

A Solution Approach to the Design of Multi-period, Multipurpose Batch Plants

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Abstract—A deterministic model for multipurpose, multiperiod batch plants was presented in a linearized form to predict the future design according to the change of demand by using a modified Benders' Decomposition. The OSL code offered by the IBM corporation as optimizer was employed for solving several example problems. The decomposition method was successful, showing remarkable reduction in the computing times as compared with those of the direct solution method. Also the heuristic used as a solution approach for the multiperiod model provided an efficient methodology to the block-structured problem by dividing the large overall problem into the manageable single period blocks.

Key words: Multipurpose Batch Plant, Decomposition, Linearization, MILP, Multiperiod

INTRODUCTION

Recently, multipurpose batch plants have been given attention due to the exploding needs of specialty chemicals and pharmaceutical products. To date, many general problem formulations for multipurpose batch plants, employing both continuous and discrete variables have not used an exact MINLP or MILP formulation to get an optimal solution [Papageorgaki and Reklaitis, 1990a, b; Wen and Chang, 1968; Nishida et al., 1974; Grossmann and Sargent, 1978; Reinhart and Rippin, 1986, 1987; Straub and Grossmann, 1990, 1992; Park and Park, 1999; Kang et al., 1996]. Treatment of discrete variables as continuous introduces a gap between the sub-optimal solution and the true optimal solution that has not been resolved to date. Therefore, a more rigorous formulation is needed at the expense of greater computing effort, which might be reduced in the near future by exploiting the problem structure. A contribution along these lines was published in 1992 by Voudouris and Grossmann [1992] who introduced binary variables for denoting discrete equipment sizes in their linearized MILP formulations. Several cases such as those of single product campaigns, multiple product campaigns, single production routes and multiple production routes were explored, but the results were not compared with previous work. To guarantee optimality, an MILP model would be preferred because if it has a special structure, then various performance enhancing techniques such as SOS, bounding, valid cuts, and so on, along with existing MILP commercial algorithms, can be used. Furthermore, a linear model takes on the role of a stepping stone, leading to a stochastic batch plant model that is considered to be more practical.

Decomposition—splitting a master problem into pieces of sub-problems—is known to be very useful for handling large scale linear programming problems. The idea was extended and exploited in mixed-variable problems by Benders [1962]. Theoretical development of a programming problem (master; which may be discrete, nonlinear etc.) and a linear programming problem (subproblem) from a mathematically complicated original problem was discussed

and a computational procedure for solving those problems was presented in his work. This work was extended to further theoretical development and industrial applications [Geoffrion, 1972; Papageorgaki, 1991; Lee, 1992; Che et al., 1999; Jung et al., 1994].

In this work, a linearized multiperiod batch plant model is solved by using a modified Bender's decomposition and a heuristic algorithm.

MODEL DEVELOPMENT: GENERAL MULTIPERIOD BATCH PLANTS

1. Deterministic Multiperiod Design Model (MINLP)

Batch plants are normally operated over multiple periods of time, with different demand levels in each period. This naturally leads to a multiperiod model, an extension to the single period model. Since the demand for products varies over the periods, the design of batch plants also must be modified accordingly.

We assume that the demands of products may vary in deterministic fashion over successive periods, that the length of the periods is known a priori (deterministic) and that the recipes of products are unchanged over time. Also, no inventory balances are considered for mathematical simplicity in formulating the model. Our goal in this type of multiperiod model would be to answer the following questions:

- How much extra equipment should be purchased whenever demand expansions occur?
- How can we predict the evolution of the plant design over multiple periods?

A multiperiod design model is proposed as an MINLP as follows.

A subscript t is introduced to denote periods that are defined as discrete time intervals. N_{et} and $N'_{e,t-1}$ denote the number of a type of equipment used in a period t and the number of equipment items of type e available in period t which were already purchased by period, $t-1$. XP_{it} symbolizes the amount of production of product i in period t .

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The objective function differs from that of the single period model in that it has two terms which denote the equipment cost and the product worth, respectively. The first term involves the amount of extra equipment to be purchased in order to meet the next period demand, and the equipment discount factor that decreases over time. This term should be minimized to suppress the purchase of extra equipment. The second term simply represents the total product sales worth. The combination of two terms balances the equipment purchase cost against the lost income from unfulfilled demands. This also means that two terms should be comparable in order of magnitude, otherwise the chosen design as well as the formulation might be far from reality.

$$\text{minimize } \sum_i \sum_e \sum_t \{ [N_{et} - N'_{e,t-1}] a_{et} V_{et}^{b_{et}} - \rho_{it} X P_{it} \} \quad (1)$$

The allocation constraints are similar to those given in our previous single period model except for an additional inequality for each subscript t . But the most important feature of the multiperiod model is shown in the connectivity constraint, which counts reuse of the same equipment over periods. By this family of constraints, the interperiod dependency in the design of batch plant is established. The minimum of the following two terms is selected as a counter for reuse of the equipment type, e .

Connectivity between periods:

$$\min[N_{et}, N_{e,t-1}] = N'_{e,t-1} \quad t=2, \dots, t^{max} \quad (2)$$

Since the formulation considers parallel units operated in phase and out of phase, the equipment bounding inequality will be stated as follows.

Equipment Bound Constraints:

$$N_{et} \geq \sum_{(i,m) \in U_e} N U_{imekt} N G_{imkt} \quad (3)$$

The batch size is simply the practical size of the minimum unit arranged in a production line. The sum of the product of the batch size and the number of batches executed over the entire horizon is the real production quantity of a product that the plant produces. This production is bounded by minimum requirement and maximum allowance of the demand.

