

Global Optimization In Multiproduct and Multipurpose Batch Design Under Uncertainty

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Abstract

This paper addresses the design of multiproduct and multipurpose batch plants with uncertainty in both product demands and in processing parameters. The uncertain demands may be described by any continuous/discrete probability distribution. Uncertain processing parameters are handled in a scenario-based approach. Through the relaxation of the feasibility requirement, the design problem with a fixed number of pieces of equipment per stage is formulated as a single large-scale nonconvex optimization problem. This problem is solved using a branch and bound technique in which a convex relaxation of the original nonconvex problem is solved to provide a lower bound on the global solution. Several different expressions for the tight convex lower bounding functions are proposed. Using these expressions, a tight lower bound on the global optimum solution can be obtained at each iteration. The α BB algorithm (Androulakis *et al.* (1995)) is subsequently employed to refine the upper and lower bounds and converge to the global solution. The tight lower bounds and the efficiency of the proposed approach is demonstrated in several example problems. These case studies correspond to large-scale global optimization problems with nonconvex constraints ranging in number from 25 to 3,750, variables ranging from 30 to 15,636 and nonconvex terms ranging from 50 to 15,000. It is shown that such large-scale multiproduct and multipurpose batch design problems can be solved to global optimality with reasonable computational effort.

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1 Introduction

Batch processes are a popular method for manufacturing products in low volume or that require several complicated steps in the synthesis procedure. The growth in the market for specialty chemicals has contributed to the demand for efficient batch plants. This paper will focus on two types of batch plant, multiproduct plants, and multipurpose plants. In the multiproduct plant, all products follow the same sequence of processing steps. Typically, one product is produced at a time in what is termed a single-product campaign (SPC). Multipurpose batch plants allow products to be processed using different sequences of equipment, and in some cases products can be produced simultaneously.

An important area of concern in the design of multiproduct and multipurpose batch plants is their ability to meet production requirements and maximize profits given uncertainties both in the market demand for the products and in the operation of the process. While significant progress has been made in the design and scheduling of batch plants, until recently the issues of flexibility and design under uncertainty have received little attention. Among the early work on the deterministic design problem, Sparrow *et al.* (1975) addressed the problem of multiproduct batch plant design via both a heuristic approach and a branch and bound formulation. This formulation assumed a single product campaign. Grossmann and Sargent (1979) presented a mixed-integer nonlinear programming (MINLP) formulation of the problem presented by Sparrow *et al.* (1975). Birewar and Grossmann (1989) incorporated the problem of scheduling in the design of multiproduct batch plants with mixed product campaigns. Voudouris and Grossmann (1992) showed that by restricting the equipment sizes to discrete values, the formulations of Grossmann and Sargent (1979) and Birewar and Grossmann (1989) could be reformulated as a series of mixed-integer linear programs (MILPs) which are more easily solved.

Among the first to address the problem of batch plant design under uncertainty in a novel way were Marketos (1975), and Johns *et al.* (1978). They divided the variables in the design problem into five categories: structural, design, state, operating, and uncertain. Structural variables describe the interconnections of the equipment in the plant. Design variables describe the size of the process equipment and are fixed once the plant is constructed. State variables are dependent variables and are determined once the design and operating variables are specified. Operating variables are those whose values can be changed in response to variations in the uncertain variables. Finally, the uncertain parameters are the quantities that can have random values which can be described by a probability distribution. Usually the uncertain parameters have normal distributions and are considered to be independent of each other. Johns *et al.* (1978) also introduced the distinction between variations which have short-term effects and those with long-term effects. Wellons and Reklaitis (1989) extended this idea, suggesting a distinction between “hard” and “soft” constraints in which the former must be satisfied for feasible plant operation, but the latter may be violated, subject to a penalty in the objective function. They considered the time required to produce a product as uncertain and developed a problem formulation.

Reinhart and Rippin (1986), (1987) addressed the problem of multiproduct batch plant design with uncertainties in both demand for the products and in technical parameters such as processing times and size factors. They restricted their designs to one piece of equipment

per stage. Fichtner *et al.* (1990) presented several variations on the problem of design with uncertain demands. They used interval methods to develop different solution procedures, including a two-stage approach and a penalty function approach. Another type of batch plant is the multipurpose plant. Shah and Pantelides (1992) proposed a scenario-based approach for the design of multipurpose batch plants with uncertain production requirements. The multipurpose approach resulted in a large-scale MILP model for which efficient techniques for obtaining good upper and lower bounds were proposed. Straub and Grossmann (1992) developed a model for the multiproduct batch design problem which takes into account uncertainties in the product demands and in equipment availability. They considered the problem of design feasibility separately from the maximization of profits and presented an approach for achieving both criteria. Subrahmanyam *et al.* (1994) addressed the problem of uncertain demands, and used a scenario-based approach with discrete probability distributions for the demands. In addition, they considered the scheduling problem as a second stage, following the design problem. Ierapetritou and Pistikopoulos (1995), (1996) considered the multiproduct batch plant design problem based on a stochastic programming formulation. They developed a relaxation of the production feasibility requirement and added a penalty term to the objective function to account for partial feasibility. Through this analysis, the problem can be reformulated as a single large-scale nonconvex optimization problem.

The scheduling strategy of a multiproduct batch plant can have a significant impact on the design. The usual single-product campaign assumption can overestimate the time required to process the products, resulting in a large overdesign of the plant equipment. Birewar and Grossmann (1989) proposed design problem formulations for both the unlimited intermediate storage (UIS) and zero-wait (ZW) mixed-product campaign strategies and also incorporated cleanup time considerations between batches.

In this paper we present a novel approach for solving the batch plant design under uncertainty problem to global optimality with reasonable computational effort. In Section 2, the SPC formulation is presented and a property that allows tighter bounds on the production variables is introduced. In Section 3, a key theoretical property is presented that allows the nonconvex formulation in Section 2 to be reformulated as a convex lower bounding problem that provides a tight lower bound on the global solution. A branch and bound algorithm for locating the global solution is developed, which is a modified version of the α BB algorithm of Androulakis *et al.* (1995). In addition, a novel approach for determining α is presented, in which α is a function of the variables participating in the nonconvex terms, rather than a constant. An illustrative example is provided to demonstrate this approach. In Section 4, the UIS design under uncertainty problem along with the corresponding scheduling problem are formulated. In Section 5, two multipurpose batch plant formulations are presented, and it is shown that the same techniques used for the multiproduct design problem can be applied to the multipurpose design problem. Finally, in Section 6, extensive computational studies and comparisons are reported.

2 Multiproduct Design Problem

The problem considered here is the design of a multiproduct batch plant with uncertain demands and processing parameters. The formulation of the model is similar to the models proposed in Sparrow *et al.* (1975) and Grossmann and Sargent (1979) for the production of N products in M stages in which each stage has N_j identical pieces of equipment for $j = 1, 2, \dots, M$, with the uncertain product demands given by a known probability distribution. In this model, production occurs in a single campaign for each product and does not take into account intermediate storage. Ierapetritou and Pistikopoulos (1995), (1996) showed that this problem can be formulated as the global optimization problem, (1).

2.1 Single-Product Campaign (SPC) Formulation

In this problem the objective is to maximize the profit, given by the expected revenues from the products less the investment costs of the plant equipment. The number of pieces of equipment per stage, N_j , are fixed. The equipment sizes, V_j , and the batch sizes, B_i , are the design variables, and the amounts of each product produced, Q_i , are the operating variables. \mathcal{N} denotes the set of products, $\mathcal{N} = \{1, \dots, N\}$, and \mathcal{M} denotes the set of processing steps, $\mathcal{M} = \{1, \dots, M\}$. The other parameters included in the model are, α_j and β_j , the fixed charge cost coefficients of the equipment at stage j ; δ , the coefficient used to annualize the capital cost; p_i , the market price of product i ; S_{ij} , the volume of the equipment in stage j needed to produce one mass unit of product i , called the size factors; t_{ij} , the amount of time needed to produce product i in one piece of equipment in stage j ; T_{Li} , the amount of time in the stage which has the longest processing time for product i , called the limiting time for product i ; H , the time horizon for the campaign; θ_i , the uncertain demand of product i ; and V_j^L and V_j^U , the bounds on the equipment sizes available for each stage j . It should be noted that the equipment sizes, V_j , are considered as continuous variables in this model.

$$\begin{aligned}
 & \max_{V_j, B_i} \quad \mathbf{E}_\theta \left[\max_{Q_i} \sum_{i=1}^N p_i Q_i \right] - \delta \sum_{j=1}^M \alpha_j N_j V_j^{\beta_j} \\
 & \text{subject to} \quad V_j \geq S_{ij} B_i & \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \\
 & \quad \sum_{i=1}^N \left(\frac{Q_i}{B_i} \right) T_{Li} \leq H \\
 & \quad Q_i = \theta_i & \forall i \in \mathcal{N} \\
 & \quad T_{Li} = \max_{j=1, \dots, M} \left\{ \frac{t_{ij}}{N_j} \right\} & \forall i \in \mathcal{N} \\
 & \quad \theta_i^L \leq \theta_i \leq \theta_i^U & \forall i \in \mathcal{N} \\
 & \quad V_j^L \leq V_j \leq V_j^U & \forall j \in \mathcal{M}
 \end{aligned} \tag{1}$$

The first set of constraints, $V_j \geq S_{ij} B_i$ are the batch size constraints. The second set of constraints, $\sum_{i=1}^N \left(\frac{Q_i}{B_i} \right) T_{Li} \leq H$ are the production horizon constraints. The third set of constraints are the production feasibility constraints which require that production meet the

market demand, $Q_i = \theta_i$. Finally, the fourth set of constraints, $T_{Li} = \max_{j=1,\dots,M} \left\{ \frac{t_{ij}}{N_j} \right\}$, define the cycle time for product i as the maximum time that product i resides in any one stage.

It can be seen that the objective function contains nonconvex terms $(N_j V_j^{\beta_j})$ as do the horizon constraints $(\frac{Q_i}{B_i})$. Employing exponential transformations,

$$V_j = \exp(v_j) \quad \forall j \in \mathcal{M} \quad (2)$$

$$B_i = \exp(b_i) \quad \forall i \in \mathcal{N} \quad (3)$$

$$T_{Li} = \exp(t_{Li}) \quad \forall i \in \mathcal{N} \quad (4)$$

as suggested by Kocis and Grossmann (1988), convexifies the continuous part of the objective function. Next, an appropriate expression for the expected value of the revenues must be provided. The calculation of the expected revenues requires the integration over an optimization problem:

$$\mathbf{E}_{\theta} \left[\max_{Q_i} \sum_{i=1}^N p_i Q_i \right] = \int_{\theta \in R(V_j, N_j)} \max_{Q_i} \left\{ \sum_{i=1}^N p_i Q_i \right\} J(\theta) d\theta \quad (5)$$

where $J(\theta)$ is the probability distribution function for the uncertain parameter θ . The integration should be performed over the feasible region of the plant, which is unknown at the design stage. Ierapetritou and Pistikopoulos (1995), (1996) showed that the demand constraint can be relaxed, allowing the integration to be performed in the region where the upper bound for Q_i is the value of the uncertain demand:

$$0 \leq Q_i \leq \theta_i \quad \forall i \in \mathcal{N} \quad (6)$$

In this paper, we consider a different relaxation of the demand constraint which involves tighter bounds on Q_i . Note that since $\theta_i^L \leq \theta_i \leq \theta_i^U$, we have:

$$\sum_{i=1}^N \theta_i^L \cdot \exp(t_{Li} - b_i) \leq \sum_{i=1}^N Q_i \cdot \exp(t_{Li} - b_i) \leq H \quad (7)$$

In this case, the production of product i , Q_i , is allowed to vary between the lower bound for the uncertain demand for that product, θ_i^L , and the predicted demand, θ_i :

$$\theta_i^L \leq Q_i \leq \theta_i \quad \forall i \in \mathcal{N} \quad (8)$$

When these new bounds for Q_i are used, along with the exponential transformations, (2), (3), and (4), the following relaxed design problem is obtained:

$$\begin{aligned}
& \max_{b_i, v_j} \int_{\theta \in R(V_j)} \max_{Q_i} \left\{ \sum_{i=1}^N p_i Q_i \right\} J(\theta) d\theta - \delta \sum_{j=1}^M \alpha_j N_j \exp(\beta_j v_j) \\
& \quad - \gamma \sum_{i=1}^N p_i (\theta_i - Q_i) \\
\text{subject to } & v_j \geq \ln(S_{ij}) + b_i & \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \\
& t_{Li} \geq \ln\left(\frac{t_{ij}}{N_j}\right) & \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \\
& \sum_{i=1}^N Q_i \cdot \exp(t_{Li} - b_i) \leq H \\
& \theta_i^L \leq Q_i \leq \theta_i & \forall i \in \mathcal{N} \\
& \ln(V_j^L) \leq v_j \leq \ln(V_j^U) & \forall j \in \mathcal{M} \\
& \min_j \ln\left(\frac{V_j^L}{S_{ij}^L}\right) \leq b_i \leq \min_j \ln\left(\frac{V_j^U}{S_{ij}^U}\right) & \forall i \in \mathcal{N}
\end{aligned} \tag{9}$$

Note that the objective function is convex with respect to the design variables, but the horizon constraints remain nonconvex. In addition, the demand constraints have been relaxed, therefore a penalty term is added to the objective function to account for the cost of unfilled orders. As the penalty parameter, γ , is increased, the production, Q_i , is driven towards the upper bound, θ_i . Due to the production horizon constraint, the batch size must be increased to accomodate the larger production. Larger batch sizes require larger equipment which increases the cost of the plant. The net result is a decrease in the expected profit. A study of the effect of the penalty parameter on the equipment and batch sizes and expected profit of the plant is shown in Example 1 in Section 6.

The following property will show that the bounds on the uncertain parameter values in the relaxed formulation (9) coincides with the feasible region of the original formulation with fixed demand, $Q_i = \theta_i$.

