therefore, the formulation (A8) with the constraint in (A9) corresponds to a nonlinear program that involves a linear objective function, linear inequalities and quasi-convex inequalities. It then follows that if a Kuhn-Tucker point exists in this nonlinear program it will correspond to the global optimum solution (see Avriel, 1976). Hence, the NLP subproblems that arise from fixing the binary variables in the MINLP given by Equations (1M2), (5M15), have a unique local optimum solution provided the production amounts for each product are strictly greater than zero.

Table 1: Size Factors for Example Problem 1 (L/kg_{product})

	Stage 1	Stage 2
product A	2.0	1.0
B	1.5	2.25

Table 2: Processing Times for Example Problem 1 (hr)

	Stage 1	Stage 2
product A	4.0	6.0
B	5.0	3.0

Table 3: Options for the Purchase of Two or Fewer Equipment Items
for Example Problem 1

case number	N^A	N_2^O	N^A	N_2^B	goals met?	production profit (x10 ³ \$)
1	0	0	0	0	no	2750
2	1	0	0	0	yes	3044
3	0	1	0	0	no	2997
4	0	0	1	0	no	3029
5	0	0	0	1	yes	3115
6	1	0	0	1	yes	3014
7	1	0	1	0	yes	3014
8	1	1	0	0	yes	3000
9	0	1	0	1	yes	3033
10	0	1	1	0	yes	3033
11	0	0	1	1	yes	3090
12	2	0	0	0	yes	2889
13	0	2	0	0	yes	2869
14	0	0	2	0	no	2998
15	0	0	0	2	yes	3084

Table 4: Progress of Upper and Lower Bounds for Example 1

iteration	Lower Bound (NLP Sub-problem)	Upper Bound (MILP Master)
1 (All $y_{jk} = 0$)	2750	3142
2 ($y_{21}^B \wedge 1$; other $y_{jk} = 0$)	3115	(no solution)

Table 5: t_{ij} (hr/batch) for Example 2

		Stage			
		1	2	3	4
product	A	6.3822	4.7393	8.3353	3.9443
	B	6.7938	6.4175	6.4750	4.4382
	D	1.0135	6.2699	5.3713	11.9213
	E	3.1977	3.0415	3.4609	3.3047

Table 6: S_{ij} (L/kg/batch) for Example 2

		Stage			
		1	2	3	4
product	A	7.9130	2.0815	5.2268	4.9523
	B	0.7891	0.2871	0.2744	3.3951
	D	0.7122	2.5889	1.6425	3.5903
	E	4.6730	2.3586	1.6087	2.7879

Table 7: Existing Equipment and the Cost of New Equipment for Example 2

stage j	V_j (L)	N_j	K_j	C_j
1	4000	1	15.28	0.1627
2	4000	1	38.20	0.4068
3	3000	2	45.84	0.4881
4	3000	1	10.18	0.1084

Table 8: Forecast of Prices (\$/kg) and Demands (kg) for Example 2

product i	P_i	Q_i
A	1.114	268 200
B	0.535	156 000
D	0.774	189 700
E	0.224	166 100

Table 9: Progress of Lower and Upper Bounds of Example 2

iteration	non-zero binary variables	Lower Bound (NLP Sub-Problem)	Upper Bound (MILP Master Problem)
1	none	460 900	532 700
2	$y^B=1$.4	513 300	523 600
3	$y_1^*=1$	461 900	-

Table 10: Optimal Solution of Example 2

$$V_4^B = 2547 \text{ L}$$

product i	n_i	B_i (kg)	T_{Li} (hr)
A	530.6	505.5	6.382
B	95.48	1634.	6.794
D	122.8	1545.	11.92
E	151.7	856.0	3.305

Table 11: Demand Forecast for Example 3 (kg)

		period 1	period 2
product	A	1,200,000	1,400,000
	B	1,000,000	1,200,000

Table 12: Price Forecast for Example 3 (\$/kg)

		period 1	period 2
product	A	1.00	0.80
	B	2.00	1.60

Table 13: Cost Equations for Example 3 (10^3 \$/yr)

period 1	Cost(V) = 30.5600 + 32.5400 (V/1000)
2	Cost(V) = 26.5739 + 28.2957 (V/1000)