Quantity Constraints:

$$B_{ikt} = \min_m \left\langle \frac{V_{et} N U_{imekt}}{S_{ime}} \right\rangle \quad (4)$$

$$X P_{it} = \sum_k n_{ikt} B_{ikt} \quad (5)$$

$$Q_{it}^{min} \leq X P_{it} \leq Q_{it}^{max} \quad (6)$$

The following constraints define the limiting cycle time, campaign duration time and total production horizon within each period. The limiting cycle time depends on how equipment is assigned to each task and on how many parallel groups exist. The production times of all products in a campaign cannot exceed the length of the campaign.

Horizon Constraints:

$$T L_{ikt} = \max_m \left\langle \frac{P_{ime} X_{imekt}}{N G_{imkt}} \right\rangle \quad (7)$$

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$$T_{kt} = \max_i \langle n_{ikt} T L_{ikt} \rangle \quad (8)$$

$$H_t \geq \sum_k T_{kt} \quad (9)$$

Parameters

$$Q_{e,t+1} = Q_{et} + Q E_{et}, \quad t=1, 2, \dots, t^{max} \quad (10)$$

where $Q E_{et}$ could be positive or negative (in certain cases, production reductions may occur).

Following contemporary practice, the cost of units and prices of commodities must be discounted with time. The discount factor is modelled as an exponential function in time.

$$a_{et} = a_{e0} e^{-\gamma(t-1)}, \quad t=1, 2, \dots, t^{max} \quad (11)$$

$$\rho_{it} = \rho_{i0} e^{-\gamma'(t-1)}, \quad t=1, 2, \dots, t^{max} \quad (12)$$

$$b_{et} = b_e = 0.6 \quad (13)$$

The symbols and notation are as follows;

- $X P_{it}$: Product Quantity Produced
- $Q E_{et}$: Expected Quantity Expansion (or Reduction)
- γ : Equipment Cost Discount Exponent
- γ' : Price Discount Exponent
- ρ_{it} : Product Sales Price

There are two practical ways to solve this model: one is to solve this formulation directly ignoring the integer character of the variables and the other is to convert it to a rigorously formulated model and to approach its solution by mean of an appropriate method. It is hard to obtain the exact optimal solution via the direct solution approach because of the nonlinearity of the model and the violation of integrality of some variables. Thus we chose the latter way as our solution method because it may attain global optimality in spite of the expected difficulties of solving large integer problems.

With this background, the model is reformulated to a linearized form (MILP).

2. Linearized Version of the Model

First, the two integer variables, N_{et} and V_{et} are represented by new binary variables. As N_{et} is an integer we obtain $N_{et} = \sum_{p=1}^{p^{max}} p Z_{pet}$ where $Z_{pet}=1$ when p item of equipment type e are used in period t and $Z_{pet}=0$ otherwise. Similarly, $V_{et} = \sum_{j=j^{min}}^{j^{max}} v_{jet} Y_{jet}$ where $Y_{jet}=1$ when size j of equipment e is used in period t and $Y_{jet}=0$ otherwise. To linearize the objective function, Eq. (1), variable α_{pjet} is introduced to represent the product of N_{et} and V_{et} as in the single period case. Thus we replace the product with α as follows:

$$N_{et} V_{et} = \sum_{p=1}^{p^{max}} p Z_{pet} \sum_{j=j^{min}}^{j^{max}} v_{jet} Y_{jet} = \sum_{p=1}^{p^{max}} \sum_{j=j^{min}}^{j^{max}} p v_{jet} \alpha_{pjet}$$

Another factor considered is reuse of equipment between periods, which is symbolized as α'_{pjet} and α''_{pjet} :

- $\alpha'_{pjet}=1$ when p items of equipment type e of size j are in period t and $t-1$ ($\alpha_{pjet} \geq \alpha_{pjet, t-1}$)
- $\alpha'_{pjet}=0$ otherwise

And

- $\alpha''_{pjet}=1$ when p items of equipment type e of size j are in period t and $t-1$ ($\alpha_{pjet} < \alpha_{pjet,t-1}$)
- $\alpha''_{pjet}=0$ otherwise

It is evident that two different variables, α'_{pjet} and α''_{pjet} , are needed because Eq. (2) also requires two exclusive mathematical formula to be represented. That is, α is used if an increase of equipment usage in the next period occurs; α'' is used otherwise.

Finally, the objective function takes the form:

$$\min \left\{ \sum_{p=1}^p \sum_{j=1}^j \sum_{e=1}^e \sum_{t=1}^t a_{et} * p * [V_{jet}^{be} \alpha_{pjet} - V_{je,t-1}^{be} (\alpha'_{pjet,t-1})] - \sum_{i=1}^i \sum_{t=1}^t \rho_{it} X P_{it} \right\} \quad (14)$$

where $a_{et} = a_{e0} e^{-\gamma(t-1)}$, $\rho_{it} = \rho_{i0} e^{-\gamma(t-1)}$

Connectivity between periods:

$$\left[\sum_{p'=p}^p \alpha_{p'jet} \right] + [\delta_{pjet}] - 2 \left[\sum_{p'=p}^p \alpha'_{pjet,t-1} \right] \geq 0 \quad \forall p; \forall j; \forall e; \forall t (\neq 1); t' = 1, \dots, t-1 \quad (15)$$

$$M' * \delta_{pjet} \geq \sum_{t'=1}^{t-1} \alpha_{pjet}, \quad M' = t^{max} \quad (16)$$

$$\delta_{pjet} \leq \sum_{t'=1}^{t-1} \alpha_{pjet}, \quad \delta \in \{0, 1\} \quad (17)$$

$$[\alpha_{pjet}] + \left[\sum_{p'=p+1}^p \alpha_{p'jet,t-1} \right] - 2[\alpha''_{pjet,t-1}] \geq 0 \quad \forall p; \forall j; \forall e; \forall t (\neq 1) \quad (18)$$

$$\sum_{p=1}^p \sum_{j=1}^j \sum_{e=1}^e \alpha_{pjet} \geq 1 \quad \forall \quad (19)$$

The connectivity between α and α' (or α'') is shown by using logical "AND" in Eq. (15) and Eq. (18). That ensures that α' (or α'') should be 1 only when the first two bracketed [] terms of those constraints are 1. The binary variable, δ is a function of t , which takes on the values zero or one according to the value of $\sum_{t'=1}^{t-1} \alpha_{pjet}$ as shown in Eqs. (16) and (17).

