Design of Single-Product Campaign Batch Plants under Demand Uncertainty

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A new method is introduced for optimally designing multiproduct batch plants under the single-product campaign (SPC) production mode. Uncertain future product demands are described with normal probability distributions, and more than one processing unit of equal size are allowed per stage. At the expense of imposing the normality assumption for product demand uncertainty and the SPC production mode, the original two-stage stochastic optimization problem is transformed into a deterministic mixed-integer nonlinear programming problem without relying on implicit or explicit discretization of the uncertain variables. This is accomplished through the explicit solution of the inner problem and the analytical integration overall product demand realizations. This problem representation and solution strategy result in savings of orders of magnitude over existing methods in computational requirements.

Introduction

Batch processing has emerged as the preferred mode of operation for many high-value added products. This is because it provides the flexibility necessary to accommodate a large number of low-volume products with customized specifications involving multiple processing steps in the same processing plant (Rippin, 1993). In this article, we consider the optimal design of multiproduct batch plants operating in single-product campaign (SPC) mode under product demand uncertainty. The defining feature of the SPC production mode is that all the batches of a given product are manufactured before production of the next product begins. In contrast, mixed-product campaign (MPC) production modes (Birewar and Grossmann, 1989a) may produce more batches per unit time at the expense of increased changeover times and cleanup costs. At the design stage, no concrete information is available for future product demand profiles over the lifetime of the plant (Rippin, 1993). Therefore, before manufacturing begins, plant capacity must be appropriately allocated to accommodate varying future product demand realizations. This allocation must establish the optimal tradeoff between product demand satisfaction and extra plant capacity. Failure to systematically set this tradeoff may lead to unnecessarily high investment cost or missed sales and, thus, market share.

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Motivated by this necessity, a number of publications have been devoted to the study of batch plant design under uncertainty. One of the first references to multiproduct batch plant design under technical and commercial uncertainty is by Johns et al. (1978). Describing the uncertain variables with probability distribution functions, the authors derived an optimal direction search procedure to maximize the expected profit in the face of uncertainty. This search for the first time demonstrated that: (i) The optimal batch plant designs with and without considering uncertainty may differ significantly; (ii) stochastic models provide much more realistic estimates for the expected profitability of batch plants than deterministic ones. Later, Reinhart and Rippin (1986, 1987) addressed the design with uncertainty in demands, processing times, and size factors based on a mathematical programming formulation. The key element of the work is the introduction of time constraints corresponding to different scenarios, leading to a design satisfying all postulated realizations of the uncertain variables. This idea was later extended by Shah and Pantelides (1992) who proposed a scenario-based approach for the design of multipurpose batch plants with uncertain production requirements yielding a large-scale mixed-integer linear (MILP) model. A conceptual formulation for batch plant design under uncertainty, which allows for staged expansions, was proposed by Wellons and Reklaitis (1989). The authors suggested a distinction between "hard" and "soft" constraints and introduced penalty terms in the objective function for the latter. After assuming that the demands change stepwise and the only uncertainty is in the time when the step-change occurs, an analytical expression for the expected value of the objective function was derived, thus enabling the solution of the model as an MINLP problem. Straub and Grossmann (1992) proposed a procedure for the evaluation and optimization of the expected stochastic flexibility in multiproduct batch plants. They integrated stochastic aspects stemming from both flexibility and reliability considerations and developed Gaussian quadrature-based procedures for establishing the optimal tradeoffs between investment cost and expected stochastic flexibility. Later, Subrahmanyam et al. (1994) addressed market uncertainty by generating scenarios based on discretized probability distributions of the product demands. Recently, Ierapetritou and Pistikopoulos (1995, 1996) contributed to the general problem of batch plant design under uncertainty. They developed a feasibility relaxation for the "soft" constraints and proposed a two-stage stochastic programming formulation. The latter is solved based on the discretization of the probability space through quadrature integration leading to a single but typically large-scale nonconvex optimization problem. Harding and Floudas (1997) proposed a global optimization procedure to solve this problem based on the αBB algorithm (Androulakis et al., 1995).

In general, there are three different approaches for formulating optimization problems in the face of uncertainty: (i) the "wait and see" formulation; (ii) the probabilistic approach; (iii) the "here and now" or the two-stage model (Vajda, 1970). The approach proven most useful as a source of reliable design information is the two-stage, or "here and now" approach (Johns et al., 1978; Wellons and Reklaitis, 1989). In the latter, the decisions are made in two stages. In the first stage, the decision variables are fixed, and in the second stage, the operating variables are adjusted based on the realization of the uncertain parameters (Prekopa, 1995). The design variables in the multiproduct batch plant design problem are the number of units and their capacity per stage, while the operating variables are the production levels (output) of each product. The difficulty associated with this undertaking is that it requires averaging of the solution of the inner optimization problem over the ensemble defined by all possible product demand realizations before the outer optimization problem is solved. Computationally, this averaging means integration over the multivariate probability space. This challenge has so far been resolved through explicit/implicit discretization of the probability space. Different integration methods are defined by their respective strategies for discretization. These are based on *a priori* discretization (Subrahmanyam et al., 1994), Gaussian quadrature integration (Straub and Grossmann, 1993; Ierapetritou and Pistikopoulos, 1996), or random sampling (Liu and Sahinidis, 1996) such as Monte-Carlo. The key advantage of the aforementioned methods lies in the fact that they are largely insensitive to the type of probability distribution selected for the uncertain demands and the adopted production policy. The main disadvantage is that computational requirements increase sharply with the number of uncertain product demands.

