Flexible Retrofit Design of Multiproduct Batch Plants

R. Fletcher[1] , J.A.J. Hall[2] , and W.R. Johns[3]

Abstract

We treat the addition of new equipment to an existing multiproduct batch plant for which new production targets and selling profits have been specified. This optimal retrofit design problem has been considered by Vaselenak et al. (1987). Their constraint that new units must be used in the same manner for all products places a restriction on the design which could readily be overcome in practice. We present a mixed-integer nonlinear programming (MINLP) formulation which eliminates this constraint. A series of examples is presented which demonstrate greater profitability for plants designed with our formulation. The examples also bring to light a further unwanted constraint in the Vaselenak, Grossmann and Westerberg formulation. In their formulation they limit batch size to the smallest unit at a stage, even when that unit is not needed. It is noted that, at the expense of some additional mathematical complexity, our formulation could be enhanced to allow reconnexion of existing units and alternate use of multiple additional units.

1. Introduction

High value or low volume products are frequently manufactured in batch or semi-batch processes. Batch processes consist of a sequence of units, the capacity of each being specified by its volume. At each stage of processing, material is fed to a unit where it is processed for a specified period of time after which it is passed on to the next stage. Reactors, tanks and centrifuges are typical batch units. Semi-batch plant includes semi-continuous stages, such as pumps and heat exchangers, whose capacity is defined by throughput rate. In principle all batch plant is semi-batch but, where the semi-continuous stages make negligible contribution to the total cost, the plant is considered to be a batch process. The total production rate of a simple batch plant is specified by two parameters, the batch size and the cycle time. The batch size is determined by the piece of equipment with the least processing volume measured in terms of the volume of the final product. The cycle time is determined by the stage with the longest processing time. Throughput can be increased either by increasing the batch size or by reducing cycle time. The batch size can be increased by increasing the size (volume) of the limiting stage, either by replacing it with a larger item or by adding volume in parallel operated in phase. The cycle time can be reduced by duplicating the equipment at the limiting stage, halving the cycle time. If appropriate, the unit could be replicated reducing the cycle time by a factor.

Multi-product batch processes are designed to make a number of related products using the same equipment operating in the same sequence. The process is operated in campaigns, when, during each campaign of a number of days or weeks, one product is made. Because the products differ, the relationship between the volume at any one stage and the final batch size differs for each product. The limiting stage and the batch size are thus likely to differ for each product. Similarly the processing times at each stage may differ and the limiting stage and cycle time are expected to differ for each product.

In this paper we analyse the case of an existing plant for which new production targets and selling profits have been specified. New equipment in the form of a *retrofit* is to be added to give an economically optimal design. The conventions we adopt generally correspond to those used in the optimal multiproduct batch plant design problem as considered by Sparrow et al. (1975) and Grossmann and Sargent (1979). We present a new mathematical formulation of the retrofit problem and use it to treat a series of examples including those previously considered by Vaselenak et al. (1987). Our new formulation eliminates unnecessary arbitrary constraints introduced by Vaselenak et al. (1987) and gives rise to more economic retrofit designs.

[1] Univ. of Dundee.

[2] Univ. of Edinburgh.

[3] Intera Sciences, 45 Station Road, Henley-on-Thames, Oxon RG9 1AT, UK. (The author to whom correspondence should be addressed)

2. Problem formulation

Products are identified by the index i and the total number manufactured is the fixed parameter N. We must determine the quantity of product i produced in any one batch—the *batch size* $B_i(kg)$. In a multiproduct batch plant all the products follow essentially the same path through the plant, passing through a sequence of *batch stages*. These are identified by index j and the total number of stages in the plant is the fixed parameter M. Each stage is assumed to consist of a number of pieces of equipment or *units* which are identical in function and operated in parallel. The number of units in a stage of the existing plant is the fixed parameter N_j^{old} and the units within a stage are identified by the index m. The size of a unit in a stage of the existing plant is $(V_j^{old})_m(l)$. As a result of the conventional scheduling assumptions made in the design problem, in a *new* plant all the units in any stage are normally identical in size. However, it is a property which we do not assume in the existing plant since it may have been the subject of previous retrofits. A simple 2-stage batch plant is illustrated in Figure 2.1.

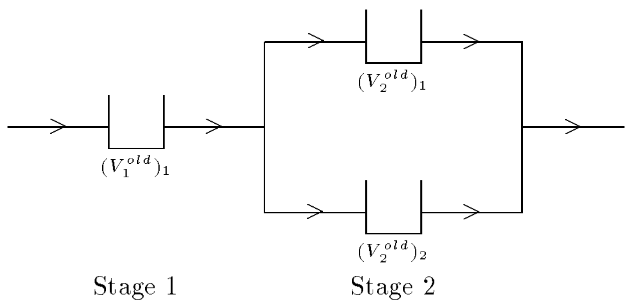

Figure 2.1. 2-stage batch plant.