Table 14: Progress of Lower and Upper Bounds of Example 3

iteration	non-zero binary variables	Lower Bound (NLP Sub-Problem)	Upper Bound (MILP Master Problem)
1	none	5070	6176
2	y_{21}^{B1}	5992	6106
3	y_{11}^{B1}, y_{21}^{B1}	6079	6088
4	y_{11}^{B1}, y_{21}^{B2}	6000	(no solution)

Table 15: Optimal Solution of Example 3

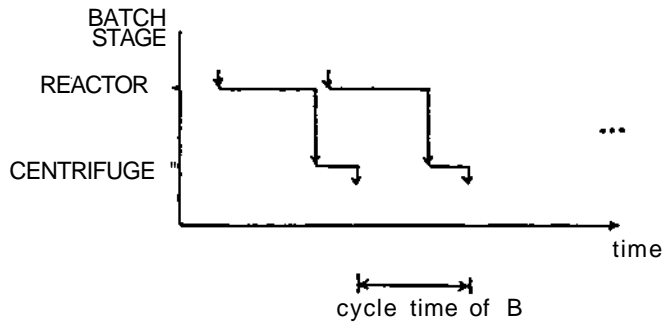
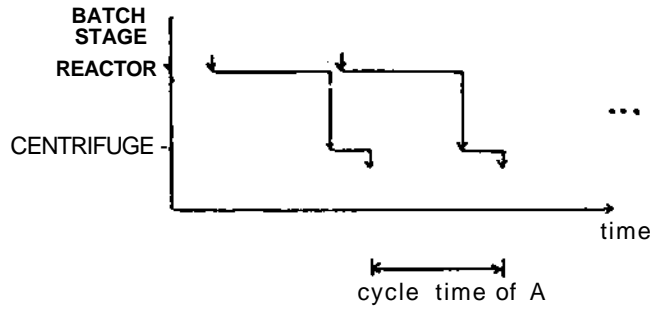
$$v_{11}^{B1} = 1310.0 \text{ L}$$

$$v_{21}^{B1} = 1760.0 \text{ L}$$

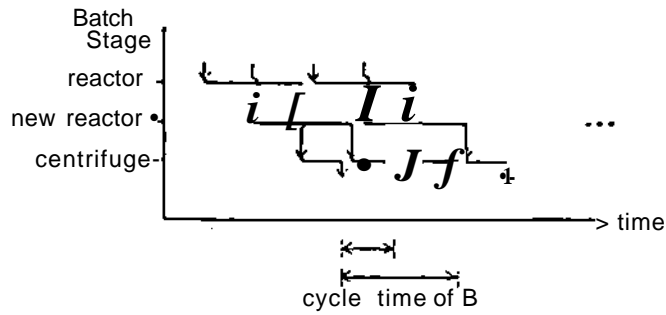
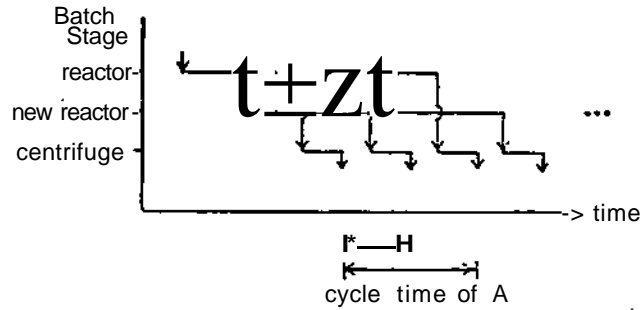
List of Figures

- Figure 1: Option C: Decrease Cycle Time
- Figure 2: Option B: Expand Batch Size
- Figure 3: Super-Structure for Retrofit Design of a Multi-Product Plant
- Figure 4: Super-Structure for Example Problem 1
- Figure 5: Bilinear Constraint Example
- Figure 6: Piece-Wise Linear Approximation of Objective Function
- Figure 7: Super-Structure for Example 2
- Figure 8: Multi-Period Demand for Products A, B, and C
- Figure 9: Super-Structure for Example 3