In this article, a novel approach is introduced for solving the design problem of multiproduct batch plants under SPC production mode when the product demands are uncertain. The approach allows for more than one processing unit of equal size per stage. At the expense of sacrificing generality by imposing the normality assumption and the SPC production mode, the original two-stage stochastic optimization problem is transformed into a deterministic convex mixed-integer nonlinear programming (MINLP) problem. The proposed approach allows for the first time the solution of large-scale batch design problems involving tens of uncertain demands. The derived analytical expressions help elicit the meaning, relative weight, and interrelationships between different elements of the model. Furthermore, an equivalence of penalizing production shortfalls and imposing a high enough probability for product demand satisfaction is revealed. Results indicate that *the number and capacities of units per stage in the optimal design depend on the imposed probability of product demand satisfaction.* Tradeoff curves typically exhibit a discontinuous behavior caused by the transition to plant designs with a different number of units at different probability levels of demand satisfaction.

Problem Definition and Overview

Given are the: (i) mean and (co)variances of the uncertain product demands; (ii) product recipe information quantified with processing times, size factors and number of production stages; (iii) capacity ranges and number of parallel processing units. The problem to be addressed can be stated as follows:

Find the optimal design of a multiproduct batch plant operating in SPC production mode such that the expected discounted cash flow return (DCFR) of the batch plant, within a prespecified time horizon, is maximized allowing for the optimal adjustment of production levels in response to every product demand realization.

The design objective, as stated above, suggests that rather than attempting to guarantee satisfaction of every possible realization of the uncertain demands, which is impossible if they are normally distributed, a flexible plant design is sought, ensuring the optimal level of product demand satisfaction. This optimal level of demand satisfaction is established by striking the proper balance between profit from sales and investment cost. This balance is quantified through the DCFR profitability measure, and it is realized through the continuous optimal adjustment of the production policy of the batch plant given the current product demand profile. Note that higher than optimal levels of demand satisfaction yield additional investment cost, which is not offset by increased profit from additional sales. Alternatively, lower than optimal levels of demand satisfaction lead to a loss of profit from unrealized sales greater than the achieved investment cost savings.

Further developments are found on the following modeling features and assumptions:

(1) The product demands are modeled as multivariate normally distributed random variables which may or may not be correlated. Correlation allows modeling situations when high demand for one product more often than not implies higher or lower demand for a different product (Petkov and Maranas, 1997). It is largely accepted that the normality assumption captures the essential features of product demand uncertainty (Nahmias, 1989). Theoretical justification of the use of normal distribution can be argued based on the cen-

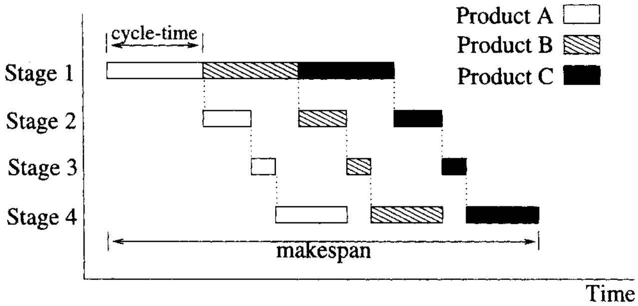

Figure 1. Gantt plot of single-product campaign (SPC) with overlapping operation.

tral limit theorem as the product demands are typically affected by a large number of stochastic events.

(2) The plant is assumed to operate in a single product campaign mode with overlapping operation (see Figure 1). Transfer times from one unit to the next are assumed to be embedded in the supplied processing times.

(3) The size factors, processing times, and profit margins are assumed to be independent of the capacity output and equipment sizes.

(4) Inventory transfers from one time horizon to the next are not considered because of the length of the time horizon (usually one year). Inventory transfer was addressed in Petkov and Maranas (1997).

(5) Equipment costs are assumed to be power functions of their capacities.

(6) Equipment capacities are assumed to be continuous. The extension to discrete sizes (see Voudouris and Grossmann, 1992) is straightforward.

(7) A number of units may operate in parallel at a particular stage to accommodate higher demands. However, all units at the same stage are assumed to have the same size.