Property 2.1 *For any design, the feasibility of the batch design problem with fixed demands, θ_i , is maintained when the demand constraints are relaxed to:*

$$\theta_i^L \leq Q_i \leq \theta_i \quad \forall i \in \mathcal{N}.$$

Proof: First the feasibility test problem is formulated as:

$$\begin{aligned}
& \min_{Q_i, u} \quad u \\
& \text{s.t.} \quad \sum_{i=1}^N Q_i \cdot \exp(t_{Li} - b_i) - H \leq u \\
& \quad Q_i - \theta_i \leq u & \forall i \in \mathcal{N} \\
& \quad \theta_i^L - Q_i \leq u & \forall i \in \mathcal{N}
\end{aligned} \tag{10}$$

For feasibility we must have that $u \leq 0$. The KKT conditions for the feasibility test problem are written:

$$\begin{aligned}\lambda \cdot \exp(t_{Li} - b_i) + \mu_i^U - \mu_i^L &= 0 \quad \forall i \in \mathcal{N} \\ \lambda + \sum_{i=1}^N \mu_i^U - \sum_{i=1}^N \mu_i^L &= 1\end{aligned}$$

where λ is the Lagrange multiplier for the production constraint, and μ_i^L and μ_i^U are the Lagrange multipliers for the bounding constraints for Q_i . Since there are N control variables, Q_i , that can be changed in response to the uncertain parameter values, then the number of active constraints of (10) is less than or equal to $(N + 1)$. By examination of the KKT conditions, it can be seen that the active set for the feasibility test problem must contain the production constraint and the constraints for the lower bound of the control variables:

$$\begin{aligned}\sum_{i=1}^N Q_i \cdot \exp(t_{Li} - b_i) - H &= u \\ \theta_i^L - Q_i &= u \quad \forall i \in \mathcal{N}\end{aligned}$$

From the second set of equations, $Q_i = \theta_i^L - u$. Substituting this into the first equation yields the following expression:

$$\sum_{i=1}^N (\theta_i^L - u) \cdot \exp(t_{Li} - b_i) - H = u$$

Rearranging to group the u terms together yields:

$$\sum_{i=1}^N \theta_i^L \cdot \exp(t_{Li} - b_i) - H = u \left(1 + \sum_{i=1}^N \exp(t_{Li} - b_i) \right)$$

It is obvious that,

$$1 + \sum_{i=1}^N \exp(t_{Li} - b_i) > 0$$

and from Equation (7) we know that,

$$\sum_{i=1}^N \theta_i^L \cdot \exp(t_{Li} - b_i) \leq H$$

otherwise there is no feasible solution to the design problem. Therefore, u is always less than or equal to zero. \square

Applying this analysis to Formulation (9) results in the nonlinear optimization problem given by Formulation (11). For the purpose of this paper, the uncertain parameters will be

considered to have a normal distribution. The Gaussian quadrature formula is derived in Appendix A.

The uncertain technical parameters investigated in this work are the size factors, S_{ij} , and the processing times, t_{ij} . The variations in these parameters are dealt with in a scenario-based approach. In this method, the uncertain technical parameters are given different discrete values in a number of scenarios, P , while the uncertain demands retain the same probability distribution in each scenario. The scenarios are given weight factors, ω^p . The object is to find the optimal design over all possible scenarios and the optimal productions in each scenario.

Using the Gaussian quadrature approach for the uncertain demands and the scenario approach for the uncertain technical parameters results in a nonlinear optimization problem, written as a minimization for the purposes of the following analysis:

$$\begin{aligned}
& \min_{b_i, v_j, Q_i^{qp}} \delta \sum_{j=1}^M \alpha_j N_j \exp(\beta_j v_j) \\
& \quad - \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \sum_{i=1}^N p_i Q_i^{qp} + \gamma \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \left\{ \sum_{i=1}^N p_i \theta_i^q - \sum_{i=1}^N p_i Q_i^{qp} \right\} \\
& \text{subject to} \quad v_j \geq \ln(S_{ij}^p) + b_i \quad \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\
& \quad \sum_{i=1}^N Q_i^{qp} \cdot \exp(t_{Li}^p - b_i) \leq H \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \quad \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \quad \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M} \\
& \quad \min_{j,p} \ln\left(\frac{V_j^L}{S_{ij}^p}\right) \leq b_i \leq \min_{j,p} \ln\left(\frac{V_j^U}{S_{ij}^p}\right) \quad \forall i \in \mathcal{N}
\end{aligned} \tag{11}$$

where

$$t_{Li}^p = \max_j \left\{ \frac{t_{ij}^p}{N_j} \right\} \quad \forall i \in \mathcal{N} \quad \forall p \in \mathcal{P} \tag{12}$$

and each t_{Li}^p is constant because both t_{ij}^p and N_j are constant. \mathcal{Q} denotes the set of quadrature points, $\mathcal{Q} = \{1, \dots, Q\}$, and \mathcal{P} denotes the set of scenarios, $\mathcal{P} = \{1, \dots, P\}$.

In Formulation (11), γ is the penalty coefficient; J^q and ω^q are the probability of each quadrature point, and its weighting factor, respectively, and θ_i^q are the parameter values associated with each point. The parameter values are calculated by the formula:

$$\theta_i^q = \frac{1}{2} \left[\theta_i^U (1 + v_i^{q_i}) + \theta_i^L (1 - v_i^{q_i}) \right] \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \tag{13}$$

where $v_i^{q_i}$ is the location of the quadrature point q_i in the $[-1, 1]$ interval, and θ_i^L, θ_i^U are the lower and upper bounds of θ_i .

Formulation (11) can be solved using a standard NLP solver such as MINOS5.4. However, these techniques cannot guarantee that the global solution will be found due to the presence of the nonconvex horizon constraints. This suggests that global optimization techniques must be developed to solve these problems.

Ierapetritou and Pistikopoulos (1995), (1996) applied the GOP algorithm of Floudas and Visweswaran (1990), (1993) for the case of a fixed number of equipment units per stage with relaxation constraint (6). In the following section, a very important theoretical property will be presented which allows very tight bounds on the global solution to be obtained in a small number of iterations.

3 Lower Bounding Problem Formulations

Note that the objective function in formulation (11) is convex, but the horizon constraints are nonconvex. In the α BB method (α -based branch and bound) of Androulakis *et al.* (1995), the procedure for finding the global solution of nonconvex problems is to construct a converging sequence of upper and lower bounds on the global solution. This is achieved by developing a convex relaxation of the original minimization problem by replacing all nonconvex terms with tight convex lower bounding functions. In particular, convex lower bounding functions for twice-differentiable nonconvex terms of generic structure are constructed by means of a separable quadratic term using the α parameter developed by Maranas and Floudas (1994b). Thus, a general nonconvex term in one variable x , $NC(x)$, would become:

$$NC(x) \geq NC(x) + \alpha(x^U - x)(x^L - x) \quad (14)$$

where x^U, x^L are the bounds on the x variable, and α is positive. As can be seen, the magnitude of the underestimator depends upon both the size of α and on the size of the current region under investigation. Maranas and Floudas (1994b) showed that:

$$\begin{aligned} \alpha \geq \max \quad & \left\{ 0, -\frac{1}{2} \min_{\mathbf{k}} \lambda_{\mathbf{k}}(x) \right\} \\ \text{s.t.} \quad & x^L \leq x \leq x^U \end{aligned} \quad (15)$$

where $\lambda_{\mathbf{k}}(x)$ are the eigenvalues of $NC(x)$. The parameter α must be large enough so that the new term is indeed convex, and as close as possible to its definition, (15). In general, the problem of finding the minimum eigenvalue is itself a nonconvex optimization problem. However, in Section 3.1, it will be shown that for the design of multiproduct batch processes under uncertainty, an exact expression for α can be obtained. Two modifications to the standard α calculation method explained above will be presented in Sections 3.4 and 3.5.

3.1 Key Theoretical Property: Formulation I

Consider the nonconvex horizon constraints. The first observation is that the horizon constraints consist of a sum of separable terms in the form of

$$x_{\mathbf{i}} \cdot \exp(y_{\mathbf{i}}) \quad (16)$$

where,

$$x_{\mathbf{i}} = Q_{\mathbf{i}}^{qp} \quad \text{and} \quad y_{\mathbf{i}} = t_{Li}^p - b_{\mathbf{i}} \quad (17)$$

As a result, a separate α can be calculated for each product $x_i \exp(y_i)$ in the summation. In order to find an exact expression for α , we have to obtain an exact calculation of the minimum eigenvalue. This requires the solution of the problem $|H - \lambda I| = 0$ where H is the Hessian of each separable nonconvex term and I is the identity matrix. Considering a general term:

$$\phi = x \cdot \exp(y) \quad (18)$$

the first derivatives are:

$$\phi_x = \exp(y) \quad \text{and} \quad \phi_y = x \cdot \exp(y) \quad (19)$$

and the second derivatives are:

$$\phi_{xx} = 0, \quad \phi_{xy} = \exp(y) \quad \text{and} \quad \phi_{yy} = x \cdot \exp(y) \quad (20)$$

Thus,

$$|H - \lambda I| = \lambda^2 - (x \exp(y)) \lambda - (\exp(y))^2 = 0 \quad (21)$$

This formula yields two real solutions,

$$\lambda_1 = \left(\frac{x + \sqrt{x^2 + 4}}{2} \right) \exp(y) > 0 \quad (22)$$

$$\lambda_2 = \left(\frac{x - \sqrt{x^2 + 4}}{2} \right) \exp(y) < 0 \quad (23)$$

Therefore λ_2 is the minimum eigenvalue for all values of x and y . In order to satisfy condition (15), we must find the minimum of λ_2 over the current domain of x and y . When x is large, the term $x - \sqrt{x^2 + 4}$ is negative and close to zero. The term decreases monotonically as x decreases. Therefore, λ_2 is minimized with respect to x when $x = x^L$. Since λ_2 is negative, it decreases monotonically as y increases, therefore λ_2 is minimized with respect to y when $y = y^U$. Substituting for x and y ,

$$\begin{aligned} x^L &= Q_i^{Lqp} \\ y^U &= t_{Li}^p - b_i^L \end{aligned}$$

The resulting expression for the minimum eigenvalue is,

$$\lambda_{i,\min}^{qp} = \left(\frac{Q_i^{Lqp} - \sqrt{(Q_i^{Lqp})^2 + 4}}{2} \right) \cdot \exp(t_{Li}^p - b_i^L) \quad (24)$$

Since Q_i^{Lqp} is always positive λ_i^{qp} is always negative, and substituting into Equation (15) the corresponding α parameter is,

$$\alpha_{1,i}^{qp} = \frac{1}{4} \left(\sqrt{(Q_i^{Lqp})^2 + 4} - Q_i^{Lqp} \right) \cdot \exp(t_{Li}^p - b_i^L) \quad (25)$$

Several conclusions can be drawn from this expression. First, if Q_i^{Lqp} is an order of magnitude greater than 4, then the term within the parentheses is a small positive number. Second, if the term $(t_{Li}^p - b_i^L)$ is negative, then the exponential term is a small positive number. As will be observed from the computational studies, in the design of multiproduct batch plants under uncertainty, the aforementioned conditions are met and hence, $\alpha_{1,i}^{qp}$ is generally a very small positive number.

Using the expression for α_1 , the convex lower bounding function for the production constraint is:

$$Q_i^{qp} \exp(t_{Li}^p - b_i) + \frac{1}{4} \left(\sqrt{(Q_i^{Lqp})^2 + 4} - Q_i^{Lqp} \right) \exp(t_{Li}^p - b_i^L) \cdot \left\{ (Q_i^{Lqp} - Q_i^{qp})(Q_i^{Uqp} - Q_i^{qp}) + (b_i^L - b_i)(b_i^U - b_i) \right\} \quad (26)$$

The resulting lower bounding problem, denoted as Formulation I is:

$$\begin{aligned} \min_{b_i, v_j, Q_i^{qp}} \quad & \delta \sum_{j=1}^M \alpha_j N_j \exp(\beta_j v_j) \\ & - \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \sum_{i=1}^N p_i Q_i^{qp} + \gamma \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \left\{ \sum_{i=1}^N p_i \theta_i^q - \sum_{i=1}^N p_i Q_i^{qp} \right\} \\ \text{subject to} \quad & v_j \geq \ln(S_{ij}^p) + b_i \quad \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\ & \sum_{i=1}^N Q_i^{qp} \cdot \exp(t_{Li}^p - b_i) + \sum_{i=1}^N \frac{1}{4} \left(\sqrt{(Q_i^{Lqp})^2 + 4} - Q_i^{Lqp} \right) \exp(t_{Li}^p - b_i^L) \cdot \\ & \left\{ (Q_i^{Lqp} - Q_i^{qp})(Q_i^{Uqp} - Q_i^{qp}) + (b_i^L - b_i)(b_i^U - b_i) \right\} \leq H \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\ & \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\ & \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M} \\ & \min_{j,p} \ln\left(\frac{V_j^L}{S_{ij}^p}\right) \leq b_i \leq \min_{j,p} \ln\left(\frac{V_j^U}{S_{ij}^p}\right) \quad \forall i \in \mathcal{N} \end{aligned} \quad (27)$$

where θ_i^q is given by Equation (13). The solution to Formulation I constitutes a lower bound on the solution of the original problem (11).

3.2 Global Optimization Algorithm - Modified α BB

A modified version of the α BB algorithm of Androulakis *et al.* (1995) is used to solve the multiproduct batch plant design problems. The goal of this procedure is to locate the global minimum solution of (11) by constructing a sequence of converging upper and lower bounds.

The approach will be described for the design problem (11) that employs the convex under-estimator (27). A similar approach can be applied for problem (61) as well.

An upper bound on the solution can be obtained by solving (11) using a local nonlinear solver such as MINOS5.4. A lower bound can be obtained by solving the convexified problem (27) also using a local solver. Since the maximum separation between the actual nonconvex terms in (11) and the convex lower bounding terms in (27) is proportional to the size of the current region $[\mathbf{v}^L, \mathbf{v}^U, \mathbf{b}^L, \mathbf{b}^U, \mathbf{Q}^L, \mathbf{Q}^U]$, the bounds on the global solution can be refined by successively partitioning the original search domain into smaller regions and solving the lower bounding problem in each region. Therefore, at each iteration the lower bound on the global solution of (11) is the minimum solution of (27) over all subregions which make up the initial search domain. This suggests a straightforward way to tighten the lower bound; at each iteration halve the subregion responsible for the minimum solution of (27). This branching and bounding procedure generates a nondecreasing sequence for the lower bound. A nonincreasing sequence for the upper bound can be generated by solving the original nonconvex problem (11) locally and updating the upper bound if this solution is less than the previous upper bound. Subregions of the original search domain may be excluded (fathomed) if the solution to the lower bounding problem (27) in this region is greater than the current upper bound.

3.2.1 Algorithmic Description

The basic steps of the algorithm are the following (only the formulation for the \mathbf{b} variables is shown):

STEP 0 - Initialization

The relative convergence tolerance, ϵ , is specified and the iteration counter, $Iter$, is set to one.

For the first iteration,

STEP 1 - Variable Bound Refinement

The global bounds on the \mathbf{v} and \mathbf{b} variables are tightened by solving the following problems (only the formulation for the \mathbf{b} variables is shown):

$$\begin{aligned}
b_i^L = \min \quad & b_i \\
\text{s.t.} \quad & v_j \geq \ln(S_{ij}^p) + b_i \quad \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\
& \sum_{i=1}^N \left\{ Q_i^{qp} \cdot \exp(t_{Li}^p - b_i) \right. \\
& \quad + \alpha_{1,i}^{qp} \cdot (Q_i^{qp,L} - Q_i^{qp}) (Q_i^{qp,U} - Q_i^{qp}) \\
& \quad \left. + \alpha_{1,i}^{qp} \cdot (b_i^L - b_i) (b_i^U - b_i) \right\} \leq H \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M} \\
& \min_{j,p} \ln\left(\frac{V_j^L}{S_{ij}^p}\right) \leq b_i \leq \min_{j,p} \ln\left(\frac{V_j^U}{S_{ij}^p}\right) \quad \forall i \in \mathcal{N}
\end{aligned} \tag{28}$$

and,

$$\begin{aligned}
b_i^U = \max \quad & b_i \\
\text{s.t.} \quad & v_j \geq \ln(S_{ij}^p) + b_i \quad \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\
& \sum_{i=1}^N \left\{ Q_i^{qp} \cdot \exp(t_{Li}^p - b_i) \right. \\
& \quad + \alpha_{1,i}^{qp} \cdot (Q_i^{qp,L} - Q_i^{qp}) (Q_i^{qp,U} - Q_i^{qp}) \\
& \quad \left. + \alpha_{1,i}^{qp} \cdot (b_i^L - b_i) (b_i^U - b_i) \right\} \leq H \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M} \\
& \min_{j,p} \ln\left(\frac{V_j^L}{S_{ij}^p}\right) \leq b_i \leq \min_{j,p} \ln\left(\frac{V_j^U}{S_{ij}^p}\right) \quad \forall i \in \mathcal{N}
\end{aligned} \tag{29}$$

The current variable bounds $[\mathbf{b}^{L,Iter}, \mathbf{b}^{U,Iter}, \mathbf{v}^{L,Iter}, \mathbf{v}^{U,Iter}, \mathbf{Q}^{L,Iter}, \mathbf{Q}^{U,Iter}]$, are then set equal to the global bounds $[\mathbf{b}^L, \mathbf{b}^U, \mathbf{v}^L, \mathbf{v}^U, \mathbf{Q}^L, \mathbf{Q}^U]$.