Figure 1: Option C: Decrease Cycle Time

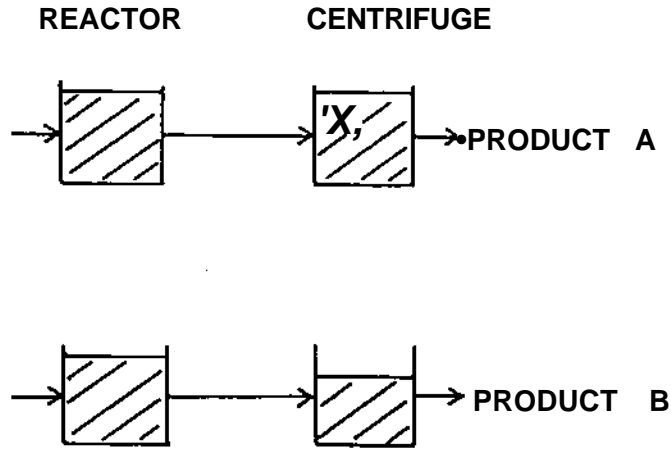


a) Existing Plant

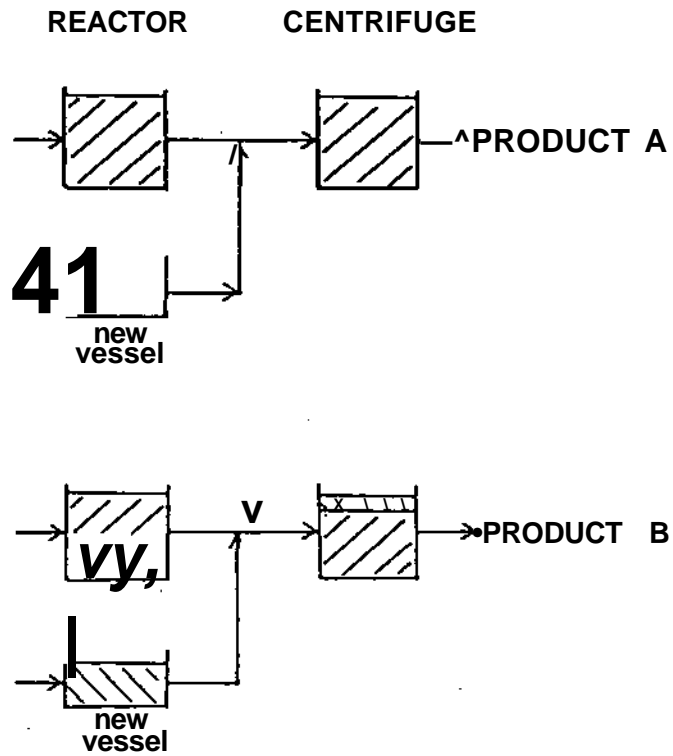


b) Modified Plant