Ierapetritou and Pistikopoulos (1995, 1996), extending the work of Johns et al. (1978) and Wellons and Reklaitis (1989), formulated the problem of multiproduct batch plant design under uncertain demands as the following two-stage optimization problem

$$\max_{V_j, B_i, N_j} E_\theta \left[\begin{array}{c} \max\limits_{Q_i} \sum\limits_{i=1}^{N} P_i Q_i \\ Q_i \le \theta_i, \quad i=1,\ldots,N \\ \sum\limits_{i=1}^{N} \left(\frac{Q_i}{B_i}\right) T_{Li} \le H \end{array} \right] - \delta \sum_{j=1}^{M} \alpha_j N_j V_j^{\beta_j}$$

subject to

$$V_j \ge S_{ij} B_i, \quad i=1,\ldots,N, \quad j=1,\ldots,M$$

$$T_{Li} = \max_{j=1,\ldots,M} \left\{ \frac{t_{ij}}{N_j} \right\}, \quad i=1,\ldots,N$$

$$V_j^L \le V_j \le V_j^U, \quad j=1,\ldots,M$$

$$N_j^L \le N_j \le N_j^U, \quad j=1,\ldots,M$$

The objective function of the outer optimization problem is composed of two terms. In the first, the expectation operator is applied to the solution of the inner optimization problem. The inner optimization problem sets the optimal operating policy for maximum profit, identified by the production levels Q_i, for a plant design V_j, B_i, N_j and a realization of the uncertain product demands θ_i. The first constraint of the inner problem safeguards against production levels exceeding product demands. The next constraint ensures that the batch plant cycle-time is not greater than the specified time horizon. The second term in the objective function of the outer problem quantifies the investment cost as the additive contribution of the respective equipment costs scaled by the discount factor. The first constraint of the outer problem determines the maximum required equipment size at each stage. The second constraint identifies the rate limiting step for every product recipe accounting for all identical parallel equipment units at each stage (SPC production mode). Finally, the last two sets of constraints impose lower and upper bounds on equipment sizes and allowable number of parallel units at each stage respectively.

Kocis and Grossmann (1988) showed that the following exponential transformations

$$V_j = \exp(v_j), \quad B_i = \exp(b_i), \quad T_{Li} = \exp(t_{Li}), \quad N_j = \exp(n_j)$$

and the binary representation of n_j

$$n_j = \left[\sum_{r=N_j^L}^{N_j^U} y_{jr} \ln(r) \right]$$

where

$$\sum_{r=N_j^L}^{N_j^U} y_{jr} = 1$$

convexify all nonconvex terms in the formulation apart from the horizon constraint. These transformations lead to the following equivalent representation of the original problem

$$\max_{v_j, b_i, y_{jr}} E_\theta \left[\begin{array}{c} \max\limits_{Q_i} \sum\limits_{i=1}^{N} P_i Q_i \\ Q_i \le \theta_i, \quad i=1,\ldots,N \\ \sum\limits_{i=1}^{N} Q_i \exp(t_{Li} - b_i) \le H \end{array} \right] - \delta \sum_{j=1}^{M} \alpha_j \exp\left(\beta_j v_j + \sum_{r=N_j^L}^{N_j^U} y_{jr} \ln(r) \right)$$

subject to

$$v_j \ge \ln(S_{ij}) + b_i, \quad i=1,\ldots,N, \quad j=1,\ldots,M$$

$$t_{Li} \ge \ln(t_{ij}) - \sum_{r=N_j^L}^{N_j^U} y_{jr} \ln(r), \quad i=1,\ldots,N, \quad j=1,\ldots,M$$

$$\sum_{r=N_j^L}^{N_j^U} y_{jr} = 1, \quad j = 1, \ldots, M$$

$$\ln(V_j^L) \leq v_j \leq \ln(V_j^U), \quad j = 1, \ldots, M$$

The main difficulty in solving the above described embedded optimization problem lies in the fact that the calculation of the expected value of the realized profits requires integration over all feasible demand realizations. Ierapetritou and Pistikopoulos (1996) first proposed a solution procedure based on Gaussian quadrature integration. In this method, the multivariate probability distribution hypersurface of the uncertain demand is discretized and for every realization θ_i^d of the uncertain demands, occurring with a probability density p^d, an optimal Q_i^d production level is defined which reduces the original formulation to a one-level optimization problem. This approach can readily accommodate different probability distribution functions and be applied to complex production modes (such as MPC). However, it requires the addition of an exponential number of variables denoting production levels and corresponding nonconvex horizon constraints.

In the following section, by exploiting the special structure of the inner problem and the properties of the normal distribution, an analytical expression for the expected value of the solution of the inner problem is derived.

Analysis

The analytical evaluation of the expected value of the inner problem requires (i) the explicit solution of the inner problem for a given uncertain demand realization; and (ii) analytical integration over all probability-weighted demand outcomes.