STEP 2 - Upper Bound on Global Solution

An initial upper bound (UB) on the global solution is obtained by solving problem (11) locally. The variable values at the solution are stored: $\mathbf{b}^{UB} = \mathbf{b}^*$, $\mathbf{v}^{UB} = \mathbf{v}^*$, $\mathbf{Q}^{UB} = \mathbf{Q}^*$.

STEP 3 - Lower Bound on Global Solution

An initial lower bound (LB) on the global solution is obtained by solving the convexified problem (27) within the refined variable bounds. The variable values at the solution are stored: $\mathbf{b}^{*,Iter}, \mathbf{v}^{*,Iter}, \mathbf{Q}^{*,Iter}$.

For all subsequent iterations ($Iter \geq 2$),

STEP 4 - Check for Convergence

If the relative difference between the upper and lower bound is greater than the convergence tolerance, $(UB - LB) / |UB + 1| > \epsilon$, then continue to STEP 5. Otherwise, the global solution has been found and the solution is:

$$\begin{aligned} f^* &\leftarrow f^{UB} \\ \mathbf{b}^* &\leftarrow \mathbf{b}^{UB} \\ \mathbf{v}^* &\leftarrow \mathbf{v}^{UB} \\ \mathbf{Q}^* &\leftarrow \mathbf{Q}^{UB} \end{aligned} \tag{30}$$

STEP 5 - Update Current Region and Lower Bound

The current search region is selected as the region containing the minimum of all stored lower bound solutions. The lower bound, LB, is updated to be the minimum of all stored solution. The current variable bounds are updated to be the bounds of the current region, and the current point is updated to the solution point of the current region.

STEP 6 - Update Upper Bound on Global Solution

The current point is used as a starting point for a local solution to problem (11). If the solution to this problem is less than the current upper bound, then the upper bound is updated to the new solution, and the variable values at the new upper bound are stored.

STEP 7 - Select Branching Variable and Partition Current Region

The current region is partitioned into two subregions by bisecting the edge corresponding to a chosen variable. The criterion for choosing the branching variable is discussed in Section 3.2.2.

STEP 8 - Solve Lower Bounding Problems

The lower bounding problem (27) is solved in both new subregions. If the solution in a region is greater than the current upper bound, then this region is guaranteed not to contain the global minimum and it is fathomed. Otherwise, the solution is stored along with the variable bounds for the region and the variable values at the solution. Return to STEP 4.

3.2.2 Analysis of the Branching Criteria

In the implementation of the α BB algorithm for the example problems discussed in Section 6, it was found that the speed of convergence was greatly affected by the choice of variables on which the subregions were partitioned (branching variable). In this section, studies on different branching criteria are presented. First, it was observed that the \mathbf{v} variables do not participate in the objective function or in any nonlinear terms and hence they should not be considered in the choice of branching variables.

The first branching criterion examined was the most straightforward one. In the current region, the variable with the longest distance between its upper and lower bounds ($x^U - x^L$), or the longest relative distance ($2(x^U - x^L)/(x^U + x^L)$) is chosen as the branching variable. This choice of criterion follows the reasoning that since the size of the approximation, $\alpha(x^L - x)(x^U - x)$, depends on the distance between x^L and x^U , then by partitioning on the variable

with the largest range, we can hopefully achieve the largest improvement in the approximation. In practice, it was found that this procedure converges to the global solution slowly.

In the second branching criterion, the entire convex lower bounding function was calculated for each variable at the solution point in the current region.

$$\alpha_{1,i}^{qp} \cdot (Q_i^{qp,L} - Q_i^{qp}) (Q_i^{qp,U} - Q_i^{qp}) \quad (31)$$

or,

$$\alpha_{1,i}^{qp} \cdot (b_i^L - b_i) (b_i^U - b_i) \quad (32)$$

The variable with the smallest value of the underestimation term (all terms are ≤ 0) is chosen as the branching variable.

Several observations were made when this criterion was used for the solution of the problems presented in this paper. First, this approach also converged to the global solution, but only slightly faster than the first method. Second, branching on the **Q** variables caused the largest improvement in the lower bound. Third, it was found that only **Q** variables were chosen as branching variables until the last iteration before convergence, and then a **b** variable was chosen.

Based on these observations, the algorithm was implemented where only branching on the **Q** variables was allowed, and then where only branching in the **b** variables was allowed. It was found that the algorithm did not converge when only the **b** variables were used as the branching variables. Further, it was observed that the algorithm converged in the same number of iterations when only the **Q** variables were used as when both the **b** and **Q** variables were used.

A third possible branching criterion is to branch only on the variables that have the largest multipliers in the objective function. The values of the probability distribution, J^q , and the weighting factors, ω^q , for the quadrature points vary over several orders of magnitude. As a result, some of the **Q** variables have a much larger effect on the objective function than others. Table 32 shows the product $\omega^q J^q$ for a 5x5 quadrature grid for a plant that produces two products, like the Illustrative Example and Example 1. As can be seen, the multiplier corresponding to the $Q_i^{3,3,p}$ variables is the largest, followed by $Q_i^{3,2,p}$, $Q_i^{2,3,p}$, $Q_i^{3,4,p}$, $Q_i^{4,3,p}$.

Initially, only the $Q_i^{3,3,p}$ variables were used as the branching variables, using the underestimation criterion, Equation (31), to select the variable to branch on. An implementation where the $Q_i^{3,3,p}$, $Q_i^{3,2,p}$, $Q_i^{2,3,p}$, $Q_i^{3,4,p}$, and $Q_i^{4,3,p}$ variables were selected as possible branching variables was also used. However, it was found that the neither of these implementations converged because the convex lower bounding functions corresponding to these variables were reduced to zero before the desired tolerance was achieved.

Finally, a combination of the second and third strategies was used as the branching criterion. The product of the objective function multiplier, $\omega^q J^q$ and the underestimation, Equation (31), is calculated for all **Q** variables. This directly determines the effect of the convex lower bounding function on the objective function. Thus, the variable with the largest product is chosen as the branching variable. This procedure was found to converge in fewer iterations than all other methods discussed above. Note that this corresponds to branching on all **Q** variables first and then branching on the **b** variables next, if needed.

3.3 Illustrative Example

In order to illustrate that a tight lower bound of the global solution can be obtained immediately by using the exact expression for α_1 , consider a small example taken from Grossmann and Sargent (1979) for the design of a batch plant that must produce two products using three stages with one piece of equipment per stage. In this example, only the demands are considered to be uncertain parameters, therefore there is only one scenario ($P = 1$). The data for this example are shown in Table 1.

The single-product campaign (SPC) formulation, (27), contains fifty-five variables and thirty-one constraint equations, not counting the variable bounds. Of the thirty-one constraints, twenty-five are nonlinear constraints containing fifty nonlinear terms. The demands have a normal distribution of $N(200,10)$ and $N(100,10)$ for products 1 and 2, respectively. Five quadrature points are used for the uncertain demand of each product. The upper and lower bound on the equipment volumes, V_j were 4500 and 500, respectively. A relative tolerance, ϵ , of 0.003 was used in this example, and the time horizon, H , was 8. The annual cost coefficient, δ , was 0.3.

The optimal design and profit is shown in Table 2, and the progression of the upper and lower bounds on the global solution for the case where the penalty term is zero is shown in Table 3. This method provides a very tight lower bound, as the lower bound is within one percent of the global solution at the first iteration, without any partitioning of the search domain. The branch and bound algorithm quickly converges to the desired tolerance.

Note that the equipment and batch sizes for the global solution increase as the γ coefficient increases. This reflects the penalty associated with not fully meeting the market demand. In addition, the computational requirements and iterations decrease as the penalty coefficient increases.

While the lower bounds provided by α_1 are very tight, it is possible to develop even tighter convex underestimators. The procedure for deriving a tighter convex lower bounding function is described in Section 3.4.

3.4 The α as a linear function: Formulation II

Note that in equation (26) the quadratic terms $(Q_i^{Uqp} - Q_i^{qp})(Q_i^{Lqp} - Q_i^{qp})$ and $(b_i^U - b_i)(b_i^L - b_i)$ are multiplied by the same α parameter. Because these terms can be of different magnitudes, it is not necessarily desirable to multiply them by the same α . To address this, a straightforward approach is to introduce a scaling factor, for example:

$$\eta_i^{qp} = \frac{Q_i^{Uqp} - Q_i^{Lqp}}{b_i^U - b_i^L} \quad (33)$$

and define a different α for each variable. Thus, the lower bounding function for a generic nonconvex term of two variables would be:

$$NC(x, y) + \alpha(x^U - x)(x^L - x) + \beta(y^U - y)(y^L - y) \quad (34)$$

where

$$\beta = \eta \cdot \alpha \quad (35)$$

For the production constraints, which have the form $NC(x, y) = x \exp(y)$, the lower bounding function, L , can be written:

$$L = x \exp(y) + \frac{\alpha}{\eta} (x^U - x)(x^L - x) + \alpha (y^U - y)(y^L - y) \quad (36)$$

First, consider η to be an arbitrary positive constant and attempt to find an expression for a constant α that maintains the convexity of L . The lower bounding function is convex if both of the eigenvalues of the Hessian of L are always positive. Both eigenvalues are positive if the following two conditions are met:

1. $\frac{\partial^2 L}{\partial x^2} + \frac{\partial^2 L}{\partial y^2} \geq 0$
2. $\frac{\partial^2 L}{\partial x^2} \frac{\partial^2 L}{\partial y^2} - \left(\frac{\partial^2 L}{\partial x \partial y} \right)^2 \geq 0$

We find that α of the form,

$$\hat{\alpha} = \frac{1}{4} \left(\sqrt{(x^L)^2 + 4\eta} - x^L \right) \exp(y^U) \quad (37)$$

guarantees that L is convex for any $\eta > 0$. Given this expression, the next step is to find η that minimizes the size of the approximation term.

$$\begin{aligned} \max_{\eta} \quad & \frac{\hat{\alpha}}{\eta} (x^U - x)(x^L - x) + \hat{\alpha} (y^U - y)(y^L - y) \\ \text{s.t.} \quad & \eta > 0 \end{aligned} \quad (38)$$

The approximation is most negative at the point $\left(\frac{x^U + x^L}{2}, \frac{y^U + y^L}{2} \right)$, so for convenience, this point will be used. Substituting for $\hat{\alpha}$ gives,

$$\begin{aligned} \max_{\eta} \quad & \frac{1}{16\eta} \left(\sqrt{(x^L)^2 + 4\eta} - x^L \right) \exp(y^U) (x^U - x^L)^2 \\ & + \frac{1}{16} \left(\sqrt{(x^L)^2 + 4\eta} - x^L \right) \exp(y^U) (y^U - y^L)^2 \\ \text{s.t.} \quad & \eta > 0 \end{aligned} \quad (39)$$

Now the stationary point with respect to η is:

$$2\eta^2 (y^U - y^L)^2 + 2\eta \frac{(x^U - x^L)^2}{\sqrt{(x^L)^2 + 4\eta}} + \left(x^L - \sqrt{(x^L)^2 + 4\eta} \right) (x^U - x^L)^2 = 0 \quad (40)$$

Solving for η results in the following expression:

$$\eta = \frac{(x^U - x^L)^2}{(y^U - y^L)^2} \pm x^L \frac{(x^U - x^L)}{(y^U - y^L)} \quad (41)$$

and the desired solution is,

$$\eta = \frac{(x^U - x^L)^2}{(y^U - y^L)^2} - x^L \frac{(x^U - x^L)}{(y^U - y^L)} \quad (42)$$

However, this term can become negative, so the definition for η must be modified so that:

$$\eta = \max \left\{ 1, \frac{(x^U - x^L)^2}{(y^U - y^L)^2} - x^L \frac{(x^U - x^L)}{(y^U - y^L)} \right\} \quad (43)$$

When the Q and b variables are substituted for x and y , the scaling factor is written:

$$\eta_i^{qp} = \max \left\{ 1, \frac{(Q_i^{Uqp} - Q_i^{Lqp})^2}{(b_i^U - b_i^L)^2} - Q_i^{Lqp} \frac{(Q_i^{Uqp} - Q_i^{Lqp})}{(b_i^U - b_i^L)} \right\} \quad (44)$$

and the α term is:

$$\hat{\alpha}_i^{qp} = \frac{1}{4} \left(\sqrt{(Q_i^{Lqp})^2 + 4\eta_i^{qp}} - Q_i^{Lqp} \right) \exp(t_{Li}^p - b_i^L) \quad (45)$$

Recall that $\hat{\alpha}$ is a constant, and thus is constrained by the most restrictive point, (x^L, y^U) , while at other points in the feasible region it may be sufficient to use a smaller value of α . The goal is to find an expression for α that is a function of the variables that maintains the convexity of the lower bounding function.

Consider the simplest function of x and y , that is, a linear function. Now the lower bounding function has the form:

$$L = x \exp(y) + \frac{\alpha_2(x)}{\eta} \cdot (x^U - x)(x^L - x) + \beta_2(y) \cdot (y^U - y)(y^L - y) \quad (46)$$

where,

$$\begin{aligned} \alpha_2(x) &= \hat{\alpha} \left(1 - c \cdot \frac{x - x^L}{x^U - x^L} \right) \\ \beta_2(y) &= \hat{\alpha} \left(1 - d \cdot \frac{y^U - y}{y^U - y^L} \right) \\ 0 &\leq c, d \leq 1 \end{aligned} \quad (47)$$

where c and d are constants. Note that at the point where the minimum eigenvalue as defined by Equation (24) is minimized, (x^L, y^U) the expressions for α_2 and β_2 reduce to:

$$\alpha_2(x^L) = \hat{\alpha} \quad (48)$$

$$\beta_2(y^U) = \hat{\alpha} \quad (49)$$

and at any other point, say (x^U, y^L) ,

$$\alpha_2(x^U) = \hat{\alpha}(1 - c) \leq \hat{\alpha} \quad (50)$$

$$\beta_2(y^L) = \hat{\alpha}(1 - d) \leq \hat{\alpha} \quad (51)$$

The constants, c and d , must be greater than zero or else no improvement in the underestimator is made. In addition, the constants must be less than or equal to unity or else the term is not a valid underestimator. The goal is to find the largest values of c and d which maintain the convexity of the lower bounding function. A procedure for determining the upper bounds on c and d is as follows:

1. Let $c = d = \frac{1}{2} \left[1 - \frac{\exp(y^L)}{4\hat{\alpha}} \left(\sqrt{(x^U)^2 + 4\eta} - x^U \right) \right]$.