Figure 2: Option B: Expand Batch Size



a) Existing Plant



b) Modified Plant

Figure 3: Super-Structure for Retrofit Design of a Multi-Product Plant

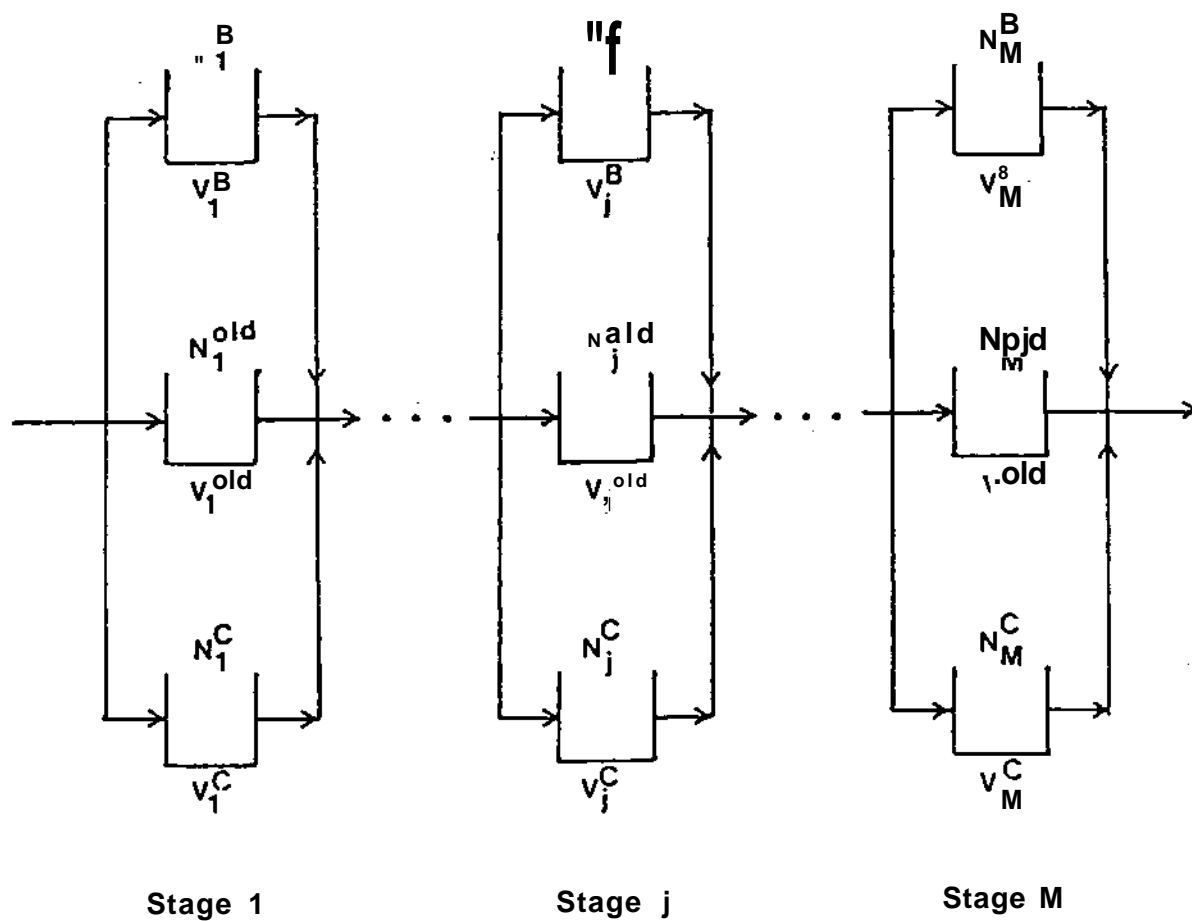