Analytical solution of inner problem

The inner (second-stage) problem can be written in the following form

$$\max_{Q_i} \sum_{i=1}^{N} P_i Q_i$$

subject to

$$Q_i \leq \theta_i, \quad i = 1, \ldots, N$$

$$\sum_{i=1}^{N} a_i Q_i \leq H$$

where

$$a_i = \exp(t_{Li} - b_i), \quad i = 1, \ldots, N$$

The solution of the inner problem identifies the optimal production levels Q_i^{opt}, which maximize profit for a given design and demand realization. Note that while production levels are not allowed to exceed product demands, production shortfalls are allowed. A new variable a_i is introduced which is equal to the ratio of the limiting production time over the batch size for product i. The new variable a_i represents the amount of time it takes to produce a unit of product i. It is a function of the design of the plant and is the only link between the inner and outer problems. For a given plant design and demand realizations, the inner problem is a linear programming (LP) problem in the space of the production levels Q_i.

The solution of the inner problem depends on whether the horizon constraint is active or inactive. If for a given demand realization the horizon constraint is satisfied, $\sum_{i=1}^{N} a_i \theta_i \leq H$, then the production levels can be driven to their respective upper bounds $Q_i^{\text{opt}} = \theta_i$ to maximize the profit. This situation arises when there is enough plant capacity to produce the desired product amounts within the specified time horizon. An illustration is given in Figure 2 where the probability density contour maps of two uncertain demands (θ_1, θ_2) (correlated) with means $(\hat{\theta}_1, \hat{\theta}_2)$ are plotted. The line $a_1 Q_1 + a_2 Q_2 \leq H$ (the horizon constraint) denotes the boundary of feasible production policies. The demand realizations at hand (θ_1, θ_2) lie below the horizon constraint, implying that the only active constraints are the demand feasibility constraints $Q_i \leq \theta_1$, $Q_2 \leq \theta_2$ denoted by the dashed lines. In this case, the feasible region of the LP has only one vertex which defines the optimal solution $(Q_1^{\text{opt}}, Q_2^{\text{opt}}) = (\theta_1, \theta_2)$.

In the second case, we have $\sum_i a_i \theta_i > H$ implying that not all product demands can be met with the existing capacity. This situation is shown in Figure 3. The horizon constraint intersects with the rectangular corner defined by the demand feasibility constraints. This gives rise to two vertices which are the candidates for the optimal solution of the LP inner problem. This means that the horizon constraint becomes active ($\sum_{i=1}^{N} a_i Q_i = H$) at the optimal solution in place of one of the demand feasibility constraints. The *a priori* identification of which demand feasibility will be inactive at the optimal solution is facilitated by rewriting the inner problem as

$$\max_{Q_i} \sum_{i=1}^{N} \left(\frac{P_i}{a_i}\right)(a_i Q_i)$$

subject to

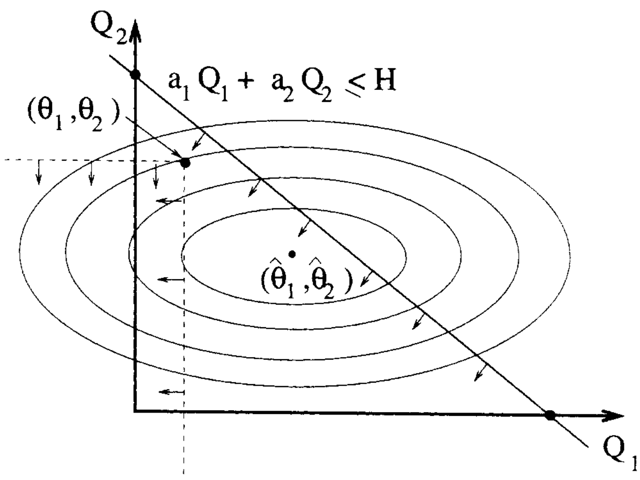

Figure 2. Inner problem: Inactive horizon constraint.

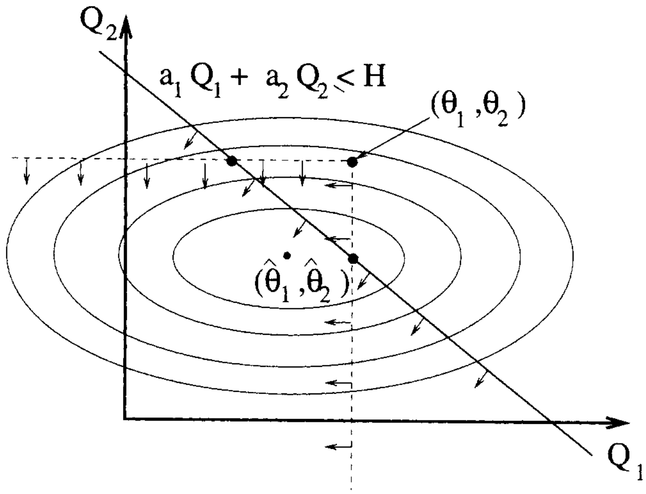

Figure 3. Inner problem: active horizon constraint.