Processing time and scheduling

Any piece of batch equipment normally goes through the basic cycle of filling, processing, emptying, cleaning and possibly waiting either empty or full. For product i in a unit of stage j this is conventionally modelled by by a *unit cycle time*, $T_{ij}(h)$, which excludes the waiting time. Grossmann and Sargent (1979) use the expression

$$T_{ij} = t_{ij} + c_{ij} B_i^{\gamma_j}$$

where $t_{ij} \geq 0$,$c_{ij} \geq 0$ and $\gamma_j \geq 0$ are fixed parameters. Vaselenak et al. (1987) take $c_{ij} = 0$ and we adopt this assumption in our formulation for reasons of comparison so the unit cycle time is t_{ij}. If there are $N_j \geq 2$ units in parallel in a stage and they are charged in turn with batches from the previous stage—operated in sequence—the *stage cycle time* is given by

$$\frac{T_{ij}}{N_j}.$$

The operating time period for the plant, $H(h)$ is typically $6\,000h$—one working year. We need to determine the number of batches, n_i of product i which are manufactured in this period. A limited overlapping production schedule is used. In this we assume that the production of batches of one product may overlap—several batches of a product may be in the plant at a given moment in time. However, we do not allow batches of different products to be in the plant at the same time. Thus the long-term production strategy assumes that a number of batches of one product are made before a changeover to another product. The scheduling problem in which several products can be manufactured simultaneously is very complex, being a 'job shop' problem and beyond the scope of this paper. Therefore, in common with Grossmann and Sargent (1979), for product i we define the *limiting cycle time*, T_{Li}—the time interval for producing successive batches—to be the maximum stage cycle time given by

$$T_{Li} = \max_{j=1\ldots M} \left(\frac{T_{ij}}{N_{ij}} \right).$$

The stage in which this is attained for a particular product is termed the 'cycle time bottleneck'. If the number of successive batches of a product that are produced is sufficiently large that the change-over time between products can be ignored, the constraint

$$\sum_{i=1}^{N} n_i T_{Li} \leq H$$

ensures that the number of batches of each product to be produced can be scheduled within the operating time period.

Batch sizes, total production and income

Each product manufactured will have different characteristics so the processing capacity required by unit mass in each piece of equipment will vary from one type of equipment to another and will be different for the various products. The processing capacity required per unit mass of product is assumed to be independent of the volume of the unit. It can, therefore, be identified with a stage. This *size factor* relates unit mass of product i in a batch leaving the plant to the volume required to process it in any unit in stage j and is the fixed parameter $S_{ij}(l/kg)$. Thus, for product i in a unit of volume V_j in stage j, we define the *unit batch size* to be V_j/S_{ij}. The *stage batch size* is the minimum unit batch size over all the units which are operated in sequence in any stage and the minimum stage batch size over all stages determines the *limiting batch size*. The stage in which this is attained is termed the 'batch size bottleneck'.

For a particular plant, the *batch processing parameters* are the number, size and limiting cycle time of batches of each product. The values of the batch processing parameters determine the total production. Sparrow et al. (1975) and Grossmann and Sargent (1979) require the quantity of product i manufactured in the operating period to be a certain mass $Q_i(kg)$ which yields the simple constraints

$$n_i B_i = Q_i \qquad i = 1, \ldots, N. \tag{2.1}$$

However, in common with Vaselenak et al. (1987), we consider Q_i as a production target which need not necessarily be achieved and the expected net income from selling unit mass of product i, p_i is introduced. This production value is the selling price offset against the cost of items such as raw materials. Hence constraints (2.1) are replaced by

$$n_i B_i \leq Q_i \qquad i = 1, \ldots, N$$

The optimal design criterion is then economic and the total production value

$$\sum_{i=1}^{N} p_i n_i B_i \tag{2.2}$$

becomes an economic optimization criterion.

Equipment cost

The volume of equipment is bounded such that in stage j the volume of a unit lies between V_j^L and V_j^U. Whether equipment is assumed to be available in either a continuous or discrete set of sizes is an important distinction when defining a model. Currently, in common with Vaselenak et al. (1987), Sparrow et al. (1975) and Grossmann and Sargent (1979), we assume that new units are available in a continuous range of sizes. The capital cost of a piece of equipment of the type to be used in stage j is conventionally accounted for by a function of the volume V of the form

$$K_j + c_j V^{r_j}$$

where $K_j \geq 0$, $c_j \geq 0$ and $r_j \geq 0$ are fixed parameters such that the minimum unit cost

$$K_j + c_j (V_j^L)^{r_j}$$

is non-zero. This cost function (with r_j typically 0.6) has been implemented in our current production code but in this paper, for comparison with Vaselenak et al. (1987), we set $r_j = 1.0$.

The retrofit design problem

Suppose that new production targets are defined. If they can be achieved with the existing plant, no alterations are necessary. If, however, the new targets cannot be reached, additional pieces of equipment may be purchased to increase the total production of some or all products and we have a retrofit design problem.

In a retrofit design problem, a revised plant configuration, operating strategy, equipment sizes and batch processing parameters must be found for which the *plant profitability*—the total production value (2.2) minus the cost of (any) new equipment—is optimal. The selection of the number of new units to add to each stage of the plant and their method of operation form the *retrofit strategy* and are discrete decisions, represented in the mathematical formulation by binary or integer variables. The volume of each new unit and the batch processing parameters can take any values, within certain bounds, and are represented by continuous variables. The decisions in the design problem thus fall into two classes, binary and real. This distinction is important since it characterizes the method of solution.