Figure 4: Super-Structure for Example Problem 1

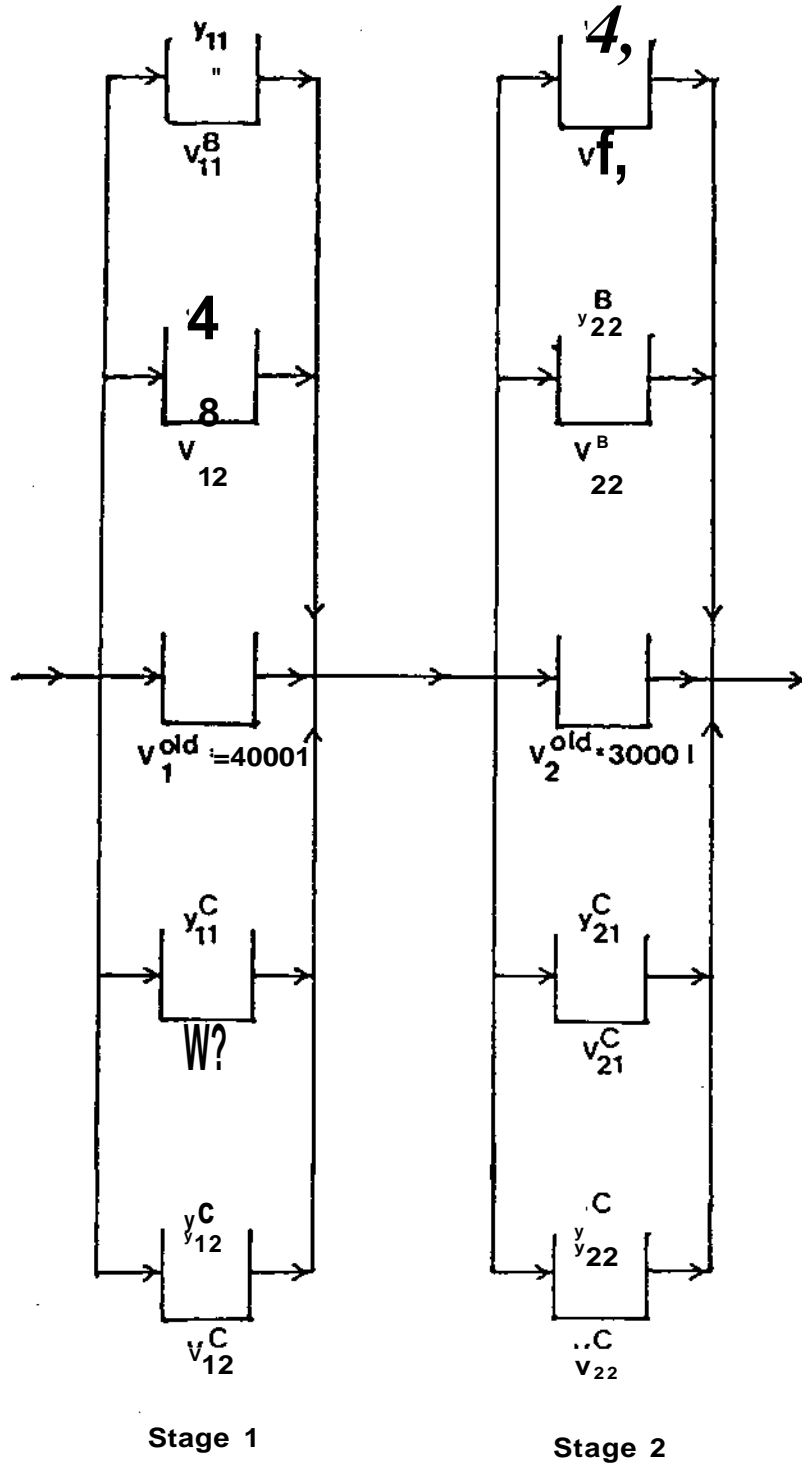
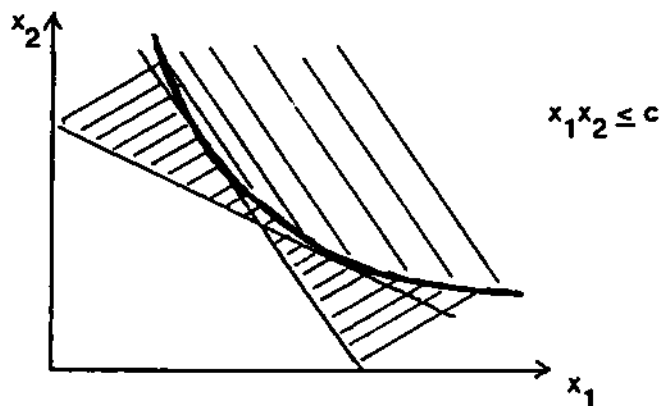
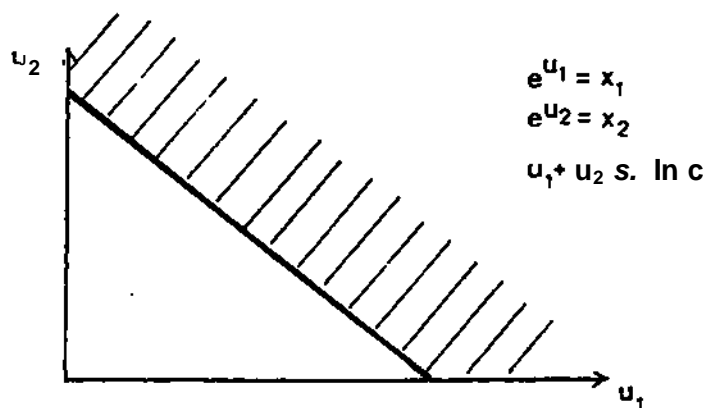