2. Check $c \leq \frac{1}{2} \left[1 - \frac{\eta \exp(2y^U)}{4\hat{\alpha}^2 \left(\frac{x^U \exp(y^U)}{2\hat{\alpha}} + 1 + d \right)} \right]$.

Check $d \leq \frac{1}{2} \left(\frac{x^L \exp(y^L)}{2\hat{\alpha}} + 1 - \frac{\eta \exp(2y^L)}{4\hat{\alpha}^2(1+c)} \right)$.

If both are satisfied, then Stop.

If one or more is not satisfied, then go to Step 3.

3. $c = \min \left\{ \frac{1}{2} \left[1 - \frac{\eta \exp(2y^U)}{4\hat{\alpha}^2 \left(\frac{x^U \exp(y^U)}{2\hat{\alpha}} + 1 + d \right)} \right], \frac{1}{2} \left[1 - \frac{\eta \exp(2y^L)}{4\hat{\alpha}^2 \left(\frac{x^U \exp(y^L)}{2\hat{\alpha}} + 1 - 2d \right)} \right] \right\}$.

4. $d = \min \left\{ 1, \frac{1}{2} + \frac{x^L \exp(y^L)}{4\hat{\alpha}} - \frac{\eta \exp(2y^L)}{8\hat{\alpha}^2(1+c)}, \frac{1}{2} + \frac{x^U \exp(y^L)}{4\hat{\alpha}} - \frac{\eta \exp(2y^L)}{8\hat{\alpha}^2(1-2c)} \right\}$.

5. Return to Step 3 and repeat until c and d converge.

A derivation of this procedure is included in Appendix B. When the Q and b variables are substituted for x and y , the α parameters are written:

$$\begin{aligned} \alpha_{2,i}^{qp}(Q_i^{qp}) &= \hat{\alpha}_i^{qp} \left(1 - c_i^{qp} \cdot \frac{Q_i^{qp} - Q_i^{Lqp}}{Q_i^{Uqp} - Q_i^{Lqp}} \right) \\ \beta_{2,i}^{qp}(b_i) &= \hat{\alpha}_i^{qp} \left(1 - d_i^{qp} \cdot \frac{b_i - b_i^L}{b_i^U - b_i^L} \right) \end{aligned} \tag{52}$$

Using the new expression for the lower bounding terms with α_2 and β_2 , Formulation II of the lower bounding problem is:

$$\begin{aligned}
& \min_{b_i, v_j, Q_i^{qp}} \delta \sum_{j=1}^M \alpha_j N_j \exp(\beta_j v_j) \\
& \quad - \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \sum_{i=1}^N p_i Q_i^{qp} + \gamma \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \left\{ \sum_{i=1}^N p_i \theta_i^q - \sum_{i=1}^N p_i Q_i^{qp} \right\} \\
\text{subject to } & v_j \geq \ln(S_{ij}^p) + b_i \quad \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\
& \sum_{i=1}^N \left\{ Q_i^{qp} \cdot \exp(t_{Li}^p - b_i) \right. \\
& \quad + \frac{1}{4\eta_i^{qp}} \left(\sqrt{(Q_i^{Lqp})^2 + 4\eta_i^{qp}} - Q_i^{Lqp} \right) \exp(t_{Li}^p - b_i^L) \\
& \quad \cdot \left(1 - c_i^{qp} \cdot \frac{Q_i^{qp} - Q_i^{Lqp}}{Q_i^{Uqp} - Q_i^{Lqp}} \right) \cdot (Q_i^{qp,L} - Q_i^{qp}) (Q_i^{qp,U} - Q_i^{qp}) \\
& \quad + \frac{1}{4} \left(\sqrt{(Q_i^{Lqp})^2 + 4\eta_i^{qp}} - Q_i^{Lqp} \right) \exp(t_{Li}^p - b_i^L) \\
& \quad \cdot \left(1 - d_i^{qp} \cdot \frac{b_i - b_i^L}{b_i^U - b_i^L} \right) (b_i^L - b_i) (b_i^U - b_i) \left. \right\} \leq H \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M} \\
& \min_{j,p} \ln\left(\frac{V_j^L}{S_{ij}^p}\right) \leq b_i \leq \min_{j,p} \ln\left(\frac{V_j^U}{S_{ij}^p}\right) \quad \forall i \in \mathcal{N}
\end{aligned} \tag{53}$$

3.4.1 Illustrative Example Revisited

Table 4 shows the results for the Illustrative Example using Formulation II and Table 5 shows the progression of the upper and lower bounds on the global solution.

Note in Table 5 that the initial lower bound is -986.777 . For the formulation using α_1 , the initial lower bound from Table 3 was -987.840 . Thus α_2 provides a tighter lower bound on the global solution than α_1 . This point is further illustrated in Table 4 where the number of iterations required to achieve the desired tolerance is less for α_2 than for the lower bounding functions using α_1 (Table 2) when $\gamma = 0$ and $\gamma = 8$. However, the CPU time required is slightly greater, most likely due to the more complicated expression for the convex lower bounding function when α_2 is used.

The optimal solutions shown in Table 4 are exactly the same for the α_1 formulation shown in Table 2, as expected.

3.5 Nonconvex Lower Bounding Function: Formulation III

In the derivation of α_1 , recall that the minimum eigenvalue of the Hessian matrix of the nonconvex term $Q_i^{qp} \cdot \exp(t_{Li}^p - b_i)$ was found to be:

$$\lambda_i^{qp} = \left(\frac{Q_i^{qp} - \sqrt{(Q_i^{qp})^2 + 4}}{2} \right) \cdot \exp(t_{Li}^p - b_i) \quad (54)$$

The minimum of this expression over the current search domain is used to calculate the constant value for α_1 . We have noted some interesting results if Equation (54) rather than its minimum is used to calculate the α parameter. In this case, the expression for α is:

$$\alpha_{3,i}^{qp} = \frac{1}{4} \left(\sqrt{(Q_i^{qp})^2 + 4} - Q_i^{qp} \right) \cdot \exp(t_{Li}^p - b_i) \quad (55)$$

Note that α_3 does not strictly satisfy the condition imposed by Equation (15). Therefore, the lower bounding function constructed using α_3 is not necessarily convex. Thus, the lower bounding problem is still a nonconvex problem and local solvers may converge to a local minimum rather than the global minimum, giving an overestimate of the lower bound. In practice, however, the algorithm never failed to converge to the correct global minimum solution when α_3 was used to construct the lower bounding function. Table 13 shows that multiple local minima can exist for these problems. For the examples studied in this paper, the local minima lie very close to the global minimum solution.

3.5.1 Illustrative Example Revisited

The advantage of using α_3 is that it provides a much tighter lower bound on the global solution than either α_1 or α_2 . These observations are demonstrated below in the Illustrative Example and in the other examples in Section 6. The number of iterations and the CPU time required to converge to the global solution are shown in Table 6. Fewer iterations were required to achieve the desired tolerance when α_3 was used than when α_1 and α_2 were used. In addition, the computational requirements were less when α_1 was used as the lower bounding function.

Table 7 shows the progressive improvement of the bounds using the proposed approach. As can be seen, the initial lower bound is very close to the global solution and the algorithm converges quickly. Recall from Table 3 that the initial lower bound when α_1 is used was -987.840 . An improved initial lower bound of -986.777 is provided by α_2 , Table 5. A much larger improvement is possible when α_3 is used, resulting in an initial lower bound of -982.171 .

4 Mixed-Product Campaign Formulation

As stated in Section 2, Formulation (11) corresponds to the multiproduct batch design problem with single-product campaigns and no intermediate storage. Since this formulation uses the maximum processing time for each product, $t_{Li} = \max_{j=1,\dots,M} \left\{ \frac{t_{ij}}{N_j} \right\}$, it overestimates the time required to process each product. This can result in an overdesign of the equipment sizes.

Figure 1 shows a comparison between a single-product campaign and a mixed-product campaign. In this case, two cycles of each product are needed to reach the required production specifications. The mixed-product campaign shown allows for unlimited storage of products

between processing stages. As can be seen, the mixed-product campaign requires less time to process the required amount of products.

In order to allow mixed-product campaigns, the horizon constraint in Formulation (11) must be replaced by an expression that takes into account the processing times in each stage, rather than the maximum processing time. This can be done in the following manner according to the analysis of Birewar and Grossmann (1989). Let n_i be the number of batches of product i over the whole production period:

$$n_i = \frac{Q_i}{B_i} \quad (56)$$

Now the total cycle time for each stage, CT_j^{tot} , must be at least as large as the sum over all products of the processing time for each product i in stage j .

$$CT_j^{tot} \geq \sum_{i=1}^N n_i t_{ij} \quad \forall j \in \mathcal{M} \quad (57)$$

Obviously, the total cycle time in each stage must be less than the horizon time, so:

$$H \geq CT_j^{tot} \geq \sum_{i=1}^N n_i t_{ij} \quad \forall j \in \mathcal{M} \quad (58)$$

Substituting for n_i results in the following expression for the new horizon constraint:

$$\sum_{i=1}^N \frac{Q_i}{B_i} t_{ij} \leq H \quad \forall j \in \mathcal{M} \quad (59)$$

Applying the exponential transformation, the Gaussian quadrature, and the scenario analysis presented in Section 2 gives the final expression for the new constraint:

$$\sum_{i=1}^N Q_i^{qp} \cdot \exp \{t_{ij}^p - b_i\} \leq H \quad (60)$$

Therefore, the global optimization problem for the design of multiproduct batch plants under uncertainty with unlimited intermediate storage and zero cleanup times is the following:

$$\begin{aligned} \min_{v_j, Q_i^{qp}} & \delta \sum_{j=1}^M \alpha_j N_j \exp(\beta_j v_j) \\ & - \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \sum_{i=1}^N p_i Q_i^{qp} + \gamma \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \left\{ \sum_{i=1}^N p_i \theta_i^q - \sum_{i=1}^N p_i Q_i^{qp} \right\} \\ \text{subject to} & \quad v_j \geq \ln(S_{ij}^p) + b_i \quad \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\ & \quad \sum_{i=1}^N Q_i^{qp} \cdot \exp(t_{ij}^p - b_i) \leq H \quad \forall j \in \mathcal{M} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\ & \quad \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\ & \quad \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M} \end{aligned} \quad (61)$$

Note that the cost of storage facilities is neglected and the batch sizes for each product are assumed to be the same at each stage. In addition, there are now $M \cdot Q \cdot P$ horizon constraints as opposed to $Q \cdot P$ horizon constraints for Formulation (11). This greatly increases the size of the problem.

For the convex lower bounding problem, the horizon constraints are replaced by their convex underestimators:

$$\sum_{i=1}^N Q_i^{qp} \exp(t_{ij} - b_i) + \alpha_{2,i}^{qp} (Q_i^{qp,L} - Q_i^{qp}) (Q_i^{qp,U} - Q_i^{qp}) + \beta_{2,i}^{qp} (b_i^L - b_i) (b_i^U - b_i) \quad (62)$$

Since each t_{ij} is used rather than the maximum over all stages, t_{Li} , the size of the exponential term in the underestimator will be larger in general than for the single-product campaign model. Due to the increased size of the UIS problem it is expected that the number of iterations needed to solve this problem and the CPU time per iteration will increase.

Once the optimal design is found, it remains to determine the schedule corresponding to the design. This problem has been formulated as a mixed-integer linear program (MILP) by Birewar and Grossmann (1989).

4.1 Illustrative Example

The results of the UIS design formulation for the Illustrative Example are shown in Table 8. Compared to the solution for the single-product campaign formulation, the volume of each of the units is substantially decreased, resulting in an increase in the optimal profit. The computational effort is also increased with the UIS formulation requiring 3.95 CPU seconds versus 1.23 CPU seconds for the SPC formulation.

5 Multipurpose Batch Plant Design

In the previous sections, two different formulations for multiproduct batch plants have been presented. In a multiproduct plant, each product uses the same equipment in a fixed sequence to perform a defined processing task. However, in many cases it may be possible to eliminate unnecessary steps in the production of one or more products, or to use some equipment for different processing tasks. In this case, the plant is called a multipurpose batch plant. Figures 2 and 3 illustrate the differences between a multiproduct batch plant and a multipurpose batch plant.

The formulation of the multipurpose batch plant design problem under uncertainty requires few modifications of the multiproduct batch design problem, and does not introduce any new nonconvex terms. It will be shown that the analysis for the lower bounding terms presented in Section 3 can be directly applied to the nonconvex terms in the multipurpose batch design problem.

5.1 Single Equipment Sequence

In the single equipment sequence model, each product requires a different sequence of processing steps, and only one route is possible for each product. A single equipment sequence multipurpose batch plant is shown in Figure 3.

This problem can be formulated as the following nonconvex global optimization problem where the products are produced in L campaigns:

$$\begin{aligned}
& \min_{v_j, b_i, C_h^{qp}, Q_i^{qp}} \quad \delta \sum_{j=1}^M \alpha_j N_j \exp(\beta_j v_j) \\
& \quad - \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \sum_{i=1}^N p_i Q_i^{qp} + \gamma \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \left\{ \sum_{i=1}^N p_i \theta_i^q - \sum_{i=1}^N p_i Q_i^{qp} \right\} \\
& \text{subject to} \quad v_j \geq \ln(S_{ij}^p) + b_i \quad \forall i \in \mathcal{N} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\
& \quad Q_i^{qp} \cdot \exp(t_{Li}^p - b_i) - \sum_{h=1}^L a_{hi} C_h^{qp} \leq 0 \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \quad \sum_{h=1}^L C_h^{qp} \leq H \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \quad \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \quad 0 \leq C_h^{qp} \leq H \quad \forall h \in \mathcal{L} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \quad \min_{j,p} \left(\frac{V_j^L}{S_{ij}^p} \right) \leq b_i \leq \min_{j,p} \left(\frac{V_j^U}{S_{ij}^p} \right) \quad \forall i \in \mathcal{N} \\
& \quad \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M}
\end{aligned} \tag{63}$$

where the new variable C_h^{qp} is the production time for campaign h for quadrature point q in period p . The parameter a_{hi} determines the possible interactions of the products in each production campaign. a_{hi} is unity if product i can be produced in campaign h and zero if not. The horizon constraint is now the sum of the production times for each campaign. Note that the nonconvex term $Q_i^{qp} \exp(t_{Li}^p - b_i)$ has not changed, nor have any new nonconvex terms been added. Therefore the lower bounding functions from Section 3 can be directly applied to formulation (63). An example problem for the design of a multipurpose single equipment sequence batch plant under uncertainty is included in Section 6.