$$\sum_{i=1}^{N} a_i Q_i \le H$$

$$a_i Q_i \le a_i \theta_i, \quad i = 1, \ldots, N$$

At the optimal solution, all $a_i Q_i$ will be driven to their respective upper bounds $a_i \theta_i$ except for that with the smallest coefficient P_i/a_i in the objective function

$$Q_i^{\text{opt}} = \theta_i, \quad i = 1, \ldots, N, \quad i \neq i^*$$

$$Q_{i^*}^{\text{opt}} = \frac{1}{a_{i^*}} \left(H - \sum_{\substack{i=1 \\ i \neq i^*}}^{N} a_i \theta_i \right)$$

where

$$i^* = \arg \min_i \left(\frac{P_i}{a_i} \right)$$

The coefficient P_i/a_i measures the profit acquired manufacturing product i per unit time (profit rate of product i). Thus, the manufacturing of products with high profit margins per unit time is favored in the inner problem. Summarizing for both cases, the following expressions for the optimal production policy Q_i^{opt} are obtained as analytical functions of the uncertain parameters θ_i

$$Q_i^{opt}(\theta) = \begin{cases} \dfrac{1}{a_{i^*}} \left(H - \sum\limits_{\substack{i=1 \\ i \neq i^*}}^{N} a_i \theta_i \right) & \text{if } i = i^* \text{ and } \sum\limits_{i=1}^{N} a_i \theta_i > H \\ \theta_i & \text{otherwise} \end{cases}$$

where

$$i^* = \arg \min_i \left(\frac{P_i}{a_i} \right)$$

Note that at the optimal operating policy all product demands are met whenever this is consistent with the horizon constraint. Otherwise, all product demands are met except for the product with the smallest profit rate whose demand is only partially satisfied.

Inspection of the optimal solution reveals that the production levels Q_i may become negative because no explicit lower bound $Q_i \ge 0$ for the production levels is imposed in the inner problem. The problem with the introduction of this bound is that a lower bound of zero also acts on the normally distributed uncertain demands θ_i which is inconsistent with the normality assumption. This dilemma demonstrates that the normality assumption for the uncertain demands can be invoked only if it samples negative product demands with a small enough probability. For example, assuming that the mean of the demands is larger than at least three times its standard deviation, negative values are sampled with only a probability of 4.3×10^{-4}. Therefore, if negative product demand values are sampled too often, the normality assumption is invalid and an alternative probability distribution such as beta or lognormal must be considered.

Nevertheless, Q_{i^*} may still assume negative values even if the product demand realizations do not sample negative values. Even with the introduction of the constraint $Q_i \ge 0$ in the inner problem, an analytical optimal solution for the production levels can still be obtained

$$Q_i^{\text{opt}}(\theta) = \begin{cases} \theta_i & \text{for } i < i^* \\ \dfrac{1}{a_{i^*}} \left(H - \sum\limits_{i=1}^{i^*-1} a_i \theta_i \right) & \text{for } i = i^* \\ 0 & \text{for } i > i^* \end{cases}$$

where the set $I = \{i | i = 1, \ldots, N\}$ has been reordered such that

$$\frac{P_1}{a_1} \ge \frac{P_2}{a_2} \ge \cdots \frac{P_N}{a_N}$$

and i^* (least profitable product) is redefined as the first i for which

$$\sum_{i=1}^{i^*} a_i \theta_i > H$$

The calculation of the expected value of the latter inner problem formulation does not decouple into a simple one-dimensional integration. In the next subsection it is shown that the expected value of the former inner problem formulation (without $Q_i \ge 0$) decompose into a single 1-D integral. This formulation, which provides an upper bound for the latter, will be employed in all subsequent developments. It can be shown that the less capacity restricted is the plant the closer the solution of the two formulations is.

Expected value of the solution of the inner problem

So far it has been shown that for a given plant design, the optimal plant operation policy depends on the realization of the random demands. This dependence renders the solution of the inner problem stochastic; thus, the calculation of its expected value requires integration over all possible realizations of the random variables.

To facilitate this calculation, first the probability α is defined which measures the likelihood that for a given plant design an uncertain demand realization will meet the horizon constraint

$$\alpha = \Pr\left[\sum_{i=1}^{N} a_i \theta_i \leq H\right]$$

This probability α is identical to the stochastic flexibility (SF) index defined by Straub and Grossmann (1992) in the context of batch plant design. They also observed that the cycle-time $CT = \sum_{i=1}^{N} a_i \theta_i$ is a normally distributed random variable as a linear combination of normal variables. Next, the probability-scaled additive property of the expectation operator is applied on the expected value of the inner problem. This is expressed as the sum of the expected value, when the uncertain demands meet the horizon constraint, times the corresponding probability α of this outcome plus the expected value when the horizon constraint is violated by the uncertain demand realization multiplied by the corresponding probability $1-\alpha$

$$E[f_{\text{inner}}^{\text{opt}}] = E\begin{bmatrix} \max\limits_{Q_i} \sum\limits_{i=1}^{N} P_i Q_i \\ Q_i \leq \theta_i, \quad i = 1, \ldots, N \\ \sum\limits_{i=1}^{N} Q_i a_i \leq H \end{bmatrix}$$

$$= \alpha E\left[\sum_{i=1}^{N} P_i Q_i^{\text{opt}}(\theta) \,\middle|\, \sum_{i=1}^{N} a_i \theta_i \leq H\right]$$

$$+ (1-\alpha) E\left[\sum_{i=1}^{N} P_i Q_i^{\text{opt}}(\theta) \,\middle|\, \sum_{i=1}^{N} a_i \theta_i \geq H\right]$$