Eqs. (15)-(18) account for the repeated use of equipment in successive periods. For instance, if the type A units of size j which were used in period 1 are reused and if one more of the same type of unit is purchased in period 2, then the duplicate indicator, α'_{1jA1} will be one while $\alpha_{2jA2}=1$ and $\alpha_{1jA1}=1$ (in this case, all α'' will be zero). Particularly, Eq. (15) and its auxiliary relations [Eqs. (16)-(17)] generally cover all cases which possibly happen while $\alpha_{pjet} \geq \alpha_{pjet,t-1}$. In other words, even if the number of unit type e used is smaller than that of the currently available items, those constraints will track the number of available items of the specific unit e and adjust α' so that the objective function has the correct unit cost terms. Let a unit type e be used over three consecutive periods in the following numbers, 3 - 2 - 5. Then, we can count the number of the reused items in periods (1-2) and (2-3) as two and three (not two and two), respectively.

Meanwhile, if some items of a unit are in idle status in the next period, then the corresponding α'' will be activated instead of α' , which reduces to zero.

Assignment of product-campaign-equipment:

$$\sum_{k \in K} \sum_{e \in P_{im}} X_{imekt} \geq 1 \quad \forall \quad \forall \quad \forall \quad (20)$$

$$\sum_{e \in P_{im}} X_{imekt} \geq 1 \quad \forall \quad \forall \quad \forall \quad \forall \quad (21)$$

$$X_{i(m-n)e'kt} + X_{imekt} + X_{i(m+1)e'kt} \leq 2 \quad n=1, m-1; e \neq e'; \forall i \forall m \forall k \forall t \quad (22)$$

$$X_{imekt} \leq \sum_{e' \in P_{im'}} X_{ime'kt} \quad \forall \quad ; \forall m; \forall e \in P_{im}; \forall k \forall t \quad (23)$$

Equipment Bounds:

$$\sum_{p=1}^p p * Z_{pet} \geq \sum_{(i,m) \in U, q=1}^q \sum_{g=1}^g q * g * \omega_{qgimekt} \quad \forall \quad \forall k \forall t \quad (24)$$

Batch Size:

$$B_{ikt} \leq \sum_{e \in P_{imj}} \sum_{j=1}^j \sum_{g=1}^g \frac{q * V_{jet}}{S_{ime}} \beta_{qjimekt} \quad \forall \quad \forall m \forall k \forall t \quad (25)$$

$$B_{ikt} \leq B_{ikt}^{max} \sum_{e \in P_{i1}} X_{i1ekt} \quad \forall \quad \forall k \forall t \quad (26)$$

$$B_{ikt} \geq B_{ikt}^{min} \sum_{e \in P_{i1}} X_{i1ekt} \quad \forall \quad \forall k \forall t \quad (27)$$

Production Demand:

Among the production demand constraints, Eq. (28) shows a distinctive feature of the production policy used in this model. Because no overproduction is allowed and extreme under-production is prevented, a lower bound and an upper bound on the production of each product are given.

$$Q_{it}^{min} \leq X P_{it} \leq Q_{it}^{max} \quad \forall \quad \forall t \quad (28)$$

$$X P_{it} = \sum_k n_{ikt} B_{ikt} \quad (5)$$

Next we introduce Eqs. (25)-(28) and (5), and obtain

$$X P_{it} \leq \sum_{k \in K} n_{ikt} \sum_{e \in P_{imj}} \sum_{j=1}^j \sum_{g=1}^g \frac{q * V_{jet}}{S_{ime}} \beta_{qjimekt} \leq \sum_{k \in K} \sum_{e \in P_{imj}} \sum_{j=1}^j \sum_{g=1}^g \frac{q * V_{jet}}{S_{ime}} \beta_{qjimekt}$$

Eq. (5) is replaced by Eq. (29). $PI_{qjimekt}$ does not reduce to zero because it is forced to be lower bounded by $X P_{it}$. Therefore, it retains the proper batch size and the related number of batches do not vanish.

$$\sum_{k \in K} \sum_{e \in P_{imj}} \sum_{j=1}^j \sum_{g=1}^g \frac{q * V_{jet}}{S_{ime}} PI_{qjimekt} \geq X P_{it} \quad \forall \quad \forall m \forall t; \quad (29)$$

$$PI_{qjimekt} \leq n_{ikt}^{max} \beta_{qjimekt} \quad \forall \quad ; \forall m; \forall e \in P_{im}; \forall k; \forall q; \forall j; \forall t \quad (30)$$

$$PI_{qjimekt} \leq n_{ikt} \quad \forall \quad ; \forall m; \forall e \in P_{im}; \forall k; \forall q; \forall j; \forall t \quad (31)$$

Production Horizon:

The same treatment is applied to the production time related constraints. However, one different manipulation must be added to eliminate nonlinearity of the form (continuous)*(binary) as shown in Eq. (35). Note that Eq. (32) does not prevent the reduction of PSI_{gimekt} to zero due to lack of any lower bound. Fortunately, we can use the nikt value form the production demand related constraints to provide PSI_{gimekt} with a lower bound as follows:

$$T_{ik} \geq \sum_{g=1}^g \frac{P_{ime}}{g} PSI_{gimekt} \quad \forall \quad \forall m; e \in P_{im}; \forall k \forall t \quad (32)$$

$$PSI_{gimekt} \leq n_{ikt}^{max} G_{gimekt} \quad \forall \forall m; e \in P_{im}; \forall k; \forall g \forall t \quad (33)$$

$$PSI_{gimekt} \leq n_{ikt} \quad \forall ; \forall m; e \in P_{im}; \forall k; \forall g \forall t \quad (34)$$

$$\sum_{g=1}^{max} \sum_{e \in P_{im}} PSI_{gimekt} \geq n_{ikt} \quad \forall \forall m; \forall k; \forall t \quad (35)$$

$$\sum_{k \in K} T_{ik} \leq H_t \quad \forall \quad (36)$$

Campaign Ordering:

$$\sum_{i \in I} CO_{ikt} \geq \sum_{i \in I} CO_{i,k+1,t} \quad \forall ; k=1,t,\dots,k^{max} \quad (37)$$

$$CO_{ikt} \geq X_{i1ekt} \quad \forall ; \forall k; \forall t \quad (38)$$

$$CO_{ikt} \leq \sum_{e \in P_{i1}} X_{i1ekt} \quad \forall ; \forall k; \forall t \quad (39)$$

To reduce degeneracy in the campaign-product assignments, the indicator variable, CO_{ikt} ensures that the smaller numbered campaign involves more products.

Subsidiary Constraints:

$$\sum_{j=j^{min}}^{j^{max}} Y_{jet} \leq 1 \quad \forall \forall t \quad (40)$$

$$\sum_{j=j^{min}}^{j^{max}} Y_{jet} \leq \sum_{(i,m) \in U, k \in K} X_{imekt} \quad \forall \forall t \quad (41)$$

$$M * \sum_{j=j^{min}}^{j^{max}} Y_{jet} \geq \sum_{(i,m) \in U, k \in K} X_{imekt} \quad \forall \forall t \quad (42)$$

where M =Maximum of $\sum_{(i,m) \in U, k \in K} X_{imekt}$

$$\sum_{p=1}^p Z_{pet} = \sum_{j=j^{min}}^{j^{max}} Y_{jet} \quad \forall \forall t \quad (43)$$

Parallel units (U) and groups (G) are accommodated by the next two relations.

$$\sum_{q=1}^q U_{qimekt} = X_{imekt} \quad \forall \forall m; e \in P_{im}; \forall k; \forall t \quad (44)$$

$$\sum_{g=1}^g G_{gimekt} = X_{imekt} \quad \forall \forall m; e \in P_{im}; \forall k; \forall t \quad (45)$$

Finally, a mathematical expression for the logical “AND” for some binary variables is presented. These are derived from the linearization of the product of two binary variables.

$$Y_{jet} + Z_{pet} - \alpha_{pjet} \leq 1 \quad \forall ; \forall j; \forall e; \forall t \quad (46)$$

$$Y_{jet} + Z_{pet} - 2 * \alpha_{pjet} \geq 0 \quad \forall ; \forall j; \forall e; \forall t \quad (47)$$

$$Y_{jet} + U_{qimekt} - \beta_{qjimekt} \leq 1 \quad \forall ; \forall m; e \in P_{im}; \forall k; \forall j; \forall q; \forall t \quad (48)$$

$$Y_{jet} + U_{qimekt} - 2 * \beta_{qjimekt} \geq 0 \quad \forall i; \forall m; e \in P_{im}; \forall k; \forall j; \forall q; \forall t \quad (49)$$

$$G_{gimekt} + U_{qimekt} - \omega_{qgimekt} \leq 1 \quad \forall i; \forall m; e \in P_{im}; \forall k; \forall j; \forall q; \forall t \quad (50)$$

$$G_{gimekt} + U_{qimekt} - 2 * \omega_{qgimekt} \geq 0 \quad \forall i; \forall m; e \in P_{im}; \forall k; \forall g; \forall q; \forall t \quad (51)$$

For all of the other constraints and variables, the reader is referred to the section on Nomenclature.

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SOLUTION METHOD AND SAMPLED RESULTS

1. Model Structure and Decomposition Method

Basically we deal with Bender's type of decomposition with slight differences from that of the single period model.

The problem can be divided into two parts: design and scheduling. In the design part, we can determine the product-campaign-unit assignment (X), and the unit sizes and numbers (α). In the latter part, the batch sizes of production lines, number of batches of products and campaign duration times will be determined. Those two parts form a master problem (an upper-level problem) which has the design aspect and a sub-problem (a lower-level problem) which deals with the scheduling aspect. The master problem variables are X and while the sub-problem(s) has two main sets of variables: one for special ordered set (SOS) and the other for logical ‘AND’. Based on the dimensionality of the X and variables, the master problem is considered to be a ‘hard’ problem from the view of MILP. On the other hand, the sub problem (in which the X and α are fixed) simply reduces to a problem involving batch sizing and appropriate division of the production horizon since most of the configuration of the batch plant is already determined.

But the multiperiod model has a linked structure composed of independent single period models (blocks). The master problem has a connection between single period models and cannot be split into blocks which would be solved independently. On the other hand, the sub-problems are nothing but a collection of independent blocks which can be dealt with one by one.

The second characteristic of this decomposition is that it has additional complicating variables denoting unit numbers and sizes. This serves to eliminate the connectivity that links one block to another in the sub-problem structure.