5.2 Multiple Equipment Sequences

In the multiple equipment sequence model, two or more alternative production routes are possible for each product. This requires defining a set of all possible routes that can be used to make product i , denoted PR_i . The multiple equipment sequence problem is formulated as follows:

$$\begin{aligned}
& \min_{v_j, b_r, C_h^{qp}, Q_i^{qp}, q_r^{qp}} \delta \sum_{j=1}^M \alpha_j N_j \exp(\beta_j v_j) \\
& - \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \sum_{i=1}^N p_i Q_i^{qp} + \gamma \sum_{p=1}^P \frac{1}{w^p} \sum_{q=1}^Q \omega^q J^q \left\{ \sum_{i=1}^N p_i \theta_i^q - \sum_{i=1}^N p_i Q_i^{qp} \right\} \\
\text{subject to } & v_j \geq \ln(S_{rj}^p) + b_r \quad \forall r \in \mathcal{R} \quad \forall j \in \mathcal{M} \quad \forall p \in \mathcal{P} \\
& \sum_{r \in PR_i} q_r^{qp} = Q_i^{qp} \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& q_r^{qp} \cdot \exp(t_{Lr}^p - b_r) - \sum_{h=1}^L a_{hr} C_h^{qp} \leq 0 \quad \forall r \in \mathcal{R} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \sum_{h=1}^L C_h^{qp} \leq H \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \theta_i^L \leq Q_i^{qp} \leq \theta_i^q \quad \forall i \in \mathcal{N} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& 0 \leq C_h^{qp} \leq H \quad \forall h \in \mathcal{L} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& 0 \leq q_r^{qp} \leq q_r^{Upq} \quad \forall r \in \mathcal{R} \quad \forall q \in \mathcal{Q} \quad \forall p \in \mathcal{P} \\
& \min_{j,p} \left(\frac{V_j^L}{S_{rj}^L} \right) \leq b_r \leq \min_{j,p} \left(\frac{V_j^U}{S_{rj}^U} \right) \quad \forall r \in \mathcal{R} \\
& \ln(V_j^L) \leq v_j \leq \ln(V_j^U) \quad \forall j \in \mathcal{M}
\end{aligned} \tag{64}$$

where

$$\begin{aligned}
q_r^{Upq} &= \theta_{P_r}^q \\
t_{Lr}^p &= \max_j t_{rj}^p
\end{aligned} \tag{65}$$

where P_r is the index for the product made in route r . The new variable q_r^{qp} represents the production of route r for quadrature point q in period p . Thus, a new constraint is that the sum over all possible routes for a product i of q_r^{qp} must equal the total production of product i , Q_i^{qp} .

Note that although q_r^{qp} has replaced Q_i^{qp} in the nonconvex term, the form of the term remains the same as in the multiproduct formulations. Therefore, the same lower bounding functions can be used for the multiple equipment sequence formulation.

$$q_r^{qp} \exp(t_{Lr}^p - b_r) + \alpha_1 \left\{ (q_r^{Lqp} - q_r^{qp})(q_r^{Upq} - q_r^{qp}) + (b_r^L - b_r)(b_r^U - b_r) \right\} \tag{66}$$

For example, if the α_1 formulation is used, the convex lower bounding function is given by equation (66).

6 Computational Studies

The following example problems illustrate the advantage of using the tight convex lower bounding functions developed in this work. The global solutions were found in a small number of iterations, even for very large problems. The algorithm presented in this paper was

implemented in GAMS and MINOS5.4 was used as a local solver. An IBM RS6000 was used to run all examples, and CPU times are reported in seconds. For all examples, five quadrature points for each product were used in the Gaussian Quadrature approximation of the expected profit integral.

6.1 Multiproduct Batch Plant Design Problems

Example 1

This example is similar to the Illustrative Example, but in this case, the size factors and processing times are taken to be uncertain parameters. Three scenarios are used to provide a range of values for the uncertain parameters. The additional scenarios increase the size of the problem. In the SPC problem formulation there are 155 variables and 93 constraint equations. These include 75 nonlinear constraints and 150 nonlinear terms. The UIS formulation also has 155 variables, but contains 225 nonlinear constraints with 450 nonlinear terms, and a total of 243 constraints. The weighting factor, w^p , was the same for each scenario and had a value of $\frac{1}{3}$. A relative tolerance of 0.003 was used in this example and the horizon time, H , was 8. The data are given in Tables 9 and 10, and the results are shown in Tables 11 and 12.

Table 12 shows that the UIS scheduling solution results in a substantial decrease in equipment and batch sizes. The decrease in equipment sizes causes an increase in the profit.

Comparing the results for Example 1 to the Illustrative Example, an increase in the CPU time is seen, which is due to the larger size of the problem in Example 1. The CPU time required for each iteration is higher for the UIS problem than for the SPC problem, but it is interesting to note that the number of iterations required for the UIS problem is one fewer than for the SPC problem using α_2 with $\gamma = 0$. Note that using α_2 gives a tighter initial lower bound than α_1 , and requires fewer iterations to converge to the global solution. Further, as was shown in Section 3.5 with the Illustrative Example, using α_3 results in a substantial improvement in the initial lower bound over α_2 .

Table 13 shows the progression of the upper and lower bounds on the global solution for Formulation I in the case where $\gamma = 0$. An upper bounding problem is solved at each iteration, using the current lower bound solution as a starting point. Note that the upper bound is equal to the global solution at iteration seven. In addition, the initial lower bound is within two percent of the initial upper bound.

Example 2

This example requires the design of a batch plant producing four products in six stages with one unit per stage. As in the Illustrative Example, only the demands are considered as uncertain parameters. The uncertain demands have the following normal distribution functions, $N(150,10)$, $N(150,8)$, $N(180,9)$, and $N(160,10)$ for products 1, 2, 3, and 4 respectively, and each are represented by five quadrature points.

The SPC problem has 649 total constraint equations, of which 625 are nonlinear constraints with 2500 nonlinear terms. The UIS formulation has 3774 total constraints, of which 3750 are nonlinear with 15000 nonlinear terms. There are a total of 2510 variables. The upper and lower bounds on the equipment volumes, V_j , were again 4500 and 500. A relative tolerance

of 0.003 was used and the horizon time was 8, the penalty coefficient, γ , was 0. The data are given in Tables 14 and 15, and the results are shown in Tables 16 and 17.

As in Example 1, the UIS scheduling formulation results in smaller equipment and batch sizes, which increases the expected profit. A tighter initial lower bound was obtained using α_2 than α_1 , and the algorithm converged in one fewer iteration. Due to the size of this problem, more computational effort was required to solve the upper and lower bounding problems than in the first two examples. In addition, notice the large increase in CPU time for the UIS formulation. When α_3 was used to construct the lower bounding functions, the lower bound on the global solution was within the specified relative tolerance in the first iteration. This example demonstrates the ability of the method to provide very tight bounds on the global solution in few iterations.

Example 3

This problem is similar to Example 2, but in this case three scenarios are used to include a range of values for the uncertain size factors and processing times. The data are shown in Tables 14 and 18. This example has 7510 variables and the SPC formulation has 1947 constraints, including 1875 nonlinear constraints with 7500 nonlinear terms. A relative tolerance of 0.015 was used. The scenario weighting factors, w^p , were $\frac{1}{3}$. The results are shown in Tables 19 and 20.

Due to the large size of this problem, the CPU time required per iteration is much larger than the previous examples. In this case, the problem formulation with α_1 took four iterations and 8640.60 CPU seconds. The α_2 solution is slightly better, requiring three iterations, but had a higher CPU time per iteration. When α_3 was used, the initial lower bound was within the specified tolerance of the upper bound, and the CPU time was substantially smaller.

Example 4

In the final example, the design of a plant which produces five products in six stages with a different (fixed) number of pieces of equipment per stage is considered. Only the demands are taken to be uncertain parameters and five quadrature points are used for each uncertain demand. This results in a large problem with 15,636 variables and 3155 constraints. Of these constraints, 3125 are nonlinear, containing 15,625 nonconvex terms.

Only the single-product campaign formulation was used for this example. The demands follow normal distributions with the following forms, $N(250,10)$, $N(150,8)$, $N(180,9)$, $N(160,6)$, and $N(120,3)$. The bounds on the V variables are 500 and 4500, and a relative tolerance of 0.015 was used. The time horizon was 6 and the penalty coefficient was 0. The processing parameters, price, and cost data are given in Tables 21 and 22, and the results are shown in Tables 23 and 24. Again, the initial lower bound provided by α_3 is the tightest, followed by α_2 . Note that in each case, the initial lower bound is extremely close to the global solution, and all formulations converged in the first iteration. Note that the CPU time required for the α_2 formulation was much higher than the other two α expressions.

6.2 Multipurpose Batch Plant Design Problems

Example 5

In this example, the task is to design a five-stage multipurpose batch plant which produces five products, as shown in Figure 3. Note that each product requires a different configuration of the plant, and only one configuration is possible for each product. Only products one and two have uncertain demands, while the remaining products have a known, fixed demand. The processing times and size factors are not considered to be uncertain. This problem has 260 variables, and 175 constraints. Of these constraints, 125 are nonlinear and each nonlinear constraint contains only one nonconvex term.

As in the illustrative example for the multiproduct design formulations, five quadrature points per uncertain demand are used to approximate the expected profit, and a cost exponent, β_j , of 0.3 and annualization coefficient, δ , of 0.6 are used. The production horizon, H , is 6.5, and the equipment cost coefficient, α_j , is 0.25. The minimum volume of each piece of equipment, V_j^U , is 500, and the maximum volume is 2000. Table 25 shows the size factors and processing times, Table 26 shows the prices and uncertain demands for each product, and Table 27 gives the values for the campaign interactions, a_{hi} .

The solution for this example is shown in Table 28 and the computational results for the different lower bounding methods are shown in Table 29. As was the case for the multiproduct examples, the α_2 formulation provides an improvement over the α_1 formulation. Again, the α_3 formulation gives a very tight initial lower bound, so that the required tolerance was achieved in the first iteration.

6.3 Comparison to Alternative Underestimating Approaches

A major advantage of the α BB approach in comparison to underestimation schemes that are based on the methods of Al-Khayyal and Falk (1983), McCormick (1976), as well as products of univariate functions is that it does not require the addition of any new constraints or variables. The effect of this advantage becomes quite pronounced as the size of the large-scale optimization problems presented in this paper increases. For example, an alternate convex lower bounding scheme is based on representing the nonconvex term as a product of univariate functions, Maranas and Floudas (1995). The nonconvex term, $Q_i^{qp} \exp(t_{Li}^p - b_i)$ is a product of two univariate functions $f(Q_i^{qp}) \cdot g(b_i)$ where $f(Q_i^{qp}) = Q_i^{qp}$ and $g(b_i) = \exp(t_{Li}^p - b_i)$. In this approach, a new variable is substituted for each nonconvex term, and convex lower bounds on the substituted variable are constructed. In this case,

$$\begin{aligned}
s_i^{qp} &= Q_i^{qp} \exp(t_{Li}^p - b_i) \\
s_i^{qp} &\geq Q_i^{Lqp} \exp(t_{Li}^p - b_i) + Q_i^{qp} \exp(t_{Li}^p - b_i^U) - Q_i^{Lqp} \exp(t_{Li}^p - b_i^U) \\
s_i^{qp} &\geq Q_i^{Uqp} \exp(t_{Li}^p - b_i) + Q_i^{qp} \exp(t_{Li}^p - b_i^L) - Q_i^{Uqp} \exp(t_{Li}^p - b_i^L)
\end{aligned} \tag{67}$$

This approach requires the addition of $N \cdot Q \cdot P$ new variables and $2 \cdot N \cdot Q \cdot P$ new constraints.

The three α BB methods are compared with the univariate functions convex lower bounding scheme in Table 30 for three examples. The advantage of the α BB approach becomes apparent as the size of the problem increases. For the illustrative example, and Example 1, the α BB methods provide tighter initial lower bounds than the alternate method. However, since the

size of the problems are not especially large, the advantage in CPU time is minimal. Example 2 is much larger than the other two examples, and the advantage of the α BB method is clearly shown. The alternate method took roughly nine times the computational effort of the α_1 method.

7 Conclusions

This paper has presented a procedure for finding the globally optimal design of multiproduct and multipurpose batch plants under uncertainty. The problem with a fixed number of equipment per stage was formulated as a single nonlinear optimization problem. The uncertain demands are represented by a Gaussian quadrature formulation, and the uncertain processing parameters are handled through a scenario-based approach. The design problem is formulated for both single-product campaign and mixed-product campaign with unlimited intermediate storage scheduling strategies. A key theoretical property has been developed, which is an analytical expression for the minimum value of α needed to form a convex lower bound of the nonconvex constraints. This property allows very tight bounds on the global solution to be generated in a small number of iterations. The α BB algorithm of Androulakis *et al.* (1995) with a modified branching criterion was used to converge to the global solution. Several example problems were presented, which demonstrate the effectiveness of the proposed approach to large-scale multiproduct and multipurpose batch design problems under uncertainty.

In addition to unlimited intermediate storage, several other mixed-product scheduling strategies have been proposed in the literature. Work is in progress to extend the global optimization method presented in this paper to the zero wait scheduling strategy, and to include clean-up times for both the unlimited intermediate storage and zero wait problems.

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A Gauss-Legendre Quadrature

We wish to estimate the integral:

$$\int_a^b f(x)dx \quad (68)$$

We approximate the function $f(x)$ with an n -th degree polynomial $p_n(x)$:

$$\int_a^b f(x)dx = \int_a^b p_n(x)dx + \int_a^b R_n(x)dx \quad (69)$$

where $R_n(x)$ is the error term.

Substitute for $f(x)$ using the Lagrange interpolating polynomial, $L^q(x)$, for $p_n(x)$ with its related error term:

$$f(x) = \sum_{q=0}^n L^q(x)f(x^q) + \prod_{q=1}^n (x - x^q) \frac{f^{n+1}(\xi)}{(n+1)!} \quad (70)$$

where,

$$L^q(x) = \prod_{j=0}^n \left(\frac{x - x^j}{x^q - x^j} \right) \quad q \neq j \quad \text{and} \quad a < \xi < b \quad (71)$$

Now to make the analysis easier, we transform the variable x ,

$$v = \frac{(x - a) + (x - b)}{b - a} \quad (72)$$

so,

$$f(x) = F(v) = \sum_{q=0}^n L^q(v)F(v^q) + \left[\prod_{q=0}^n (v - v^q) \right] Q_n(v) \quad (73)$$

where $Q_n(v)$ is an n th degree polynomial and,

$$L^q(v) = \prod_{j=0}^n \frac{(v - v^j)}{(v^q - v^j)} \quad q \neq j \quad (74)$$

Now the integral is given by:

$$\int_{-1}^1 f(x)dx = \int_{-1}^1 F(v)dv = \int_{-1}^1 \sum_{q=0}^n L^q(v)F(v^q)dv + \int_{-1}^1 \left[\prod_{q=0}^n (v - v^q) \right] Q_n(v)dv \quad (75)$$

Since $F(v^q)$ are fixed values, they can be taken outside the integral:

$$\begin{aligned} \int_{-1}^1 F(v)dv &\approx \sum_{q=0}^n F(v^q) \int_{-1}^1 L^q(v)dv \\ &\approx \sum_{q=0}^n \hat{\omega}^q \cdot F(v^q) \end{aligned} \quad (76)$$

where $\hat{\omega}^q$ are weighting factors and depend on the number of points n used in the approximation. These values can be found from tables.

Finally, we must select the quadrature points v^q . The object is to select them in such a way so that the error term vanishes. The orthogonality property of the Legendre polynomials is used to establish the v^q values, and these can be found in tables. For the five-point quadrature formula used in this work, the weighting factors, $\hat{\omega}^q$, and the roots, v^q , are given in Table 31.