After substituting the previously derived expression for $Q_i^{\text{opt}} = Q_i^{\text{opt}}(\theta)$ we obtain

$$E[f_{\text{inner}}^{\text{opt}}] = \alpha E\left[\sum_{i=1}^{N} P_i \theta_i \,\middle|\, \sum_{i=1}^{N} a_i \theta_i \leq H\right]$$

$$+ (1-\alpha) E\left[\sum_{\substack{i=1 \\ i \neq i^*}}^{N} P_i \theta_i \,\middle|\, \sum_{i=1}^{N} a_i \theta_i \geq H\right]$$

$$+ (1-\alpha) E\left[\frac{P_{i^*}}{a_{i^*}}\left(H - \sum_{\substack{i=1 \\ i \neq i^*}}^{N} a_i \theta_i\right) \,\middle|\, \sum_{i=1}^{N} a_i \theta_i \geq H\right]$$

This relation can be further simplified by adding the expression

$$(1-\alpha) E\left[P_{i^*} \theta_{i^*} \,\middle|\, \sum_{i=1}^{N} a_i \theta_i \geq H\right]$$

to the second term of the previous expression and subtracting it from the third term. This gives

$$E[f_{\text{inner}}^{\text{opt}}] = \sum_{i=1}^{N} P_i \hat{\theta}_i$$

$$- (1-\alpha) \frac{P_{i^*}}{a_{i^*}} E\left[\sum_{i=1}^{N} a_i \theta_i - H \,\middle|\, \sum_{i=1}^{N} a_i \theta_i - H \geq 0\right]$$

Next, the terms under the expectation operator are standardized to enable the analytical calculation of the integral. This involves subtracting the means and dividing by the standard deviations

$$E[f_{\text{inner}}^{\text{opt}}] = \sum_{i=1}^{N} P_i \hat{\theta}_i - (1-\alpha) \frac{P_{i^*}}{a_{i^*}} \left\{ \left(\sum_{i=1}^{N} a_i \hat{\theta}_i - H \right) \right.$$

$$\left. + \sigma_{ct} E\left[\frac{\sum_{i=1}^{N} a_i (\theta_i - \hat{\theta}_i)}{\sigma_{ct}} \,\middle|\, \frac{\sum_{i=1}^{N} a_i (\theta_i - \hat{\theta}_i)}{\sigma_{ct}} \geq \frac{H - \sum_{i=1}^{N} a_i \hat{\theta}_i}{\sigma_{ct}} \right] \right\}$$

Here σ_{ct} is the standard deviation of the normally distributed cycle time CT which has a mean of

$$\hat{CT} = \sum_{i=1}^{N} a_i \hat{\theta}_i$$

and a variance of

$$\sigma_{ct} = \sqrt{\sum_{i=1}^{N} a_i^2 \operatorname{Var}(\theta_i) + 2 \sum_{i=1}^{N} \sum_{i'=i+1}^{N} a_i a_{i'} \operatorname{Cov}(\theta_i, \theta_{i'})}$$

The last conditional expectation can be written as $E[x \mid x \geq -K]$ where

$$x = \frac{\sum_{i=1}^{N} a_i (\theta_i - \hat{\theta}_i)}{\sigma_{ct}}$$

is a standardized normally distributed random variable (that is, $N[0,1]$). The parameter

$$K = \frac{\sum_{i=1}^{N} a_i \hat{\theta}_i - H}{\sigma_{ct}}$$

measures the discrepancy between the required mean cycle time and available horizon divided by the standard deviation of the cycle time. The larger the value of K, the less sufficient are the available resources to meet the product demands within the specified time horizon H. The application of the definition of the expectation of a standard normal distribution truncated at $x = -K$ yields

$$E[x|x \geq -K] = \frac{\frac{1}{\sqrt{2\pi}}\int_{-K}^{+\infty} x e^{-(1/2)x^2}dx}{\frac{1}{\sqrt{2\pi}}\int_{-K}^{+\infty} e^{-(1/2)x^2}dx} = \frac{f(K)}{\Phi(K)}$$

where f denotes the standardized normal distribution function. In addition, the probability $(1-\alpha)$ of having $\Sigma_{i=1}^{N} a_i\theta_i \geq H$ can be related to K as follows

$$(1-\alpha) = \Pr\left[\sum_{i=1}^{N} a_i\theta_i \geq H\right]$$

$$= \Pr\left[\frac{\sum_{i=1}^{N} a_i(\theta_i - \hat{\theta}_i)}{\sigma_{ct}} \geq \frac{H - \sum_{i=1}^{N} a_i\hat{\theta}_i}{\sigma_{ct}}\right] = \Phi(K)$$