The procedure of implementing this algorithm will be described next. Its flow diagram is shown in Fig. 1. Starting with the master problem with known input of the campaign lengths, the related sub-problem can be solved from the first period to last. The input of campaign duration times makes the master problem linear (MILP). The process starts with an equal division of the entire horizon.

If infeasibility occurs, the computation returns to the master problem with an integer cut of the assignment variables. Otherwise, the

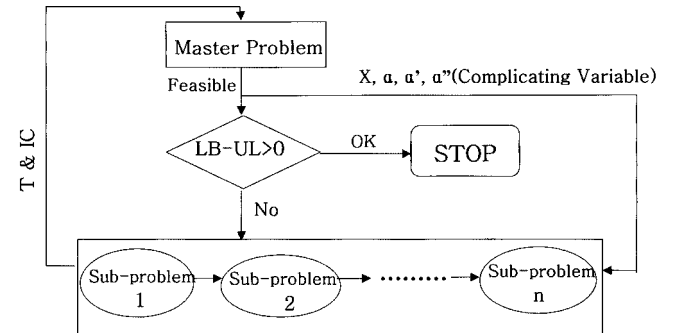


Fig. 1. Flow diagram of decomposition in multiperiod model.

X: product-campaign-unit assignment

α : unit size and number allocation

α', α'' : reuse indication of α between adjacent periods

T: campaign duration time updated

IC: integer cut of current integer solution

updated campaign duration times as well as the integer cut are added to the master problem. The updated data of campaign duration times will lead to the master problem. The updated data of campaign duration times will lead to a re-search of the feasible domain of the MP solution to avoid missing of possible local minimal points.

The lower bound given by the master problem is compared with the current upper bound resulting from the feasible solutions of the sub-problems. If the lower bound exceeds or is equal to the upper bound, then the process stops because there will be no further feasible set of solutions to the master problem. Otherwise, the process will be resumed.

2. Modified Method (Heuristic)

In a multiperiod model, the major difficulty in applying the Bender's type of decomposition to its solution originates from the master problem. A solution of the master problem is supposed to yield values of the complicating variables - product-unit-campaign allocation and unit numbers and sizes. This, however, does not normally give the optimal solution in reasonable computation time due to the complicated interconnectivity between periods, which often leads the branching and bounding procedure to extensive enumeration. The relatively weak relation of the assignment variables to the objective function and the large number of possible combinations of the assignments to be searched through the process are the main reasons of the slow convergence to MP optimality.

Therefore, we need a modified solution method, particularly for the MP. Another decomposition of the MP into period subproblems was carried out as follows.

2-1. Partition and Heuristic Optimization in MP

Sub-MP's (SMP) were set up for all periods considered. The first SMP is solved and its solution α is used for solution of the next SMP. After the last SMP is solved, we have to check for the possibility that another combination of α and α' , excluding the current point, may produce a better configuration. Thus a so-called 'cut' of α is added to the first SMP in the next iteration. When the objective value is not improved with further iterations (until one equipment unit with a size and a type is added only in period 1), the iteration process is terminated to accept the best value as optimal solution.

2-2. Major Decomposition

With fixed X , α and α' , each partitioned sub-problem is solved.

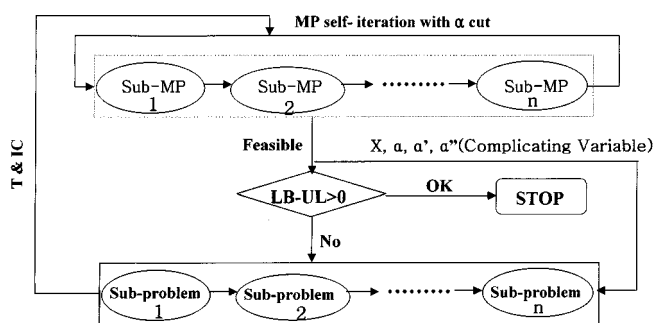


Fig. 2. Flow diagram of heuristic decomposition in multiperiod model.

X : product-campaign-unit assignment

α : unit size and number allocation

α' , α'' : reuse indication of α between adjacent periods

T : campaign duration time updated

IC : integer cut of current integer solution

The next stage is to create a new MP with properly generated integer cuts of X , α' and α'' and to solve it. If the termination condition is not satisfied, the iteration continues.

A schematic diagram of this heuristic algorithm is presented in Fig. 2.

3. Usefulness of Decomposition Algorithm

The MP is a relaxation of the original problem. Hence its feasible region completely covers the solution sets of the original problem. In other words, the feasible solution set of the original problem is just a subset of those of the MP. Hence if, through iteration, every solution set of the MP is explored, we can ensure that the optimal solution is necessarily obtained.

Let S_{MP} denote the set of MP solutions, S_{SP} set of SP solutions and S_{OP} set of original problem solutions.

Then,

$$S_{MP} \supseteq S_{SP}, S_{MP} \supseteq S_{OP}$$

After each iteration, we find the next better solution in MP (to exclude the previous solution, integer cuts are necessary). So we expect the lower bounds to increase as the iterations proceed and finally the lower bound will exceed the upper bound or all solutions of the MP will be explored exhaustively.

Then, we do not have to keep iterating because those two conditions guarantee that we reached true optimum of the original problem, if one exists. Therefore, exhaustive investigation of the feasible region of MP results in exhaustive investigation of that of OP, which produces the optimal solution.

From

$$S_{MP} \supseteq S_{OP} \supseteq S_{SP}$$

$$\min S_{MP} \supseteq \min S_{OP} \supseteq \min S_{SP}$$

If $\min S_{MP} \geq \min S_{SP}$ (termination condition for iterations), then,

$$\min S_{OP} = \min S_{SP} = \min S_{MP}$$

This proves the sufficiency of the decomposition method used for global optimum(linear model).