New units may be added to any stage in parallel with existing units. This forms a new plant configuration for which an operating strategy must be defined. The operating strategy for each new unit allows the following options.

1. Operate in phase with existing unit m effectively to increase its capacity—option B_m.
2. Operate in sequence with the existing units to decrease the stage cycle time—option C.

The formulation of the retrofit problem used by Vaselenak et al. (1987)—the VGW formulation—assumes that either option B_m is taken for all products or option C is taken for all products. Our formulation of the problem—the FHJ formulation—allows the operating strategy to be chosen independently for each product. Thus, for product i, a particular new unit may be operated using option B_{m_i} *or* option C. It is also possible that a new unit may not be used to process a particular product. The greater flexibility of the FHJ formulation is illustrated in the example introduced in Table 2.1 below.

Depending on the location of the bottlenecks, production can be increased either by option B_m to allow larger batches of some products to be processed or by option C to reduce the limiting cycle time for some products. The FHJ formulation is presented as a mixed integer nonlinear programming (MINLP) problem in Section 3. A quantitative comparison between the FHJ and VGW formulations is made using the examples in Section 4. Conclusions regarding the merits of the two formulations are offered in Section 5.

Before going on to a more complex examples, a simple illustration of the options allowed by the alternative formulations will be given for the manufacture of products P_1 and P_2 using the basic plant illustrated in Figure 1. In the existing plant, the two units of stage 2 are operated alternately to give the least possible cycle time. All three units have the same volume v. The cycle time and size factor data are given in Table 2.1.

	Unit Cycle Times, t_{ij}		Size Factors, S_{ij}	
product	stage 1	stage 2	stage 1	stage 2
P_1	1/2	2	v	$v/2$
P_2	1	1	$v/2$	v

Table 2.1 Example cycle times and size factors for products P_1 and P_2

The production for the existing plant is given as case 1 in Table 2.2. The other cases considered are

case 2: new unit in stage 1 of size v operated in phase for both products,

case 3a: new unit in stage 1 of size v operated in sequence for both products,

case 3b: new unit in stage 1 of size $v/2$ operated in sequence for both products,

case 4a: new unit in stage 1 of size v operated in phase for P_1 and in sequence for P_2,

case 4b: new unit in stage 1 of size $v/2$ not used for P_1 and in sequence for P_2 and

case 5: no new units added but the two existing units in stage 2 operated in sequence for P_1 and in phase for P_2.

Case		Operation		Cycle Times			Batch Sizes			Rate
		Stage		Stage		limit	Stage		limit	
		1	2	1	2		1	2		
1	P_1	-	C	1/2	1	1	1	2	1	1
	P_2	-	C	1	1/2	1	2	1	1	1
2	P_1	B	C	1/2	1	1	2	2	2	2
	P_2	B	C	1	1/2	1	4	1	1	1
3a	P_1	C	C	1/4	1	1	1	2	1	1
	P_2	C	C	1/2	1/2	1/2	2	1	1	2
3b	P_1	C	C	1/4	1	1	1/2	2	1/2	1/2
	P_2	C	C	1/2	1/2	1/2	1	1	1	2
4a	P_1	B	C	1/2	1	1	2	2	2	2
	P_2	C	C	1/2	1/2	1/2	2	1	1	2
4b	P_1	-	C	1/2	1	1	1	2	2	1
	P_2	C	C	1/2	1/2	1/2	2	1	1	2
5	P_1	-	C	1/2	1	1	1	2	1	1
	P_2	-	B	1	1	1	2	2	2	2

Table 2.2 Illustrative retrofit operation strategies for products $P_1$and P_2

The production for Case 1—the existing plant—is calculated as follows:

The cycle times for stage 1 are as given in Table 2.1. For stage 2, the cycle times are reduced by a factor of 2 because the two units operate alternately. The batch sizes are calculated from v/S_{ij}. The production rate of each product is then simply calculated from (batch size limit)/(cycle time limit).

Case 2 is one of the retrofit expansions permitted by the VGW formulation. The effective volume in stage 1 is doubled by adding a unit of size v in parallel with the existing unit and operating it in phase. Cycle times are unaltered but batch sizes in stage 1 are increased to $2v/S_{ij}$. Case 3a is an alternative retrofit expansion allowed by the VGW formulation. The effective cycle time for stage 1 is halved by adding a unit of size v which is operated in sequence with the original unit. These two alternative ways of adding the unit of size v either enable the production rate of P_1 or of P_2 to be doubled.

Both cases 2 and 3a are also allowed in the FHJ formulation. FHJ does, however, allow an additional way of adding a single unit of size v to stage 1 and this expansion is illustrated as case 4a. The additional unit is operated in phase for P_1 and in sequence for P_2. This simple modification to the operating strategy enables the production rates of *both* products to be doubled at no extra cost above that for cases 2 or 3a.