Figure 5: Bilinear Constraint Example



a) Bilinear Constraint



b) Transformed Constraint

Figure 6: Piece-Wise Linear Approximation of Objective Function

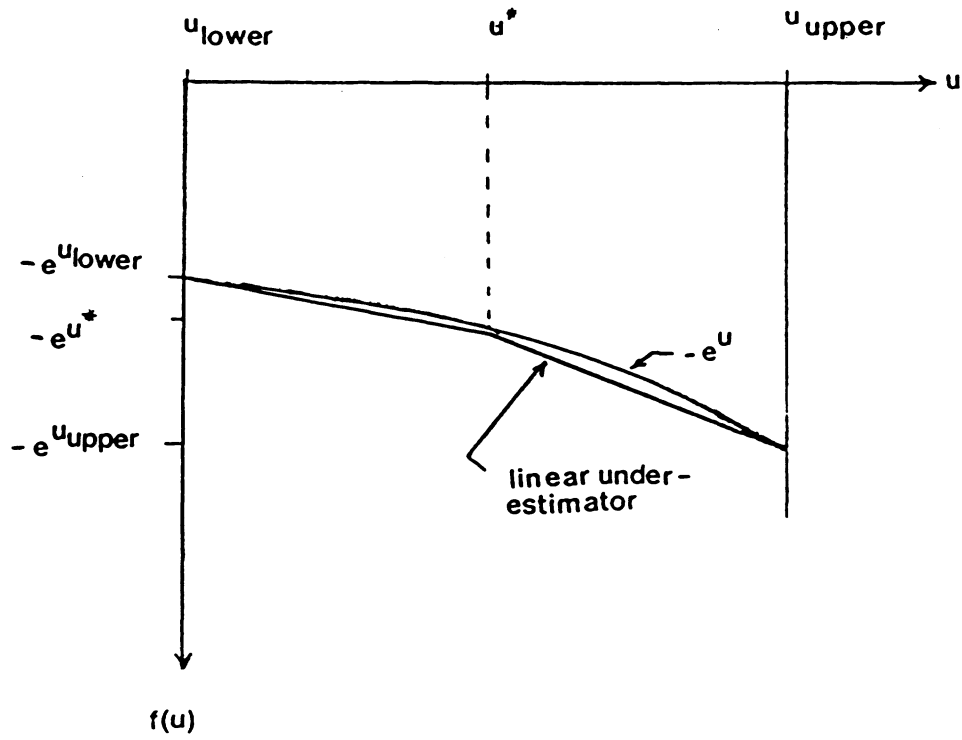