Note that the integration limits are -1 and 1, which is required by the Gauss-Legendre quadrature formula. However, we are interested in integrating between arbitrary numbers a and b . This can be done simply by transforming the quadrature formula to the desired interval as follows:

$$x = \frac{a(1-v) + b(1+v)}{2} \quad (77)$$

and the integral becomes,

$$\int_a^b f(x)dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{a(1-v) + b(1+v)}{2}\right) dv \quad (78)$$

Now using the standard Gauss-Legendre quadrature formula, the right-hand integral can be approximated by,

$$\int_a^b f(x)dx \approx \frac{b-a}{2} \sum_{q=1}^n \hat{\omega}^q \cdot f\left(\frac{a(1-v^q) + b(1+v^q)}{2}\right) \quad (79)$$

For the formulations discussed in this paper, the following substitution is made:

$$\omega^q = \frac{b-a}{2} \hat{\omega}^q \quad (80)$$

resulting in the following Gauss-Legendre quadrature formula:

$$\int_a^b f(x)dx \approx \frac{b-a}{2} \sum_{q=1}^n \omega^q \cdot f\left(\frac{a(1-v^q) + b(1+v^q)}{2}\right) \quad (81)$$

It still remains to calculate the joint probability density function, J , for the uncertain parameters. For a single continuous random variable, y , the normal density function, $f(y)$ is:

$$f(y) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(y-\mu)^2}{2\sigma^2}\right\} \quad (82)$$

where μ is the mean and σ is the standard deviation of the distribution.

In general, a multivariate normal density function is very complicated to calculate. However, since we have assumed that all uncertain parameters are independent, the joint probability density function is simply the product of the individual density functions:

$$J(y_1, \dots, y_m) = \prod_{i=1}^m \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left\{ -\frac{(y_i - \mu_i)^2}{2\sigma_i^2} \right\} \quad (83)$$

and with a quadrature formulation,

$$J^q(y_1^q, \dots, y_m^q) = \prod_{i=1}^m \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left\{ -\frac{(y_i^q - \mu_i)^2}{2\sigma_i^2} \right\} \quad (84)$$

Now, for two uncertain demand parameters represented by five quadrature points each, the product $\hat{\omega}^q J^q$ is given by the 5x5 grid shown in Table 32. Note that the terms in the center of the grid are several orders of magnitude greater than the terms on the edges.

B Derivation of Upper Bounds for c and d

The task is to find the upper bounds for the constants c and d that maintain the convexity of the lower bounding function:

$$L = x \exp(y) + \frac{\alpha_2}{\eta} (x^U - x)(x^L - x) + \beta_2 (y^U - y)(y^L - y)$$

where,

$$\begin{aligned}\alpha_2 &= \hat{\alpha} \left(1 - c \cdot \frac{x - x^L}{x^U - x^L} \right) \\ \beta_2 &= \hat{\beta} \left(1 - d \cdot \frac{y^U - y}{y^U - y^L} \right)\end{aligned}$$

Recall that L is convex if both of the eigenvalues of the Hessian matrix are positive, which is equivalent to satisfying the following two conditions:

1. $\frac{\partial^2 L}{\partial x^2} + \frac{\partial^2 L}{\partial y^2} \geq 0$
2. $\frac{\partial^2 L}{\partial x^2} \frac{\partial^2 L}{\partial y^2} - \frac{\partial^2 L}{\partial x \partial y} \geq 0$

The second derivatives of L are:

$$\begin{aligned}L_{xx} &= \frac{\partial^2 L}{\partial x^2} = \frac{2\hat{\alpha}}{\eta} \left(1 - c \cdot \frac{3x - x^U - 2x^L}{x^U - x^L} \right) \\ L_{yy} &= \frac{\partial^2 L}{\partial y^2} = 2\hat{\alpha} \left(\frac{x \exp(y)}{2\hat{\alpha}} + 1 + d \cdot \frac{3y - 2y^U - y^L}{y^U - y^L} \right) \\ L_{xy} &= \frac{\partial^2 L}{\partial x \partial y} = \exp(2y)\end{aligned}$$

Substituting the second derivatives into the second convexity condition gives the following expression:

$$F = \frac{4\hat{\alpha}^2}{\eta} \left[1 - c \cdot \frac{3x - x^U - 2x^L}{x^U - x^L} \right] \left[\frac{x \exp(y)}{2\hat{\alpha}} + 1 + d \cdot \frac{3y - 2y^U - y^L}{y^U - y^L} \right] - \exp(2y) \geq 0 \quad (85)$$

As an initial estimate of the upper bounds on c and d , the observation is made that both

$$\left[1 - c \cdot \frac{3x - x^U - 2x^L}{x^U - x^L} \right] \quad \text{and} \quad \left[\frac{x \exp(y)}{2\hat{\alpha}} + 1 + d \cdot \frac{3y - 2y^U - y^L}{y^U - y^L} \right]$$

must always be positive, otherwise the second convexity condition will be violated. This observation gives the following bounds:

$$c > \frac{1}{2} \quad (86)$$

$$d > \frac{1}{2} + \frac{x^L \exp(y^L)}{4\hat{\alpha}} \quad (87)$$

However, these bounds only guarantee that the first term in the second convexity condition is always positive, they do not guarantee that the condition is always satisfied. In order to find tighter upper bounds on c and d , one needs to find the point at which F is minimized and then determine the bounds on c and d that guarantee that F is non-negative at the minimum. To find the minimum, find all of the stationary points of F .

$$\begin{aligned} \frac{\partial F}{\partial x} \Big|_{(x^*, y^*, c^*, d^*)} &= \frac{4\hat{\alpha}^2}{\eta} \left[\frac{-3c^*}{x^U - x^L} \right] \left[\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1 + d^* \cdot \frac{3y^* - 2y^U - y^L}{y^U - y^L} \right] \\ &\quad + \frac{4\hat{\alpha}^2}{\eta} \left[1 - c^* \cdot \frac{3x^* - x^U - 2x^L}{x^U - x^L} \right] \left[\frac{\exp(y^*)}{2\hat{\alpha}} \right] = 0 \\ \frac{\partial F}{\partial y} \Big|_{(x^*, y^*, c^*, d^*)} &= \frac{4\hat{\alpha}^2}{\eta} \left[1 - c^* \cdot \frac{3x^* - x^U - 2x^L}{x^U - x^L} \right] \left[\frac{x^* \exp(y^*)}{2\hat{\alpha}} + \frac{3d^*}{y^U - y^L} \right] - 2\exp(2y^*) = 0 \\ \frac{\partial F}{\partial c} \Big|_{(x^*, y^*, c^*, d^*)} &= \frac{4\hat{\alpha}^2}{\eta} \left[-\frac{3x^* - x^U - 2x^L}{x^U - x^L} \right] \left[\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1 + d^* \cdot \frac{3y^* - 2y^U - y^L}{y^U - y^L} \right] = 0 \\ \frac{\partial F}{\partial d} \Big|_{(x^*, y^*, c^*, d^*)} &= \frac{4\hat{\alpha}^2}{\eta} \left[1 - c^* \cdot \frac{3x^* - x^U - 2x^L}{x^U - x^L} \right] \left[\frac{3y^* - 2y^U - y^L}{y^U - y^L} \right] = 0 \end{aligned}$$

where each (x^*, y^*, c^*, d^*) that satisfies these conditions is a stationary point. By examining the derivative of F with respect to d , either

$$y^* = \frac{2y^U + y^L}{3} \quad \text{or} \quad c^* = \frac{x^U - x^L}{3x^* - x^U - 2x^L}.$$

It is evident that $y^* = \frac{2y^U + y^L}{3}$ otherwise the derivative of F with respect to y reduces to:

$$0 - 2\exp(2y^*) = 0 \quad \longrightarrow \quad y^* = -\infty$$

By the same argument with the derivative of F with respect to c , either

$$x^* = \frac{x^U + 2x^L}{3} \quad \text{or} \quad d^* = -\frac{y^U - y^L}{3y^* - 2y^U - y^L} \left(\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1 \right)$$

and $x^* = \frac{x^U + 2x^L}{3}$, otherwise $y^* = \infty$. Now x^* and y^* can be substituted into the first two equations of the stationarity condition in order to solve for c^* and d^* :

$$\begin{aligned} c^* &= \left(\frac{x^U - x^L}{3} \right) \left(\frac{\exp(y^*)}{x^* \exp(y^*) + 2\hat{\alpha}} \right) \\ d^* &= \left(\frac{y^U - y^L}{6} \right) \left(\frac{\eta \exp(2y^*)}{\hat{\alpha}^2} - \frac{x^* \exp(y^*)}{\hat{\alpha}} \right) \end{aligned}$$

Therefore there is only one stationary point of F . Now it is necessary to determine the type of the stationary point. This can be done by evaluating the eigenvalues of the Hessian matrix of F at the stationary point. This results in the following fourth-order characteristic polynomial:

$$\begin{aligned}
& \lambda^4 \\
& + \left(\frac{4\hat{\alpha}^2}{\eta} \right) \left[2 \left(\frac{\exp(y^*)}{2\hat{\alpha}} \right)^2 \frac{1}{\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1} - \frac{\exp(y^*)}{2\hat{\alpha}} \left(x^* - 4\eta \frac{\exp(y^*)}{2\hat{\alpha}} \right) \right] \cdot \lambda^3 \\
& + \left(\frac{4\hat{\alpha}^2}{\eta} \right)^2 \left[\left(\frac{3}{x^U - x^L} \right)^2 \left(\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1 \right)^2 - \left(\frac{3}{y^U - y^L} \right)^2 \right. \\
& \quad - \left. \left(\frac{\exp(y^*)}{2\hat{\alpha}} \right)^2 \left(1 - 2\eta \left(\frac{\exp(y^*)}{2\hat{\alpha}} \right)^2 \frac{1}{\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1} \right)^2 \right. \\
& \quad \left. - 2 \left(\frac{\exp(y^*)}{2\hat{\alpha}} \right)^3 \frac{1}{\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1} \left(x^* - 4\eta \frac{\exp(y^*)}{2\hat{\alpha}} \right) \right] \cdot \lambda^2 \\
& + \left(\frac{4\hat{\alpha}^2}{\eta} \right)^3 \left[- 2 \left(\frac{3}{y^U - y^L} \right)^2 \left(\frac{\exp(y^*)}{2\hat{\alpha}} \right)^2 \frac{1}{\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1} \right. \\
& \quad \left. - \left(\frac{3}{x^U - x^L} \right)^2 \left(\frac{\exp(y^*)}{2\hat{\alpha}} \right) \left(\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1 \right)^2 \left(x^* - 4\eta \frac{\exp(y^*)}{2\hat{\alpha}} \right) \right] \cdot \lambda \\
& + \left(\frac{4\hat{\alpha}^2}{\eta} \right)^4 \left(\frac{3}{y^U - y^L} \right)^2 \left(\frac{3}{x^U - x^L} \right)^2 \left(\frac{x^* \exp(y^*)}{2\hat{\alpha}} + 1 \right)^2 = 0
\end{aligned}$$

In order to determine whether the four roots of the polynomial are all positive, all negative, or a combination of positive and negative, consider a general fourth-order polynomial:

$$(\lambda - a)(\lambda - b)(\lambda - c)(\lambda - d) = 0$$

when expanded, this equation becomes:

$$\begin{aligned}
\lambda^4 - (a + b + c + d)\lambda^3 & + (ab + ac + ad + bc + bd + cd)\lambda^2 \\
& - (abc + abd + acd + bcd)\lambda + abcd = 0
\end{aligned}$$

Note that the constant term in the characteristic polynomial for the Hessian is always positive. This term corresponds to the $(abcd)$ term in the general fourth-order polynomial. Therefore, the roots of the characteristic polynomial are either all positive, all negative, or two positive and two negative.

Next, consider the term which multiplies λ^2 , $(ab + ac + ad + bc + bd + cd)$. If the roots are all positive or all negative, then this term must be positive. However, if this term is negative, then there must be two positive and two negative roots. It can be shown for the characteristic polynomial that this term is maximized when $x^L = 0$. When this is substituted, the term simplifies to:

$$\begin{aligned}
& \left(\frac{y^U - y^L}{3 \exp(\frac{y^U - y^L}{3})} + 1 \right)^2 - \left(\frac{x^U}{y^U - y^L} \right)^2 \\
& - \left(\frac{y^U - y^L}{3 \exp(\frac{y^U - y^L}{3})} \right)^2 \left(1 - 2 \left(\frac{1}{\exp(\frac{y^U - y^L}{3})} \right)^2 \left(\frac{1}{\frac{y^U - y^L}{3 \exp(\frac{y^U - y^L}{3})} + 1} \right) \right)^2 \\
& - 2 \left(\frac{1}{\exp(\frac{y^U - y^L}{3})} \right)^3 \left(\frac{1}{\frac{y^U - y^L}{3 \exp(\frac{y^U - y^L}{3})} + 1} \right) \left(\left(\frac{y^U - y^L}{3} \right)^3 - 4 \left(\frac{y^U - y^L}{3} \right)^2 \left(\frac{1}{\exp(\frac{y^U - y^L}{3})} \right) \right)
\end{aligned}$$

This expression allows us to solve for the x^U , in terms of y^U, y^L , where the term changes from negative to positive, denoted by $x^{U,crit}$.

$$x^{U,crit} = \pm \frac{3n\sqrt{n}}{(n + \exp(n)) \exp(2n)} \sqrt{\exp(6n) + 2(n+1)\exp(5n) + n(n+4)\exp(4n) - 2n(n^2 - 6)\exp(2n) + 12n^2 \exp(n) - 4n}$$

where,

$$n = \frac{y^U - y^L}{3}$$

The upper bound on x is always positive, so we are only interested in the positive solution. It can be shown that $x^{U,crit}$ increases monotonically with n , and for $x^U < x^{U,crit}$, the term which multiplies λ^2 is positive, and for $x^U > x^{U,crit}$, the term is negative. We can scale the \mathbf{x} variables independently of the \mathbf{y} variables and force $x^U > x^{U,crit}$ for all x . In fact, for the problems examined in this paper $x^{U,crit} = 2.79$, while the smallest x^U is 60.

As a result, the coefficient that multiplies λ^2 is always negative. This means that the characteristic polynomial for the eigenvalues has two positive roots and two negative roots, thus the stationary point is a saddle point. Therefore, the second convexity condition, (85), must be at a minimum somewhere on the *boundary of the feasible region*. We can now use this fact to develop upper bounds on the constants, c and d .

The second convexity condition is a parametric function $f(x, y; c, d)$ where x, y are variables and c, d are parameters. The goal is to determine where this function is a minimum in order to obtain upper bounds on c and d . First, we examine each of the "faces" of the feasible region, $(x^L, y), (x^U, y), (x, y^L), (x, y^U)$. We take the gradient of the second convexity condition with respect to the independent variable on each face of the feasible region and set it equal to zero to find the stationary points of the surface on the face. Then we take the second derivative to determine what type of point the stationary point is.