4. Test Results of Computer Experiments

Four example problems were depicted in the Tables and their computation results were demonstrated visually in Figs. 2 through 5.

4-1. Example Problem 1

The direct decomposition method and heuristic decomposition method were both tested for this 2-period example.

The comparison of computation times involve two methods. Us-

Table 1. Processing times and size factor [()] for tasks in Problem 1

Product. task	Equipment type			
	E1	E2	E3	E4
A.T1	5(1.2)		4.5(1.25)	
A.T2		3(1.3)		
A.T3			4.5(1.1)	
B.T1		6(1.4)		
B.T2	4(1.15)			3(1.2)
C.T1			7.5(1.5)	
C.T2		6.5(1.2)		
C.T3	6(1.1)			5(1.2)

Table 2. Possible unit capacity data in Problem 1

Unit type	v_e	N_e^{max}	a_{eo}
E1	2000, 3000, 4000	3	200
E2	2000, 3000	3	220
E3	2000, 3000	3	280
E4	2000, 3000, 4000	3	360

Table 3. Production demands in Problem 1

	Product	Demand range $\times 10^5$	Value coeff., ρ_{io}
Period 1	A	2.4-3.0	0.05
	B	2.0-2.5	0.05
	C	2.4-3.0	0.05
Period 2	A	4.8-6.0	0.05
	B	4.0-5.0	0.05
	C	4.8-6.0	0.05

Table 4. Comparison of computation times by two methods (heuristic vs direct decomposition)

Heuristic	CPU (sec)	Obj. value	Decomp.	CPU (sec)
MP1	20.60	21575.65		
MP2	20.15	3475.65	MP1	181.82
MP3	22.24	8745.65		
SP1	52.67	5150.99	SP1	52.67
MP4	14.99	7918.44	MP2	545.48

Table 5. Production demands in Problem 2

	Product	Demand range $\times 10^5$	Value coeff., ρ_{io}
Period 1	A	2.4-3.0	0.05
	B	2.0-2.5	0.05
	C	2.4-3.0	0.05
Period 2	A	4.8-6.0	0.05
	B	4.0-5.0	0.05
	C	4.8-6.0	0.05
Period 3	A	6.4-8.0	0.05
	B	8.0-10.0	0.05
	C	5.6-7.0	0.05

ing the direct method, the solution time required was 779.97 seconds, while only 130.65 seconds was consumed using the heuristic decomposition method (Table 4). Considering that the majority of the computation time for the direct method is due to the difficulty of the master problems involved, the partitioning of the master problem has obviously brought remarkable enhancement in solution time.

Note that 'MP(SP) n ' denotes 'in the n -th master(sub) problem'.

4-2. Example Problem 2

The same input data as that of example problem 1 was used except that the number of periods was increased to three. This problem requires 1737/900 (integer/continuous) variables in total. The production horizon is 6,000 hours in each period and the maximum allowable number of parallel processing groups is chosen to be two.

The direct decomposition method was unable to obtain the optimal solution due to the excessive number of iterations executed dur-

Table 6. Solution for scheduling in Problem 2

	Batch size	No. batches	Campaign length
Period 1	BA _A , 1538	n _A , 195	T ₁ , 1049.7
	BA _B , 1429	n _B , 175	T ₂ , 1349.7
	BA _C , 1667	n _C , 180	T ₃ , 975.3
Period 2	BA _A , 1538	n _A , 390	T ₁ , 2099.4
	BA _B , 1429	n _B , 350	T ₂ , 1950.6
	BA _C , 1667	n _C , 260	T ₃ , 1950.0
Period 3	BA _A , 1538	n _A , 293	T ₁ , 4533.2
	BA _B , 1429	n _B , 755	T ₂ , 1466.8
	BA _C , 1667	n _C , 604	T ₃ , 0.0

ing even an MP solution. However, the heuristic decomposition method resulted in a (sub) optimal solution in reasonable time since the partitioned sub-master problems (SMP) were each easily solved because of the elimination of the interconnectivity relations and the small number of binary variables involved in each SMP.

The first optimization of MP was completed in three iterations. That was followed by sub-problem solution to give optimal scheduling information. In the second attempt of the MP solution, the best solution after the first solution is found to be greater than the upper bound. This means that further search (iteration) is not necessary since no better solution can be expected through further iterations. Therefore, we found the optimal solution that is shown in Table 6.

In the optimal design configuration given in Fig. 3, note that the design for period 3 is distinguished from the design of period 1 and 2 by the campaign arrangement. The common use of most units in all production lines forces the plant to have multiple serial campaigns as long as the production horizon provides enough time for meeting minimum demands. Meanwhile, in period 3 where the production demand increased to a higher level, the number of campaigns was reduced by the joint production of B and C. The joint production of B and C requires one more item of each type of equipment, E1 and E2.

4-3. Example Problem 3

The input data for example problem 3 are shown in Tables 8, 9 and 10; the number of integer variables involved in the formulation is 1842.