Case 3b illustrates an unfortunate constraint imposed by the VGW formulation when adding units to reduce cycle time for all products. In case 3a the production rate for P_2 is doubled by halving its cycle time in stage 1 and hence its limiting cycle time. In stage 1 the size of vessel required to process the limiting batch size for P_2 is $v/2$ so, in operation, the vessels of size v will be half full. Thus, adding a vessel of size $v/2$ to stage 1 would allow the cycle time for P_2 to be halved whilst maintaining the limiting batch size. However, we are also required to use the new vessel in stage 1 to halve the cycle time for P_1. The cycle time bottleneck for P_1 is in stage 2 so we gain no overall benefit from this reduction. Unfortunately, the current limiting batch size requires a processing volume v in stage 1. Thus, operating vessels of size $v/2$ and v in sequence in stage 1 halves the stage 1 batch size and hence limiting batch size for P_1. Hence the production rates are halved for P_1 and doubled for P_2. This operating strategy is illustrated in case 3b. If only we could simply not use the new unit for P_1! Case 4b does just this but is only allowed by the FHJ formulation. The new unit of size $v/2$ in stage 1 is used to halve the cycle time for P_2 as in case 3b. For product P_1 we consider the new unit to be operated in phase with the original but, since the available capacity is $3v/2$ and the requirement given by the batch size bottleneck is v, the new unit is effectively unused in the production of P_1. Hence the production rate is doubled for P_2 and maintained for P_1.

Finally, case 5 shows how a simple modification to the operating strategy of the existing plant enables the production rate of P_2 to be doubled *without adding any new equipment*. The problem of maximizing the output from an existing plant by 're-sequencing' existing equipment is also of practical interest. This is the subject of current research by Fletcher et al. which also allows new equipment to be added.

The simple illustrations of Table 2.2 demonstrate that the FHJ formulation provides the potential to give a greater increase in production rate than the VGW formulation for the same cost or the same increase for a lesser cost. The example also illustrates the qualitative difference between the VGW and FHJ formulations. The detailed mathematical formulation of the FHJ optimization is given in Section 3 and its application to the VGW problems given in Section 4.

3. Formulation and solution

A retrofit strategy is determined by discrete decisions represented in the formulation below by binary variables. New units within stage j are identified by index k and the decision to add a particular new unit is indicated by the binary variable y_{jk} taking the value 1. The maximum number of new units which can be added to stage j and to the plant as a whole are denoted by Z_j and Z^U respectively. The operating strategy option B_m or C with product i for the k^{th} new unit in stage j is indicated by one of the binary variables $(y^B_{ijk})_m$ or y^C_{ijk} taking the value 1.

In stage j the k^{th} new unit is of volume V_{jk}. Corresponding to the operating strategy selected for product i the *processing volume* required is represented by the variable $(V^B_{ijk})_m$ or V^C_{ijk}. The bounds on all variables are given in the nomenclature.

MINLP formulation

The objective function for the problem is the maximization

$$\max \sum_{i=1}^{N} p_i n_i B_i - \sum_{j=1}^{M} \sum_{k=1}^{Z_j} (K_j y_{jk} + c_j V_{jk}). \tag{3.1}$$

Production targets give the constraints

$$n_i B_i \leq Q_i \qquad i = 1, \ldots, N. \tag{3.2}$$

The limiting cycle time of product i is given by

$$T_{Li} = \max_{j=1\ldots M} \left(\frac{t_{ij}}{N_{ij}} \right), \quad \text{where} \quad N_{ij} = N_j^{old} + \sum_{k=1}^{Z_j} y^C_{ijk}$$

which yields constraints

$$N_j^{old} + \sum_{k=1}^{Z_j} y^C_{ijk} \geq t_{ij}/T_{Li} \qquad \begin{array}{l} i = 1, \ldots, N \\ j = 1, \ldots, M. \end{array} \tag{3.3}$$

The operating time period gives the constraint

$$\sum_{i=1}^{N} n_i T_{Li} \leq H. \tag{3.4}$$

The bound on the total number of new units yields the constraint

$$\sum_{j=1}^{M} \sum_{k=1}^{Z_j} y_{jk} \leq Z^U. \tag{3.5}$$

To ensure that new units when used satisfy the lower bound on their volume we require the constraints

$$V_{jk} \geq y_{jk} V_j^L \qquad \begin{array}{l} j = 1,\ldots,M \\ k = 1,\ldots,Z_j. \end{array} \tag{3.6}$$

The requirement that, for each product, each new unit is either operated in phase with an existing unit or in sequence gives the constraints

$$y_{jk} = \sum_{m=1}^{N_j^{old}} (y_{ijk}^B)_m + y_{ijk}^C \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j. \end{array} \tag{3.7}$$

When new units are added to stage j and used in phase with existing units, the requirement that the volume is sufficient to process the batch size yields the *option B capacity constraints*

$$\sum_{k=1}^{Z_j} (V_{ijk}^B)_m + (V_j^{old})_m \geq S_{ij} B_i \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ m = 1,\ldots,N_j^{old}. \end{array} \tag{3.8}$$

It can be observed that if, for some retrofit strategy, $(y_{ijk}^B)_m = 1$ and the optimal processing volume $(V_{ijk}^B)_m = 0$ then in stage j new unit k is not used to process product i.