The $x = x^U$ Face:

The gradient of F with respect to y :

$$\left. \frac{\partial F}{\partial y} \right|_{x^U} = \frac{4\hat{\alpha}^2}{\eta} [1 - 2c] \left[\frac{x^U \exp(y)}{2\hat{\alpha}} + \frac{3d}{y^U - y^L} \right] - 2 \exp(2y)$$

So the stationary point with respect to y is:

$$y^* = \ln \left\{ \frac{\hat{\alpha} x^U [1 - 2c]}{2\eta} + \sqrt{\left(\frac{\hat{\alpha} x^U [1 - 2c]}{2\eta} \right)^2 + \frac{8\hat{\alpha}^2}{\eta} [1 - 2c] \left(\frac{3d}{y^U - y^L} \right)} \right\}$$

And the second derivative evaluated at y^* is:

$$\begin{aligned} \frac{\partial^2 F}{\partial y^2} \Big|_{x^U, y^*} &= \left(\frac{\hat{\alpha} x^U [1 - 2c]}{\eta} - 4 \right) \left(\frac{\hat{\alpha} x^U [1 - 2c]}{\eta} + \right. \\ &\quad \left. 2\sqrt{\left(\frac{\hat{\alpha} x^U [1 - 2c]}{2\eta} \right)^2 + \frac{8\hat{\alpha}^2}{\eta} [1 - 2c] \left(\frac{3d}{y^U - y^L} \right)} \right) \end{aligned}$$

It can be shown that the second derivative is always negative at y^* , thus y^* is always a maximum. This means that the minimum of F on the $(x = x^U)$ face of the feasible region must occur at either the (x^U, y^L) or (x^U, y^U) corner.

The $x = x^L$ Face:

The gradient of F with respect to y :

$$\frac{\partial F}{\partial y} \Big|_{x^L} = \frac{4\hat{\alpha}^2}{\eta} [1 + c] \left[\frac{x^L \exp(y)}{2\hat{\alpha}} + \frac{3d}{y^U - y^L} \right] - 2\exp(2y)$$

So the stationary point with respect to y is:

$$y^* = \ln \left\{ \frac{\hat{\alpha} x^L [1 + c]}{2\eta} + \sqrt{\left(\frac{\hat{\alpha} x^L [1 + c]}{2\eta} \right)^2 + \frac{8\hat{\alpha}^2}{\eta} [1 + c] \left(\frac{3d}{y^U - y^L} \right)} \right\}$$

And the second derivative evaluated at y^* is:

$$\begin{aligned} \frac{\partial^2 F}{\partial y^2} \Big|_{x^L, y^*} &= \left(\frac{\hat{\alpha} x^L [1 + c]}{\eta} - 4 \right) \left(\frac{\hat{\alpha} x^L [1 + c]}{\eta} + \right. \\ &\quad \left. 2\sqrt{\left(\frac{\hat{\alpha} x^L [1 + c]}{2\eta} \right)^2 + \frac{8\hat{\alpha}^2}{\eta} [1 + c] \left(\frac{3d}{y^U - y^L} \right)} \right) \end{aligned}$$

It can be shown that the second derivative is always negative at y^* , thus y^* is always a maximum. This means that the minimum of F on the $(x = x^L)$ face of the feasible region must occur at either the (x^L, y^L) or (x^L, y^U) corner.

The $y = y^U$ Face:

The gradient of F with respect to x :

$$\left. \frac{\partial F}{\partial x} \right|_{y^U} = \frac{4\hat{\alpha}^2}{\eta} \left[\frac{-3c}{x^U - x^L} \right] \left[\frac{x \exp(y^U)}{2\hat{\alpha}} + 1 + d \right] + \frac{4\hat{\alpha}^2}{\eta} \left[1 - c \cdot \frac{3x - x^U - 2x^L}{x^U - x^L} \right] \frac{\exp(y^U)}{2\hat{\alpha}}$$

So the stationary point with respect to x is:

$$x^* = \frac{x^U - x^L}{3c} + \frac{x^U + 2x^L}{6} - \frac{\hat{\alpha}}{\exp(y^U)} [1 + d]$$

And the second derivative evaluated at x^* is:

$$\left. \frac{\partial^2 F}{\partial x^2} \right|_{x^*, y^U} = - \frac{12c\hat{\alpha} \exp(y^U)}{\eta(x^U - x^L)}$$

It is easily shown that the second derivative is always negative at x^* , thus x^* is always a maximum. This means that the minimum of F on the $(y = y^U)$ face of the feasible region must occur at either the (x^L, y^U) or (x^U, y^U) corner.

The $y = y^L$ Face:

The gradient of F with respect to x :

$$\left. \frac{\partial F}{\partial x} \right|_{y^L} = \frac{4\hat{\alpha}^2}{\eta} \left[\frac{-3c}{x^U - x^L} \right] \left[\frac{x \exp(y^L)}{2\hat{\alpha}} + 1 - 2d \right] + \frac{4\hat{\alpha}^2}{\eta} \left[1 - c \cdot \frac{3x - x^U - 2x^L}{x^U - x^L} \right] \frac{\exp(y^L)}{2\hat{\alpha}}$$

So the stationary point with respect to x is:

$$x^* = \frac{x^U - x^L}{3c} + \frac{x^U + 2x^L}{6} - \frac{\hat{\alpha}}{\exp(y^L)} [1 - 2d]$$

And the second derivative evaluated at x^* is:

$$\left. \frac{\partial^2 F}{\partial x^2} \right|_{x^*, y^L} = - \frac{12c\hat{\alpha} \exp(y^L)}{\eta(x^U - x^L)}$$

It is easily shown that the second derivative is always negative at x^* , thus x^* is always a maximum. This means that the minimum of F on the $(y = y^L)$ face of the feasible region must occur at either the (x^L, y^L) or (x^U, y^L) corner.

Since the minimum of F for each face of the feasible region always occurs at one of the corner points, then the minimum of F for the whole feasible region must occur at a corner point. As a result of this analysis, it suffices to examine F at each of the corner points of the feasible region in order to determine the bounds on c and d .

$$F(x^U, y^U; c, d) = (1 - 2c) \left(\frac{x^U \exp(y^U)}{2\hat{\alpha}} + 1 + d \right) - \frac{\eta \exp(2y^U)}{4\hat{\alpha}^2} \geq 0 \quad (88)$$

$$F(x^L, y^L; c, d) = (1 + c) \left(\frac{x^L \exp(y^L)}{2\hat{\alpha}} + 1 - 2d \right) - \frac{\eta \exp(2y^L)}{4\hat{\alpha}^2} \geq 0 \quad (89)$$

$$F(x^L, y^U; c, d) = (1 + c) \left(\frac{x^L \exp(y^U)}{2\hat{\alpha}} + 1 + d \right) - \frac{\eta \exp(2y^U)}{4\hat{\alpha}^2} \geq 0 \quad (90)$$

$$F(x^U, y^L; c, d) = (1 - 2c) \left(\frac{x^U \exp(y^L)}{2\hat{\alpha}} + 1 - 2d \right) - \frac{\eta \exp(2y^L)}{4\hat{\alpha}^2} \geq 0 \quad (91)$$

Equation (88) provides an upper bound on c in terms of d , and this upper bound decreases as d decreases:

$$c \leq \frac{1}{2} \left[1 - \frac{\eta \exp(2y^U)}{4\hat{\alpha}^2 \left(\frac{x^U \exp(y^U)}{2\hat{\alpha}} + 1 + d \right)} \right]$$

Equation (89) provides an upper bound on d in terms of c , and this upper bound decreases as c decreases:

$$d \leq \frac{1}{2} \left(\frac{x^L \exp(y^L)}{2\hat{\alpha}} + 1 - \frac{\eta \exp(2y^L)}{4\hat{\alpha}^2(1 + c)} \right)$$

Equation (90) provides no upper bounds for c or d . Finally, Equation (91) gives an upper bound for both c and d :

$$\left(1 + \frac{x^U \exp(y^L)}{2\hat{\alpha}} \right) c + d - 2cd \leq \frac{1}{2} \left[1 + \frac{x^U \exp(y^L)}{2\hat{\alpha}} - \frac{\eta \exp(2y^L)}{4\hat{\alpha}^2} \right]$$

In order for the values for c and d to be valid, they must satisfy the bounds given above. Using these bounding equations, a procedure can be developed to determine the largest c and d that satisfy these criteria.

Now we have derived upper bounds on c and d that guarantee that the second convexity condition is always satisfied. It still remains to show that the first convexity condition is satisfied. Substituting for the second derivatives, the condition is written:

$$x \exp(y) - \frac{2c\hat{\alpha}}{\eta(x^U - x^L)} (2x - x^U - x^L) + \frac{2\hat{\alpha}}{\eta} \left(1 - c \cdot \frac{x - x^L}{x^U - x^L} \right) - 2d\hat{\alpha} + 2\hat{\alpha}(1 - d) \geq 0$$

It can be shown that this expression is minimized at the point $(x^L, y^L; c^L, d^U)$. As a worst case scenario, we use the upper bound for d given by Equation (87), which is the largest possible

upper bound for d . Substituting in the values for each of the variables and parameters reduces the first convexity condition to the following expression:

$$\frac{2\hat{\alpha}}{\eta} \geq 0$$

This expression is always satisfied, thus the first convexity condition is satisfied when c and d are chosen within the bounds given by Equations (86) and (87).

Size Factors				Processing Times				Investment Cost Coefficients			Prices of Products	
Product	Stage			Product	Stage			Stage	α_j	β_j	Product	p_i
	1	2	3		1	2	3					
1	2	3	4	1	8	20	8	1	5	0.6	1	5.5
2	4	6	3	2	16	4	4	2	5	0.6	2	7.0
								3	5	0.6		

Table 1: Data for Illustrative Example

γ value	Optimal Profit	Optimal Design: α_1					Iterations	CPU s
		V_1	V_2	V_3	B_1	B_2		
Single-Product Campaign								
0	979.186	1800	2700	3600	900	450	4	1.30
4	937.424	1908	2861	3815	954	477	4	0.86
8	934.854	1972	2958	3945	986	493	3	0.59

Table 2: Results for Illustrative Example (SPC)

α_1			
Iteration	Upper Bound	Lower Bound	Relative Difference
1	-979.180	-987.840	0.00884
2	-979.185	-984.106	0.00502
3	-979.186	-982.404	0.00328
4	-979.186	-981.278	0.00213

Table 3: Progression of Upper and Lower Bounds for Illustrative Example, ($\gamma = 0$)

γ value	Optimal Profit	Optimal Design: α_2					Iterations	CPU s
		V_1	V_2	V_3	B_1	B_2		
Single-Product Campaign								
0	979.186	1800	2700	3600	900	450	3	1.47
4	937.424	1908	2861	3815	954	477	4	1.90
8	934.854	1972	2958	3945	986	493	2	0.71

Table 4: Results for Illustrative Example (SPC)

$\alpha_2(Q), \beta_2(b)$			
Iteration	Upper Bound	Lower Bound	Relative Difference
1	-979.180	-986.777	0.00775
2	-979.185	-983.599	0.00451
3	-979.186	-982.093	0.00297

Table 5: Progression of Upper and Lower Bounds for Illustrative Example, ($\gamma = 0$)

γ value	Optimal Profit	Optimal Design: α_3					Iterations	CPU s
		V_1	V_2	V_3	B_1	B_2		
Single-Product Campaign								
0	979.186	1800	2700	3600	900	450	2	0.75
4	937.424	1908	2861	3815	954	477	2	0.56
8	934.854	1972	2958	3945	986	493	1	0.18

Table 6: Results for Illustrative Example (SPC)

$\alpha_3(Q, b)$			
Iteration	Upper Bound	Lower Bound	Relative Difference
1	-979.180	-982.171	0.00305
2	-979.186	-980.880	0.00173

Table 7: Progression of Upper and Lower Bounds for Illustrative Example, ($\gamma = 0$)

γ value	Optimal Profit	Optimal Design: α_2					Iterations	CPU s
		V_1	V_2	V_3	B_1	B_2		
Mixed Product Campaign with UIS								
0	1197.132	1200	1800	2400	600	300	2	2.10

Table 8: Results for Illustrative Example (UIS)

Investment Cost Coefficients			Prices of	
Stage	α_j	β_j	Products	
1	5	0.6	Product	p_i
2	5	0.6	1	5.5
3	5	0.6	2	7.0

Table 9: Cost and Price Data for Example 1

Scenario	Size Factors				Processing Times			
	Product	Stage			Product	Stage		
		1	2	3		1	2	3
1	1	2.5	3.5	4.5	1	7	19	7
	2	4.5	6.5	3.5	2	15	3	3
2	1	1.5	2.5	3.5	1	9	21	9
	2	3.5	5.5	2.5	2	17	5	5
3	1	2	3	4	1	8	20	8
	2	4	6	3	2	16	4	4

Table 10: Processing Parameter Data for Example 1

γ value	Optimal Profit	Optimal Design				
		V_1	V_2	V_3	B_1	B_2
Single-Product Campaign						
0	876.582	2159	3119	3886	864	480
4	841.932	2285	3300	4112	914	508
8	827.730	2410	3481	4338	964	536
Unlimited Intermediate Storage						
0	1097.265	1509	2113	2716	604	325

Table 11: Solution for Example 1

γ	Using α_1			Using α_2			Using α_3		
	Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s
Single-Product Campaign									
0	-892.825	13	27.57	-890.861	5	14.55	-882.530	4	11.65
4	-860.249	14	22.30	-857.797	6	13.55	-848.045	5	11.39
8	-843.390	11	18.30	-840.534	4	7.83	-831.612	2	4.48
Unlimited Intermediate Storage									
0	-1103.856	5	40.73	-1103.196	4	29.41	-1100.653	2	18.22

Table 12: Computational Results for Example 1

Iteration	Upper Bound	Lower Bound	Relative Difference
1	-876.5781766	-892.8253296	0.01851
2	-876.5795104	-887.0662490	0.01195
3	-876.5818400	-887.0645756	0.01194
4	-876.5818403	-886.9900931	0.01186
5	-876.5818403	-885.8041489	0.01050
6	-876.5818403	-882.0419320	0.00622
7	-876.5818419	-880.8482292	0.00486
8	-876.5818419	-880.8463604	0.00485
9	-876.5818419	-879.8040916	0.00367
10	-876.5818419	-879.8022239	0.00366
11	-876.5818419	-879.6526083	0.00349
12	-876.5818419	-879.6408780	0.00348
13	-876.5818419	-879.0291303	0.00278

Table 13: Progression of Upper and Lower Bounds for Example 1, ($\alpha_1; \gamma = 0$)

Investment Cost Coefficients			Prices of Products	
Stage	α_j	β_j		
1	10	0.6	Product	p_i
2	10	0.6		
3	10	0.6		
4	10	0.6		
5	10	0.6		
6	10	0.6		
			1	3.5
			2	4.0
			3	3.0
			4	2.0

Table 14: Cost and Price Data for Examples 2 and 3

Size Factors							Processing Times						
Product	Stage						Product	Stage					
	1	2	3	4	5	6		1	2	3	4	5	6
1	8.0	2.0	5.2	4.9	6.1	4.1	1	7.0	8.3	6.0	7.0	6.5	8.0
2	0.7	0.8	0.9	3.8	2.1	2.5	2	6.8	5.0	6.0	4.8	5.5	5.8
3	0.7	2.6	1.6	3.4	3.2	2.9	3	4.0	5.9	5.0	6.0	5.5	4.5
4	4.7	2.3	1.6	2.7	1.2	2.5	4	2.4	3.0	3.5	2.5	3.0	2.8