After incorporating the expressions for the conditional expectation and probability $1-\alpha$, the expected value of the solution of the inner problem yields

$$E[f_{\text{inner}}^{\text{opt}}] = \sum_{i=1}^{N} P_i\hat{\theta}_i - \frac{P_{i^*}}{a_{i^*}}\sigma_{ct}[K\Phi(K) + f(K)]$$

where

$$K = \frac{\sum_{i=1}^{N} a_i\hat{\theta}_i - H}{\sigma_{ct}}$$

and

$$\sigma_{ct} = \sqrt{\sum_{i=1}^{N} \sigma_i^2 \mathrm{Var}(\theta_i) + 2\sum_{i=1}^{N}\sum_{i'=i+1}^{N} a_i a_i \mathrm{Cov}(\theta_i, \theta_{i'})}$$

$$i^* = \arg\min_i \left(\frac{P_i}{a_i}\right)$$

Inspection of the derived functionalities reveals that the optimum expected profit is equal to the profit incurred without any resource limitations, penalized by the profit rate of the least profitable product, times the standard deviation of the cycle time, times a monotonically increasing function of K. This demonstrates that higher uncertainty and larger discrepancies between the required mean cycle time and available horizon have a negative effect on the optimum expected profit.

Single-Stage Problem Reformulation

The derivation of an analytical expression for the expected value of the optimum of the inner problem enables recasting of the original two-stage formulation as a single-stage problem whose objective function is defined as

$$\max \sum_{i=1}^{N} P_i\hat{\theta}_i - \frac{P_{i^*}}{a_{i^*}}\sigma_{ct}[K\Phi(K) + f(K)] - \delta\sum_{j=1}^{M} \alpha_j \exp\left[\beta_j v_j + \sum_{r=N_j^L}^{N_j^U} y_{jr}\ln(r)\right]$$

where

$$K = \frac{\sum_{i=1}^{N} a_i\hat{\theta}_i - H}{\sigma_{ct}}$$

$$\sigma_{ct} = \left[\sum_i a_i^2 \mathrm{Var}(\theta_i) + 2\sum_{i=1}^{N}\sum_{i'=i+1}^{N} a_i a_{i'}\mathrm{Cov}(\theta_i, \theta_{i'})\right]^{1/2}$$

$$a_i = \exp(t_{Li} - b_i)$$

$$i^* = \arg\min_i \left(\frac{P_i}{a_i}\right)$$

Inspection of the above definition for the objective function reveals a number of nonconvexities in the objective function and defining relations. In the following section, a number of transformations are introduced for eliminating most, and in some cases all, nonconvexities.

Transformations

(1) The batch plant design affects the selection of the least profitable product i^* through the a_i variables. The systematic identification of i^* can be accomplished by introducing the binary variables

$$x_i = \begin{cases} 1, & \text{if } i = i^* \\ 0, & \text{otherwise} \end{cases}$$

and expressing the "uncertainty-induced" penalty term in the objective function as

$$\left(\sum_{i=1}^{N} x_i \frac{P_i}{a_i}\right)\sigma_{ct}[K\Phi(K) + f(K)] \text{ subject to } \sum_{i=1}^{N} x_i = 1$$

(2) The nonconvex ratio of σ_{ct} over a_i in the objective function is replaced with a new variable w_i defined as

$$w_i = \left(\sum_{i'} r_{ii'}^2 \mathrm{Var}(\theta_{i'}) + 2\sum_{i'=1}^{N}\sum_{i''=i'+1}^{N} r_{ii'}r_{ii''}\mathrm{Cov}(\theta_{i'}, \theta_{i''})\right)^{1/2}, \quad i = 1, \ldots, N$$

where

$$r_{ii'} = \exp(t_{Li'} - b_{i'} - t_{Li} + b_i), \quad i, i' = 1, \ldots, N$$

At the optimal solution, the necessary optimality Karush Kuhn Tucker (KKT) (Bazaraa et al., 1993) conditions, with respect to w_i and $r_{ii'}$, yield positive multipliers for both equations. This indicates that they can be equivalently relaxed into the following convex inequalities

$$w_i \geq \left[\sum_{i'} r_{ii'}^2 \mathrm{Var}(\theta_{i'}) + 2 \sum_{i'=1}^{N} \sum_{i''=i'+1}^{N} r_{ii'} r_{ii''} \mathrm{Cov}(\theta_{i'}, \theta_{i''}) \right]^{1/2}, \quad i = 1, \ldots, N$$

$$r_{ii'} \geq \exp(t_{Li'} - b_{i'} - t_{Li} + b_i), \quad i, i' = 1, \ldots, N$$

An elegant proof of convexity for the expression denoting the square root of the variance of the cycle time can be found in (Kataoka, 1963).

(3) The resulting products between binary x_i and continuous w_i variables in the objective function can be linearized exactly based on the Glover (1975) transformation

$$x_i w_i^L \leq z_i \leq x_i w_i^U$$

$$w_i - (1 - x_i) w_i^U \leq z_i \leq w_i - (1 - x_i) w_i^L$$

This is accomplished at the expense of introducing a new set of variables z_i.