As shown in Table 8, the task-equipment assignment is unique,

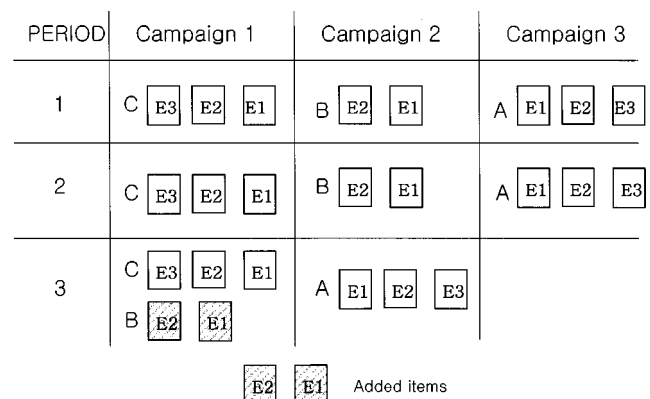
**Fig. 3. Optimal configuration of test Problem 2.**

Table 7. Result of computation times of Problem 2

Problem	Obj. value	CPU (sec)
MP1	-17550.51	34.22
MP2	-26756.15	51.20
MP3	-8250.52	38.81
SP1	-26479.0	128.46
MP4	-1505.67	31.41

Table 8. Processing times and size factor [()] for tasks in test Problem 3

Product. task	Equipment type				
	E1	E2	E3	E4	E5
A.T1	5(1.2)				
A.T2	6(1.2)				
A.T3	4.5(1.2)				
B.T1	3.5(1.2)				
B.T2	2(1.2)				
B.T3	5(1.2)				
C.T1	7.2(1.2)				
C.T2	5.5(1.2)				
C.T3	3(1.2)				
D.T1	4.8(1.2)				
D.T2	3.6(1.2)				

Table 9. Possible unit capacity data in Problem 3

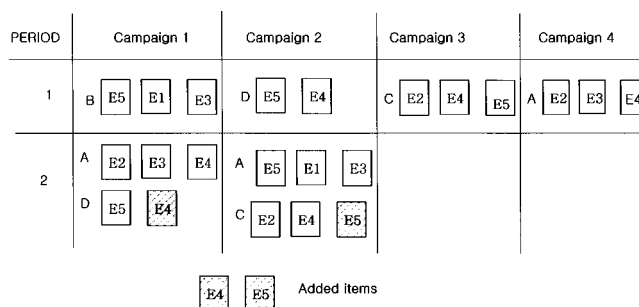
Unit type	v_e	N_e^{max}	a_{eo}
E1	2000, 3000, 4000	3	200
E2	2000, 3000	3	220
E3	2000, 3000	3	280
E4	2000, 3000, 4000	3	300
E5	2000, 3000	3	350

Table 10. Production demands in Problem 3

	Product	Demand range $\times 10^5$	Value coeff., p_{io}
Period 1	A	4.0-5.0	0.03
	B	4.0-5.0	0.03
	C	4.0-5.0	0.03
	D	4.0-5.0	0.03
Period 2	A	8.0-10.0	0.03
	B	8.0-10.0	0.03
	C	6.4-8.0	0.03
	D	8.0-10.0	0.03

and the main concern of the design in this problem will be about the campaign rearrangement. Fig. 4 shows that the large increase in the demand (nearly double) within the same horizon (6,000 hours) has resulted in the joint production of (A, D) and (B, C) in the same period. Thus, one more item each of E4 and E5 must be purchased at the beginning of period 2.

It is obvious that as problem size grows the computing efforts greatly increase as shown in Tables 4, 7 and 12.

**Fig. 4. Optimal configuration of test Problem 3.****Table 11. Solution for scheduling in Problem 3**

	Batch size	No. batches	Campaign length
Period 1	BA_A , 1667	n_A , 240	T_1 , 1392.9
	BA_B , 1667	n_B , 279	T_2 , 1439.7
	BA_C , 1667	n_C , 240	T_3 , 1727.7
	BA_D , 1667	n_D , 300	T_4 , 1439.7
Period 2	BA_A , 1667	n_A , 500	T_1 , 2999.4
	BA_B , 1667	n_B , 600	T_2 , 3000.6
	BA_C , 1667	n_C , 417	T_3 , 0.0
	BA_D , 1667	n_D , 625	T_4 , 0.0

Table 12. Result of computation times of Problem 3

Problem	Obj. Value	CPU (sec)
MP1	35797.33	219.31
MP2	53777.33	431.06
SP1	34615.71	1029.21
MP3	49822.34	229.74

4-4. Example Problem 4

All previous test problems dealt with the expansion in demand for every product. At times a general multiperiod batch plant must also deal with a decrease in some of the demands, which requires the plant design to be more flexible according to the market need. This example considers a case in which the demands for two products decrease while that for the third still increases. All the related input data is shown in Tables 1, 2 and 13 (actually modified from the data of problem 2).

In this case as shown in Fig. 5, compared to Fig. 3, there were

Table 13. Production demands in Problem 4

	Product	Demand range $\times 10^5$	Value coeff., p_{io}
Period 1	A	2.4-3.0	0.05
	B	2.0-2.5	0.05
	C	2.4-3.0	0.05
Period 2	A	4.8-8.0	0.05
	B	4.0-5.0	0.05
	C	4.8-7.0	0.05
Period 3	A	6.4-6.0	0.05
	B	8.0-10.0	0.05
	C	5.6-6.0	0.05

Table 14. Result of computation times of Problem 4

Problem	Obj. value	CPU (sec)
MP1	-37140.	470.84
MP2	-25620.	874.9
SP1	-36436.4	92.04
MP3	-14882.6	552.28

PERIOD	Campaign 1	Campaign 2	Campaign 3
1	C E3 E2 E1	B E2 E1	A E1 E2 E3
2	C E3 E2 E1 B E2 E1	A E1 E2 E3	
3	C E3 E2 E1 B E2 E1	B E2 E1 A E1 E2 E3	

Fig. 5. Optimal configuration of test Problem 4.

two added equipment items required in period 2 but none are added in period 3, and campaign rearrangement [from (B, C) and (A) to (B, C) and (A, B)] suffices to allow the production demands to be met in that period.