Suppose we replace (3.7) by inequalities which allow $y_{ijk}^C = 0$ and $(y_{ijk}^B)_m = 0 \; \forall m$ if $y_{jk} = 1$. This forces $(V_{ijk}^B)_m = 0$ and might seem a more obvious way to represent a new unit not being used for product i. However, this could allow distinct assignments of binary variables to lead to identical designs—a source of redundancy which should be avoided.

When new units are added to stage j and used in sequence with existing units, we have the *option C capacity constraints* which ensure that the volumes of the units operated in sequence are sufficient to process the batch size.

$$U\left(1 - y_{ijk}^C\right) + V_{ijk}^C \geq S_{ij} B_i \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j. \end{array} \tag{3.9}$$

where U is a large number which ensures that this constraint is satisfied when $y_{ijk}^C = 0$.

The restrictions on the processing volume of new units give constraints

$$\begin{array}{l} (V_{ijk}^B)_m \leq V_{jk} \\ (V_{ijk}^B)_m \leq U (y_{ijk}^B)_m \end{array} \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j \\ m = 1,\ldots,N_j^{old} \end{array} \tag{3.10}$$

and

$$\begin{array}{l} V_{ijk}^C \leq V_{jk} \\ V_{ijk}^C \leq U y_{ijk}^C \end{array} \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j. \end{array} \tag{3.11}$$

Distinct assignments of new units are guaranteed by the constraints

$$y_{jk} \geq y_{j\,k+1} \qquad \begin{array}{l} j = 1,\ldots,M \\ k = 1,\ldots,Z_j - 1. \end{array} \tag{3.12}$$

Exponential transformations to remove non-convex bilinearities

The problem defined by (3.1–3.12) is one of mixed integer nonlinear programming (MINLP). An efficient algorithm for solving convex MINLP problems is described by Duran and Grossmann (1986). The algorithm of Duran and Grossmann is described for a minimization problem so, for the purpose of theoretical discusstion, it is convenient to consider the minimization of (3.1) with a change of sign. However, when discussing the practical implications of optimal designs for the examples in Section 3, the value of the original objective function (3.1) is used. This is also done by Vaselenak et al. (1987).

The formulation above also contains non-convex bilinear functions in (3.1), (3.2) and (3.4) and these must be removed. As described by Vaselenak et al. (1987), suitable exponential transformations of the variables involved can be used to achieve this. The details for our formulation are identical so we simply present the reformulated problem.

Defining the following variables:

$$\begin{aligned} x_{1i} &= \ln n_i \\ x_{2i} &= \ln B_i \qquad i = 1,\ldots,N \\ x_{3i} &= \ln T_{Li} \end{aligned} \tag{3.13}$$

we obtain the MINLP formulation below.

$$\min\ -\sum_{i=1}^{N} p_i \exp(x_{1i} + x_{2i}) + \sum_{j=1}^{M}\sum_{k=1}^{Z_j}(K_j y_{jk} + c_j V_{jk}) \tag{3.14}$$

subject to

mixed integer linear constraints

$$x_{1i} + x_{2i} \le \ln Q_i \qquad i = 1,\ldots,N, \tag{3.15}$$

$$-V_{jk} \le -y_{jk} V_j^L \qquad \begin{array}{l} j = 1,\ldots,M \\ k = 1,\ldots,Z_j, \end{array} \tag{3.16}$$

$$-\sum_{k=1}^{Z_j}(V_{ijk}^B)_m + S_{ij}B_i \le (V_j^{old})_m \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ m = 1,\ldots,N_j^{old}, \end{array} \tag{3.17}$$

$$-V_{ijk}^C + S_{ij}B_i \le U(1 - y_{ijk}^C) \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j, \end{array} \tag{3.18}$$

$$\begin{aligned} -V_{jk} + (V_{ijk}^B)_m &\le 0 \\ (V_{ijk}^B)_m &\le U(y_{ijk}^B)_m \end{aligned} \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j \\ m = 1,\ldots,N_j^{old}, \end{array} \tag{3.19}$$

$$\begin{aligned} -V_{jk} + V_{ijk}^C &\le 0 \\ V_{ijk}^C &\le U y_{ijk}^C \end{aligned} \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j, \end{array} \tag{3.20}$$

integer linear constraints

$$\sum_{j=1}^{M}\sum_{k=1}^{Z_j} y_{jk} \le Z^U. \tag{3.21}$$

$$\sum_{m=1}^{N_j^{old}} (y_{ijk}^B)_m + y_{ijk}^C - y_{jk} = 0 \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M \\ k = 1,\ldots,Z_j, \end{array} \tag{3.22}$$

$$-y_{jk} + y_{j\,k+1} \le 0 \qquad \begin{array}{l} j = 1,\ldots,M \\ k = 1,\ldots,Z_j - 1, \end{array} \tag{3.23}$$

nonlinear constraints

$$t_{ij}\exp(-x_{3i}) \le N_j^{old} + \sum_{k=1}^{Z_j} y_{ijk}^C \qquad \begin{array}{l} i = 1,\ldots,N \\ j = 1,\ldots,M, \end{array} \tag{3.24}$$

$$\sum_{i=1}^{N} \exp(x_{1i} + x_{3i}) \le H \tag{3.25}$$

and

$$\exp(x_{2i}) - B_i \le 0 \qquad i = 1,\ldots,N. \tag{3.26}$$

Solving the MINLP problem

The algorithm of Duran and Grossmann (1986) solves a MINLP problem by solving a sequence of subproblems. These alternate between nonlinear programming (NLP) and mixed-integer linear programming (MILP). Indexed by k, they commence with NLP^1.