Table 15: Processing Parameter Data for Example 2

Optimal Profit	Optimal Design									
	V_1	V_2	V_3	V_4	V_5	V_6	B_1	B_2	B_3	B_4
Single-Product Campaign										
750.184	2875	1407	1869	2385	2192	1569	359	628	541	612
Unlimited Intermediate Storage										
830.338	2703	1323	1757	2045	2061	1475	338	538	509	575

Table 16: Solution of Example 2 for $\gamma = 0$

Using α_1			Using α_2			Using α_3		
Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s
Single-Product Campaign								
-757.247	6	551.56	-756.238	5	471.74	-751.566	1	35.65
Unlimited Intermediate Storage								
-836.851	5	2942.32	-835.903	4	4325.90	-831.717	1	398.18

Table 17: Computational Results for Example 2

Scenario	Size Factors							Processing Times						
	Product	Stage						Product	Stage					
		1	2	3	4	5	6		1	2	3	4	5	6
1	1	8.0	2.0	5.2	4.9	6.1	4.1	1	7.0	8.3	6.0	7.0	6.5	8.0
	2	0.7	0.8	0.9	3.8	2.1	2.5	2	6.8	5.0	6.0	4.8	5.5	5.8
	3	0.7	2.6	1.6	3.4	3.2	2.9	3	4.0	5.9	5.0	6.0	5.5	4.5
	4	4.7	2.3	1.6	2.7	1.2	2.5	4	2.4	3.0	3.5	2.5	3.0	2.8
2	1	8.5	2.5	5.7	5.4	6.6	4.6	1	6.0	7.3	5.0	6.0	5.5	7.0
	2	1.2	1.3	1.4	4.3	2.6	3.0	2	5.8	4.0	5.0	3.8	4.5	4.8
	3	1.2	3.1	2.1	3.9	3.7	3.4	3	3.0	4.9	4.0	5.0	4.5	3.5
	4	5.2	2.8	2.1	3.2	1.7	3.0	4	1.4	2.0	2.5	1.5	2.0	1.8
3	1	7.5	1.5	4.7	4.4	5.6	3.6	1	8.0	9.3	7.0	8.0	7.5	9.0
	2	0.2	0.3	0.4	3.3	1.6	2.0	2	7.8	6.0	7.0	5.8	6.5	6.8
	3	0.3	2.1	1.1	2.9	2.7	2.4	3	5.0	6.9	6.0	7.0	6.5	5.5
	4	4.2	1.8	1.1	2.2	0.7	2.0	4	3.4	4.0	4.5	3.5	4.0	3.8

Table 18: Processing Parameter Data for Example 3

Optimal Profit	Optimal Design									
	V_1	V_2	V_3	V_4	V_5	V_6	B_1	B_2	B_3	B_4
552.665	3036	1726	2036	2714	2357	1894	357	631	557	584

Table 19: Solution of Example 3 for $\gamma = 0$

Using α_1			Using α_2			Using α_3		
Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s
-562.382	3	8640.60	-561.391	2	5469.87	-554.386	1	1211.85

Table 20: Computational Results for Example 3

Investment Cost Coefficients				Prices of	
Stage	α_j	β_j	N_j	Products	
1	0.25	0.6	3	Product	p_i
2	0.25	0.6	2	1	3.5
3	0.25	0.6	3	2	4.0
4	0.25	0.6	2	3	3.0
5	0.25	0.6	1	4	2.0
6	0.25	0.6	2	5	4.5

Table 21: Cost and Price Data for Example 4

Size Factors							Processing Times						
Product	Stage						Product	Stage					
	1	2	3	4	5	6		1	2	3	4	5	6
1	7.9	2.0	5.2	4.9	6.1	4.2	1	6.4	4.7	8.3	3.9	2.1	1.2
2	0.7	0.8	0.9	3.4	2.1	2.5	2	6.8	6.4	6.5	4.4	2.3	3.2
3	0.7	2.6	1.6	3.6	3.2	2.9	3	1.0	6.3	5.4	11.9	5.7	6.2
4	4.7	2.3	1.6	2.7	1.2	2.5	4	3.2	3.0	3.5	3.3	2.8	3.4
5	1.2	3.6	2.4	4.5	1.6	2.1	5	2.1	2.5	4.2	3.6	3.7	2.2

Table 22: Processing Parameter Data for Example 4

Optimal Profit	Optimal Design										
	V_1	V_2	V_3	V_4	V_5	V_6	B_1	B_2	B_3	B_4	B_5
3731.079	2789	1901	1836	2460	2187	1982	353	724	683	593	528

Table 23: Solution of Example 4 for $\gamma = 0$

Using α_1			Using α_2			Using α_3		
Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s
-3731.406	1	1232.75	-3731.251	1	7051.85	-3731.132	1	2089.49

Table 24: Computational Results for Example 4

Size Factors						Processing Times					
Product	Stage					Product	Stage				
	1	2	3	4	5		1	2	3	4	5
1	3.2	2.5	—	—	—	1	9.0	6.0	—	—	—
2	—	—	1.0	1.5	—	2	—	—	3.9	6.2	—
3	—	2.7	—	—	2.3	3	—	5.5	—	—	3.5
4	3.1	—	1.1	—	—	4	7.5	—	4.5	—	—
5	—	—	—	1.7	2.8	5	—	—	—	7.1	4.0

Table 25: Processing Parameter Data for Example 5

Product	Mean	Std. Dev.	Price
1	200	10	55
2	150	10	70
3	150	0	60
4	150	0	65
5	150	0	70

Table 26: Product Demand and Price Data for Example 5

Campaign	Product				
	1	2	3	4	5
1	1	1	0	0	0
2	0	1	1	0	0
3	0	0	1	1	0
4	0	0	0	1	1
5	1	0	0	0	1

Table 27: Campaign Interactions for Example 5

Optimal Profit	Multipurpose Batch Plant: Optimal Design									
	V_1	V_2	V_3	V_4	V_5	B_1	B_2	B_3	B_4	B_5
33.725	1481	1157	526	682	1071	463	454	429	478	383

Table 28: Solution of Example 5 for $\gamma = 0$

Using α_1			Using α_2			Using α_3		
Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s	Initial LB	No. of Iters.	CPU s
Single-Equipment Sequence								
38.991	6	14.47	35.127	3	5.02	33.807	1	1.32

Table 29: Computational Results for Example 5

Lower Bounding Approach	Initial LB	Number of Iterations	CPU s	Number of Variables	Number of Constraints
Illustrative Example: $\gamma = 0$					
α_1	-987.840	4	1.30	55	31
α_2	-986.777	3	1.47	55	31
α_3	-982.180	2	0.75	55	31
Univariate Functions	-990.076	10	2.01	105	131
Example 1: $\gamma = 0$					
α_1	-892.825	13	27.57	155	93
α_2	-890.861	5	14.55	155	93
α_3	-882.530	4	11.65	155	93
Univariate Functions	-900.901	10	14.38	305	393
Example 2					
α_1	-757.247	6	551.56	2510	649
α_2	-756.238	5	471.74	2510	649
α_3	-751.566	1	35.65	2510	649
Univariate Functions	-796.887	8	4825.96	5010	5649

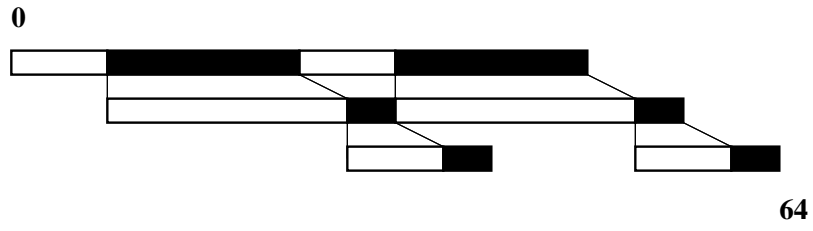
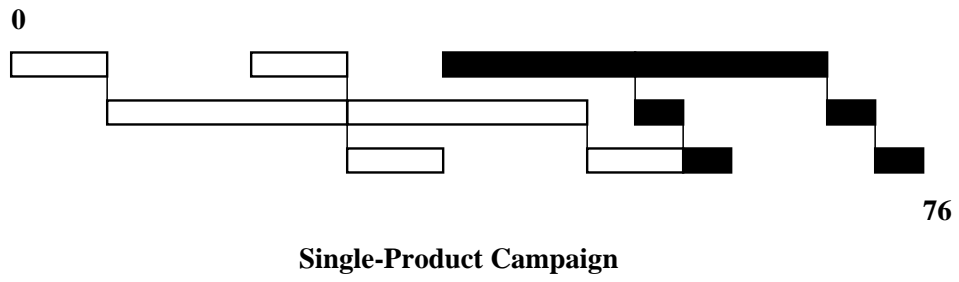
Table 30: Comparison of Lower Bounding Strategies

q	v^q	$\hat{\omega}^q$
1	-0.9061798459	0.23692885
2	-0.5384693101	0.4786286705
3	0	0.56888889
4	0.5384693101	0.4786286705
5	0.9061798459	0.23692885

Table 31: Five-Point Gaussian Quadrature Parameters

$\hat{\omega}^q J^q \cdot 10^3$: 5x5 Quadrature					
q_1/q_2	1	2	3	4	5
1	0.00000018	0.00002489	0.00030092	0.00002489	0.00000018
2	0.00002489	0.00352407	0.04260490	0.00352407	0.00002489
3	0.00030092	0.04260490	0.51508041	0.04260490	0.00030092
4	0.00002489	0.00352407	0.04260490	0.00352407	0.00002489
5	0.00000018	0.00002489	0.00030092	0.00002489	0.00000018

Table 32: Objective Function Multipliers



 **Product A**
 **Product B**

Figure 1: Comparison of campaign strategies

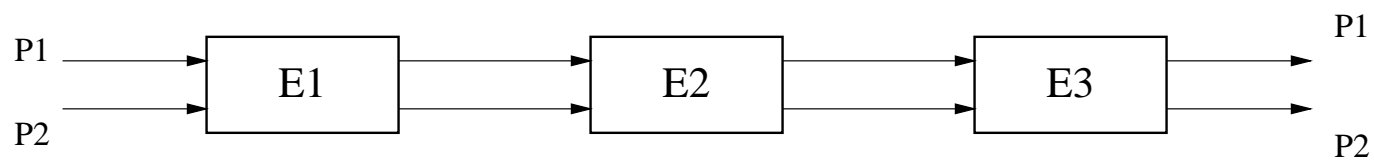


Figure 2: A multiproduct batch plant

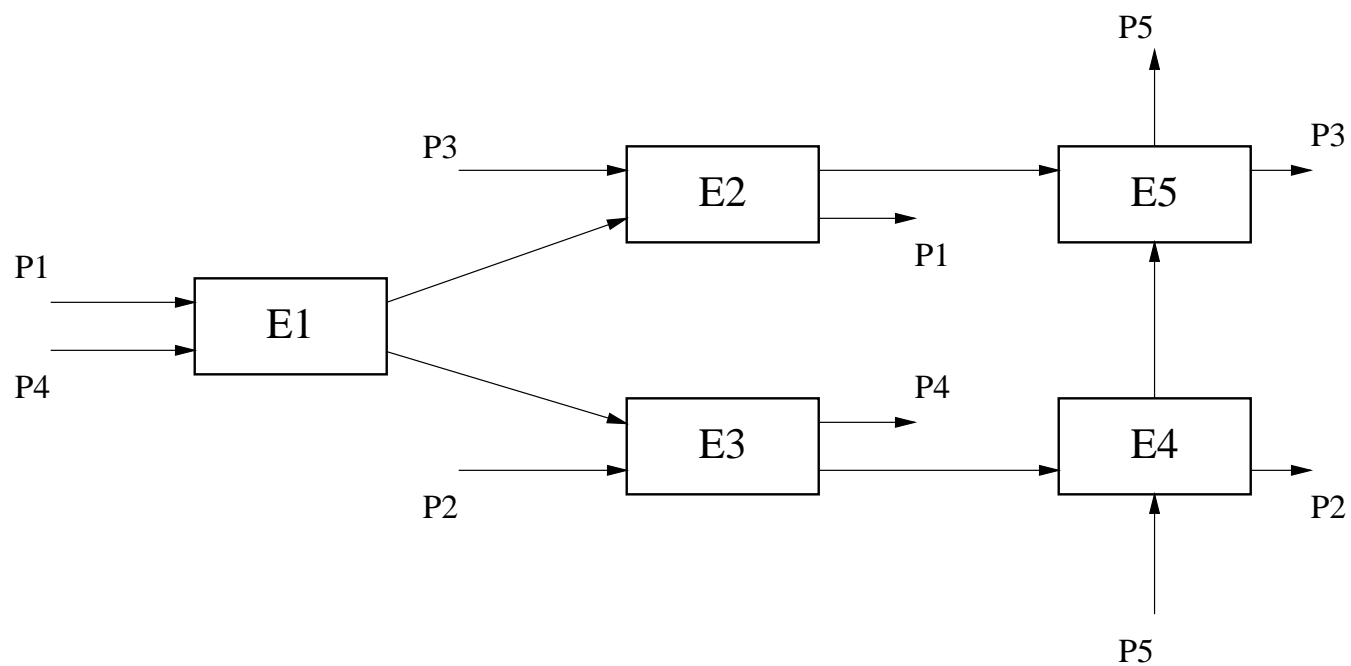


Figure 3: A multipurpose batch plant: single equipment sequence (Example 5)

List of Tables

1	Data for Illustrative Example	43
2	Results for Illustrative Example (SPC)	44
3	Progression of Upper and Lower Bounds for Illustrative Example, ($\gamma = 0$) . .	45
4	Results for Illustrative Example (SPC)	46
5	Progression of Upper and Lower Bounds for Illustrative Example, ($\gamma = 0$) . .	47
6	Results for Illustrative Example (SPC)	48
7	Progression of Upper and Lower Bounds for Illustrative Example, ($\gamma = 0$) . .	49
8	Results for Illustrative Example (UIS)	50
9	Cost and Price Data for Example 1	51
10	Processing Parameter Data for Example 1	52
11	Solution for Example 1	53
12	Computational Results for Example 1	54
13	Progression of Upper and Lower Bounds for Example 1, ($\alpha_1; \gamma = 0$)	55
14	Cost and Price Data for Examples 2 and 3	56
15	Processing Parameter Data for Example 2	57
16	Solution of Example 2 for $\gamma = 0$	58
17	Computational Results for Example 2	59
18	Processing Parameter Data for Example 3	60
19	Solution of Example 3 for $\gamma = 0$	61
20	Computational Results for Example 3	62
21	Cost and Price Data for Example 4	63
22	Processing Parameter Data for Example 4	64
23	Solution of Example 4 for $\gamma = 0$	65
24	Computational Results for Example 4	66
25	Processing Parameter Data for Example 5	67
26	Product Demand and Price Data for Example 5	68
27	Campaign Interactions for Example 5	69
28	Solution of Example 5 for $\gamma = 0$	70
29	Computational Results for Example 5	71
30	Comparison of Lower Bounding Strategies	72
31	Five-Point Gaussian Quadrature Parameters	73
32	Objective Function Multipliers	74

List of Figures

1	Comparison of campaign strategies	75
2	A multiproduct batch plant	76
3	A multipurpose batch plant: single equipment sequence (Example 5)	77