CONCLUSION AND RECOMMENDATIONS

The single period model was extended to the multiperiod case in which the change of the design is considered according to the change of demands. The model for multiple periods was established in a different way from the single period model in which the demands must be met (the order must always be fulfilled). That is, since the multiperiod model represents a long-term plant planning and design, the overproduction in every period could cause waste of resources and over-utilization of equipment under a no inventory system. But to avoid the complicated formulation that an inventory system might cause we presented the plant model without an inventory system, focusing only on minimization of the net investment cost for the given periods. The net investment cost is comprised of the equipment cost the revenue loss, which is defined as the lost income due to unfulfilled order. The objective function is simply the necessary equipment cost which must be expended to minimize the revenue loss for the set of periods.

For this model, a two-level decomposition was applied: the first partition was implemented in the same manner as in the single period model while the second partition was implemented for each sub problem associated with each period. Each sub problem associated with a given period could be solved in increasing order of periods with a heuristic which links the independent blocks to one another. Thus, this implies that as long as each block can be solved by using reasonable computing effort, the entire optimization of the model will become tractable.

However, there are some further points to be considered in the solution approaches and the model development.

First, since even the single period model basically includes too many integer variables, causing computational difficulties, there is a serious limitation on the tractable problem size. Therefore, some heuristics (or approximation) just like in the solution method used in the multiperiod model solution should be analyzed for larger problems.

Secondly, expansion of the multiperiod model may be considered to inventory when the number of periods is increased and their duration becomes shorter.

The introduction of inventory between periods allows overproduction in some periods and will require modifying the present model. The difficulty here lies in the increase of the mathematical complexity.

NOMENCLATURE

i	: product
m	: task
e	: equipment type
k	: campaign
t	: period
N_e	: number of units of type e
V_e	: unit capacity of type e
T_k	: campaign length
TL_k	: limiting cycle time
B_{ik}	: batch size
Q_i	: production quantity
H_i	: production horizon
X_{imekt}	: product-task-equipment-campaign-period assigning variable

All others were explained in the text.

REFERENCES

- Benders, J. F., "Partitioning Procedures for Solving Mixed-variables Programming Problems," *Numerische Mathematik*, **4**, 238 (1962).
- Cho, K. W., Yeo, Y. K. and Kim, M. K., "Application of Partitioning and Tearing Techniques to Sulfolane Extraction Plant," *Korean J. Chem. Eng.*, **16**, 462 (1999).
- Geoffrion, A. M., "Generalized Benders Decomposition," *J. of Opt. Theo. and Appl.*, **10**(4), 237 (1972).
- Grossmann, I. E. and Sargent, R. W. H., "Optimum Design of Chemical Plants with Uncertain Parameters," *AIChE J.*, **24**, 1021 (1978).
- Grossmann, I. E. and Sargent, R. W. H., "Optimum Design of Multipurpose Chemical Plant," *Ind. Eng. Chem. Process Des. Dev.*, **18**(2), 343 (1979).
- Jung, S. H., Lee, I.-B., Yang, D. R. and Chang, K. S., "Synthesis of Maximum Energy Recovery Networks in Batch Processes," *Korean J. Chem. Eng.*, **11**, 162 (1994).
- Kang, M. S., Kim, I. W. and Park, S., "Stage Efficiency Estimation by Modified MIMT using NLP," *Korean J. Chem. Eng.*, **13**, 159 (1996).
- Lee, B., "Optimal Scheduling of Batch Processes for Heat Integration," PhD Thesis, Purdue University, W. Lafayette, IN (1992).
- Nichida, N., Ichikawa, A. and Tazaki, E., "Synthesis of Optimal Process Systems with Uncertainty," *Ind. Eng. Chem. Process Des. Dev.*, **13**, 209 (1974).
- Papageorgaki, S., "Design of Multipurpose Batch Plants Using Mathe-

- mathematical Programming Techniques," PhD Thesis, Purdue University, W. Lafayette, IN (1991).
- Papageorgaki, S. and Reklaitis, G. V., "Optimal Design of Multi-Purpose Batch Plants 1. Problem Formulation," *Ind. Eng. Chem. Res.*, **29**, 2054 (1990).
- Papageorgaki, S. and Reklaitis, G. V., "Optimal Design of Multi-Purpose Batch Plants 2. A Decomposition Strategy," *Ind. Eng. Chem. Res.*, **29**, 2062 (1990).
- Park, S. Y. and Park, S., "Nonlinear Control of a Batch Ester-interchange Reactor," *Korean J. Chem. Eng.*, **16**, 745 (1999).
- Reinhart, H. J. U. and Rippin, D. W. T., "Design of Flexible Batch Chemical Plants," Presented at AIChE spring national meeting, New Orleans, LA (1986).
- Reinhart, H. J. U. and Rippin, D. W. T., "Design of Flexible Multiproduct Plants. A New Procedure for Optimal Equipment Sizing under Uncertainty," Presented at AIChE annual meeting, New York (1987).
- Straub, D. A. and Grossmann, I. E., "Integrated Statistical Metric of Flexibility for Systems with Discrete State and Continuous Parameter Uncertainties," *Comput. Chem. Eng.*, **14**(9), 967 (1990).
- Straub, D. A. and Grossmann, I. E., "Evaluation and Optimization of Flexibility in Multiproduct Batch Plants," *Comput. Chem. Eng.*, **16**, 69 (1992).
- Voudouris, V. T. and Grossmann, I. E., "MILP Reformulations for Batch Process Design with Discrete Equipment Sizes," *Ind. Eng. Chem. Res.*, **31**, 1315 (1992).
- Wen, C. Y. and Chang, T. M., "Optimal Design of Systems Involving Parameter Uncertainty," *Ind. Eng. Chem. Process Des. Dev.*, **7**, 49 (1968).