The NLP problems correspond to the MINLP problem with fixed assignments of the binary variables so the MINLP algorithm requires an initial assignment. Physically, the solution of MILP^k determines a retrofit strategy for which optimal values for the volumes of new units and the batch processing parameters are determined by the solution of NLP^{k+1}. Unless we have some heuristic or intuitive idea of the optimal retrofit strategy, we choose the initial assignment of binary variables which corresponds to the unmodified plant. Its optimal batch processing parameters are always of interest since if the new production targets are achieved then it solves the MINLP problem.

The MILP problems minimize a piecewise linear approximation to the MINLP objective function—linearizations being made at the solution of each NLP problem—subject to the linear constraints and a set of linear approximations for each nonlinear constraint of the MINLP problem, together with constraints (integer cuts) which make previous assignments infeasible.

The algorithm yields the global solution to a convex MINLP problem since convex NLP problems have unique global solutions and linearizations of convex functions underestimate them. This ensures that the feasible region of the MINLP problem is included in that of the MILP problems and that the set of linearizations of the MINLP objective function underestimate it. However, in the MINLP defined by (3.13–3.26) the negative exponentials of the term representing production value in the objective function are concave.

Despite the non-convexities in (3.14), it is shown by Vaselenak et al. (1987) that if the binary variables are fixed the resulting NLP problem has a unique optimal solution. However, linearizations of the negative exponentials in (3.14) *overestimate* the MINLP objective function so a system of piecewise linear underestimators must be set up as described by Vaselenak et al. (1987). Hence the algorithm of Duran and Grossmann can be shown to find the global solution of the formulation presented above.

The resulting MILP problems yield many highly degenerate LP problems. The solution of these has led to advances in the LP method of Fletcher (1988) which are described by Fletcher and Hall (1990).

4. Examples

Three examples are presented. The first two are due to Vaselenak et al. (1987) and demonstrate that a retrofit strategy giving greater profit exists within the FHJ formulation. The third example demonstrates a situation where the FHJ formulation results in a strategy which is considerably better than that obtained using the VGW formulation. Such a situation is likely to arise wherever there are significant differences in times and size factors between products at each stage, and their bottlenecks lie in different stages.

Each example has been solved using both formulations. The results are presented in terms of the sequence of retrofit strategies considered during the solution of each problem using the algorithm of Duran and Grossmann (1986). The operation option for each basic configuration is indicated by the entry B_m if a new unit is to be operated in phase with existing unit m and C if it is to be operated in sequence with existing units. With our formulation, if a new unit is not used in the manufacture of a particular product, this is indicated by the entry N.

Example 1

The data for this example are given in Table 4.1.1 and the sequence of retrofit strategies considered using the VGW and FHJ formulations are given in Tables 4.1.2 and 4.1.3 respectively.

	stage 1	stage 2
product	$t_{ij}(h)$	
P_1	4.0	6.0
P_2	5.0	3.0
product	$S_{ij}(l/kg)$	
P_1	2.0	1.0
P_2	1.5	2.25
N_j^{old}	1	1
$V_j^{old}(l)$	4 000	3 000
Z_j	2	2
$K_j(£)$	30 560	30 560
$c_j(£/l)$	32.54	32.54
$V_j^L(l)$	0	0
$V_j^U(l)$	4 000	3 000
product	$p_i(£/kg)$	$Q_i(kg)$
P_1	1.0	1 200 000
P_2	2.0	1 000 000

Table 4.1.1. Data for example 1

The value of the objective function for the optimal design with the FHJ formulation shows an improvement of only 0.3% over that for the VGW formulation. This is due to the relatively large production value compared with cost of new units. However, since the new production targets are attained using both optimal designs, the cost of the new equipment can be used to compare the respective designs. The VGW formulation required the purchase of £85 450 worth of new equipment. The corresponding value for the FHJ formulation was £75 950 which represents a saving of 11%.

NLP	new units		operation	objective
k	stage	size(l)	all products	£
1	–	–	–	2 750 000
2	2	1 687	B_1	3 115 000

Table 4.1.2. Retrofit strategies considered using the VGW formulation

NLP	new units		operation		objective
k	stage	size(l)	P_1	P_2	£
1	–	–	–	–	2 750 000
2	2	1 687	N	B_1	3 115 000
3	1	1 358	B_1	C	3 125 000
4	2	1 395	C	B_1	3 124 000

Table 4.1.3. Retrofit strategies considered using the FHJ formulation

Example 2

For this example the data are given in Table 4.2.1 and the sequence of retrofit strategies considered are given in Table 4.2.2 for the VGW formulation and Table 4.2.3 for the FHJ formulation.