Figure 7: Super-Structure for Example 2

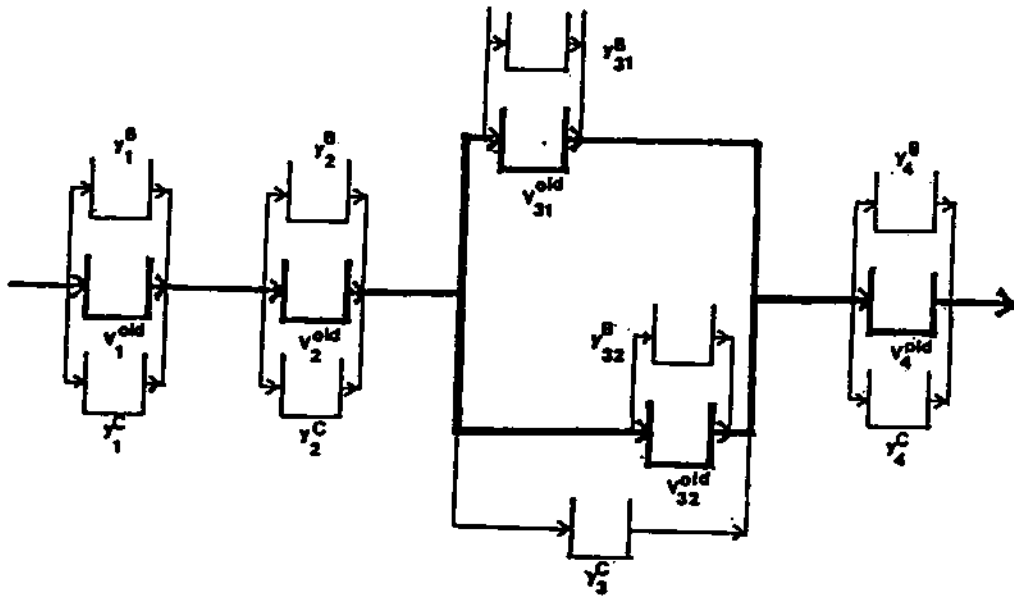


Figure 8: Multi-Period Demand for Products A, B, and C

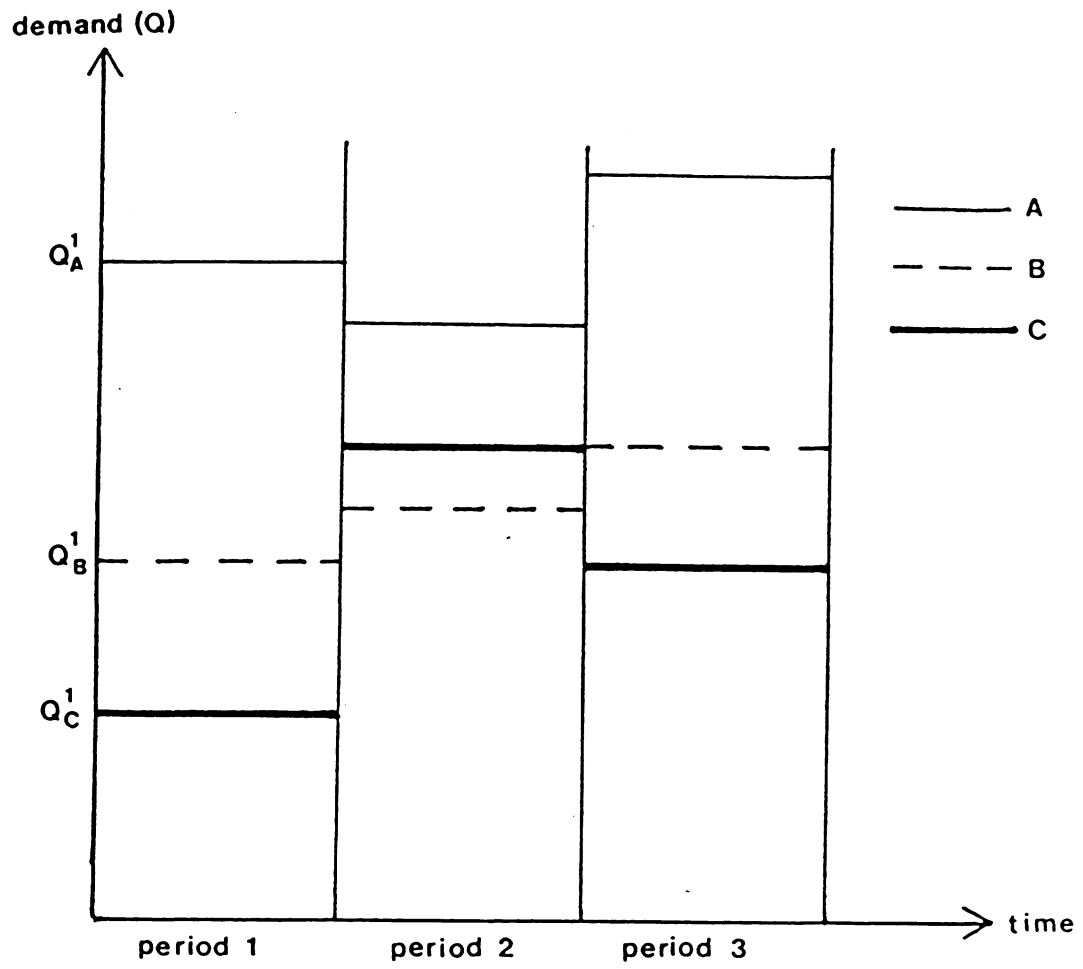


Figure 9: Super-Structure for Example 3