	stage 1	stage 2	stage 3	stage 4
product		$t_{ij}(h)$		
P_1	6.3822	4.7393	8.3353	3.9443
P_2	6.7938	6.4175	6.4750	4.4382
P_3	1.0135	6.2699	5.3713	11.9213
P_4	3.1977	3.0415	3.4609	3.3047
product		$S_{ij}(l/kg)$		
P_1	7.9130	2.0815	5.2268	4.9523
P_2	0.7891	0.2871	0.2744	3.3951
P_3	0.7122	2.5889	1.6425	3.5903
P_4	4.6730	2.3586	1.6087	2.7879
N_j^{old}	1	1	2	1
$V_j^{old}(l)$	4 000	4 000	3 000	3 000
Z_j	2	2	2	2
$K_j(£)$	15 280	38 200	45 840	10 180
$c_j(£/l)$	16.27	40.68	48.81	10.84
$V_j^L(l)$	0	0	0	0
$V_j^U(l)$	4 000	4 000	3 000	3 000
product	$p_i(£/kg)$	$Q_i(kg)$		
P_1	1.114	268 200		
P_2	0.535	156 000		
P_3	0.774	189 700		
P_4	0.224	166 100		

Table 4.2.1. Data for example 2

The value of the objective function for the optimal design with the FHJ formulation again shows only a small improvement (0.7%) over that for the VGW formulation. The production targets are not achieved with either of the optimal designs. With the VGW formulation less was spent on new equipment but the value of the additional production obtained using the FHJ formulation more than makes up for this.

NLP	new units		operation	objective
k	stage	size(l)	all products	£
1	–	–	–	461 400
2	4	2 547	B_1	518 000

Table 4.2.2. Retrofit strategies considered using the VGW formulation

NLP	new units		operation				objective
k	stage	size(l)	P_1	P_2	P_3	P_4	£
1	–	–	–	–	–	–	461 400
2	4	2 547	N	B_1	B_1	N	518 000
3	4	3 000	N	B_1	C	C	521 800

Table 4.2.3. Retrofit strategies considered using the FHJ formulation

Example 3

Table 4.3.1 gives the data for this example and the sequence of retrofit strategies considered using the VGW and FHJ formulations are given in Tables 4.3.2 and 4.3.3 respectively.

	stage 1	stage 2
product	$t_{ij}(h)$	
P_1	4.7	10.1
P_2	4.1	3.8
P_3	2.9	2.7
P_4	5.3	11.8
product	$S_{ij}(l/kg)$	
P_1	4.8	2.0
P_2	3.6	4.9
P_3	3.9	5.6
P_4	8.3	3.6
N_j^{old}	1	1
$V_j^{old}(l)$	4 000	3 000
Z_j	2	2
$K_j(£)$	12 800	11 400
$c_j(£/l)$	13.63	12.14
$V_j^L(l)$	1 000	1 000
$V_j^U(l)$	4 000	3 000
product	$p_i(£/kg)$	$Q_i(kg)$
P_1	0.63	290 000
P_2	0.53	300 000
P_3	0.44	350 000
P_4	1.09	140 000

Table 4.3.1. Data for example 3

With the FHJ formulation the value of the objective function for the optimal design shows an improvement of 12% over that for the VGW formulation. The new production targets are attained with both optimal designs so, as in Example 1, the cost of the new equipment can be used to compare the respective designs. The VGW formulation required the purchase of £96 400 worth of new equipment. The corresponding value for the FHJ formulation was £32 000 which is a saving of 67%.

The optimal solution with the FHJ formulation involves adding one new unit of volume 1 699l in parallel with the existing one in stage 2 at a cost of £32 000 and using it in sequence for P_1 and P_4 and in phase for P_2 and P_3. Within the VGW formulation it is reasonable, therefore, to consider the following retrofit strategy. Add two new units to stage 2 in parallel with the existing one. One is operated in phase with the original and the other in sequence (for all products). Clearly, adding units each of volume 1 699l allows the same production levels to be attained as with the optimal solution using our formulation. These production levels were all at their upper bounds giving a total production value of £648 300. When the cost of the new units (£64 000) is deducted, the profitability is £584 300. Why is this not the optimal solution using the VGW formulation?

The answer is that we are forced to halve the cycle time for P_2 and P_3 to no practical advantage since their cycle time bottlenecks are in stage 1 but add a larger unit simply to maintain their limiting batch sizes which occur in stage 2. If the upper bound on the volume of new units is raised, it is found that the optimal new unit volumes for the retrofit strategy are one of volume 1 631l operating in phase with the original and one of volume 4 631l operating in sequence. The extra cost of the larger unit reduces the profitability to £549 500 and the optimal retrofit strategy remains that corresponding to NLP^4 above. Thus we see in practice the effect of the constraint on the design problem in the VGW formulation which was highlighted in the simple example in Section 2.

NLP	new units		operation	objective
k	stage	size(l)	all products	£
1	–	–	–	386 500
2	2	3 000	C	490 100
3	1	3 465	B_1	
	2	2 137	B_1	550 900
4	1	2 624	B_1	
	2	3 000	C	551 900
5	1	3 733	C	
	2	2 568	C	542 000

Table 4.3.2. Retrofit strategies considered using the VGW formulation

NLP	new units		operation				objective
k	stage	size(l)	P_1	P_2	P_3	P_4	£
1	–	–	–	–	–	–	386 500
2	2	1 699	C	B_1	B_1	C	616 300

Table 4.3.3. Retrofit strategies considered using the FHJ formulation

Comparison of formulations

Example 2 shows that it is not always possible to compare the formulations in terms of the expenditure on new equipment since the production value generally will not be the same if the production targets are not reached. When the two formulations are considered in terms of the profitability of the optimal retrofit design offset against the profitability of the existing plant the performance of the two formulations is compared in Table 4.4.

Examples	1	2	3
VGW formulation	13%	12%	43%
FHJ formulation	14%	13%	59%

Table 4.4. Comparison of formulations

5. Conclusions

The new formulation for optimal multiproduct batch plant design presented in the paper includes the formulation presented by Vaselenak et al. (1987) as a subset. Thus the new formulation will give rise to designs at least as good as those obtained using the VGW formulation. The examples also throw up a case which reveals a further shortcoming in the MINLP formulation adopted by Vaselenak et al. (1987) whereby the solutions that they obtain do not meet the optimum that they claim to achieve, ie the best profitability adding units either all in parallel or all in sequence.

It is therefore concluded that the new retrofit optimization formulation presented here represents a significant advance on previous practice and should be adopted. It should be noted, however, that even this formulation excludes plant designs that could easily be achieved in practice, eg by re-sequencing existing equipment or grouping new equipment in alternative ways for different products. The new formulation is currently being evaluated by Fletcher et al. and will be published in the near future.

It should be noted that each greater degree of operating flexibility introduces a larger number of binary (decision) variables. For the formulation above, the NLP subproblems are simple and the dominant cost in solving the MINLP problem is that of solving the MILP problems. Their computational cost is essentially related to the number of integer variables and our formulation requires $O(N)$ times as many as the formulation of Vaselenak et al. (1987), where N is the number of products. Thus, for problems with a large number of products, our formulation is potentially more expensive. For the examples studied, however, both formulations can be solved in a few seconds on a SUN 3/60 workstation.

In the future we expect our physical models to represent more realistic chemical engineering design problems which will include non-linear relationships between the performance parameters and the detailed physical dimensions that determine the cost of equipment. We should also allow for it to be more economic to use standard equipment sizes. Both these developments favour our new formulation. First, more complex relationships will tend to make the solution of tht NLP subproblems the dominant cost and there is no indication that our formulation consistently generates more NLP subproblems. Secondly, the treatment of standard equipment sizes requires that some of our real variables are replaced by non-binary integer variables. These variables are more difficult to handle than binaries and will impact equally on the VGW and FHJ formulations, thus reducing the difference in size between the MILP problems. For the present we are, therefore, convinced that the benefits in improved designs achievable by using the FHJ formulation outweigh any marginal differences in computational complexity.

The further development that we propose is to allow reallocation of existing equipment and alternate use of new units where more than one new unit per stage is added. This formulation may require a sufficient number of additional binary variables to make MILP run times excessive and requires further investigation.

The future developments that we anticipate, with larger nonlinear, nonconvex problems with non-integer and binary variables are not well treated with current MINLP codes. We therefore see further development of mathematical techniques to be complementary to advances in batch plant design.

Nomenclature

The parameters which define the problem are

$N =$ The number of products manufactured

$M =$ The number of stages in the production

$N_j^{old} =$ The number existing units in stage j

$(V_j^{old})_m =$ The volume of existing unit m in stage j

$t_{ij} =$ The unit cycle time of product i in stage j

$H =$ The operating time period

$S_{ij} =$ The size factor of product i in stage j

$K_j =$ The annualized fixed charge of a new unit in stage j

$c_j =$ The annualized cost coefficient of a new unit in stage j

$Q_i =$ The upper bound on production of product i

$p_i =$ The expected net profit per unit of product i

$V_j^L =$ The minimum volume of new units in stage j

$V_j^U =$ The maximum volume of new units in stage j

$Z_j =$ The maximum number of units which can be added to stage j

$Z^U =$ The maximum number of units which can be added to the plant

The solution space is defined by the following variables with the limits given in brackets.

$n_i =$ The number of batches of product i (≥ 0)

$B_i =$ The batch size of product i (≥ 0)

$T_{Li} =$ The limiting cycle time of product i (≥ 0)

$V_{jk} =$ The volume of new unit k in stage j $(V_j^U \leq V_{jk} \leq V_j^L)$

$(V_{ijk}^B)_m =$ The volume required in new unit k in stage j for product i to use it in phase with existing unit m (≥ 0)

$V_{ijk}^C =$ The volume required in new unit k in stage j for product i to use it in sequence with existing units (≥ 0)

$y_{jk} =$ The binary variable for new unit k in stage j $(0, 1)$

$(y_{ijk}^B)_m =$ The binary variable of new unit k in stage j for product i to use it in phase with existing unit m $(0, 1)$

$y_{ijk}^C =$ The binary variable of new unit k in stage j for product i to use it in sequence with existing units $(0, 1)$

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