(4) Application of the KKT conditions to the newly defined objective function and defining constraints with respect to K yields at the optimal solution:

$$-\left(\sum_{i=1}^{N} P_i z_i \right) \Phi(K) + \lambda_K = 0$$

This implies that the Lagrange multiplier λ_K of the defining equality for K at the optimal solution will always be positive. Therefore, the defining equality for K can be relaxed into the inequality

$$K \sigma_{ct} \geq \sum_{i=1}^{N} a_i \hat{\theta}_i - H$$

which is convex for a fixed K.

(5) The KKT optimality conditions with respect to σ_{ct} yield

$$+ K \lambda_K + \lambda_{\sigma_{ct}} = 0$$

implying that $\lambda_{\sigma_{ct}} \geq 0$ when $K \leq 0$ and $\lambda_{\sigma_{ct}} \leq 0$ when $K \geq 0$. This means that the defining relation for σ_{ct} can be written as

$$\mathrm{sign}(K) \left[\sigma_{ct} - \left(\sum_i a_i^2 \mathrm{Var}(\theta_i) + 2 \sum_{i=1}^{N} \sum_{i'=i+1}^{N} a_i a_{i'} \mathrm{Cov}(\theta_i, \theta_{i'}) \right)^{1/2} \right] \leq 0$$

where

$$\mathrm{sign}(K) = \begin{cases} 1, & \text{if } K > 0 \\ 0, & \text{if } K = 0 \\ -1, & \text{if } K < 0 \end{cases}$$

which is convex for $K \leq 0$ and concave for $K \geq 0$ (fixed K).

(6) Finally, the necessary optimality conditions with respect to a_i yield

$$-\hat{\theta}_i \lambda_K - \lambda_{\sigma_{ct}} \frac{\mathrm{Var}(\theta_i) + \sum_{i' \neq i} a_{i'} \mathrm{Cov}(\theta_i, \theta_{i'})}{\sigma_{ct}} + \lambda_{a_i} = 0, \quad i = 1, \ldots, N$$

For $K \leq 0$, λ_{a_i} is always positive at the optimal solution and the defining equation for a_i can be written as the following convex inequality

$$a_i \geq \exp(t_{Li} - b_i), \quad i = 1, \ldots, N$$

However, for $K \geq 0$ the sign of λ_{a_i} cannot be predetermined. Depending on the relative magnitude of the terms in the KKT necessary optimality conditions the defining equation for a_i relaxes into convex or concave expressions.

Formulation

Based on the above described transformations, the optimal batch design problem with product demand uncertainty can be expressed as the following mixed-integer nonlinear programming (MINLP) problem

$$\max \sum_i^N P_i \hat{\theta}_i - \sum_i P_i z_i [K \Phi(K) + f(K)] - \delta \sum_{j=1}^{M} \alpha_j \exp\left(\beta_j v_j + \sum_{r=N_j^L}^{N_j^U} y_{jr} \ln(r) \right)$$

subject to

$$\left. \begin{aligned} x_i w_i^L \leq z_i \leq x_i w_i^U \\ w_i - (1 - x_i) w_i^U \leq z_i \leq w_i - (1 - x_i) w_i^L \end{aligned} \right\}, \quad i = 1, \ldots, N$$

$$w_i \geq \left[\sum_{i'} r_{ii'}^2 \mathrm{Var}(\theta_{i'}) + 2 \sum_{i'=1}^{N} \sum_{i''=i'+1}^{N} r_{ii'} r_{ii''} \mathrm{Cov}(\theta_{i'}, \theta_{i''}) \right]^{0.5}, \quad i = 1, \ldots, N$$

$$r_{ii'} \geq \exp(t_{Li'} - b_{i'} - t_{Li} + bi), \quad i, i' = 1, \ldots, N$$

$$K \sigma_{ct} \geq \sum_{i=1}^{N} a_i \hat{\theta}_i - H$$

$$0 \geq \mathrm{sign}(K) \left\{ \sigma_{ct} - \left[\sum_i a_i^2 \mathrm{Var}(\theta_i) + 2 \sum_{i=1}^{N} \sum_{i'=i+1}^{N} a_i a_{i'} \mathrm{Cov}(\theta_i, \theta_{i'}) \right]^{1/2} \right\}$$

$$\left.\begin{array}{ll} a_i \ge \exp(t_{Li} - b_i), & K \le 0 \\ a_i = \exp(t_{Li} - b_i), & \text{otherwise} \end{array}\right\}, \quad i = 1, \ldots, N$$

$$t_{Li} \ge \ln(t_{ij}) - \sum_{r=N_j^L}^{N_j^U} y_{jr} \ln(r), \quad i = 1, \ldots, N, \; j = 1, \ldots, M$$

$$v_j \ge \ln(S_{ij}) + b_i, \quad i = 1, \ldots, N, \; j = 1, \ldots, M$$

$$\ln\left(V_j^L\right) \le v_j \le \ln\left(V_j^U\right), \quad j = 1, \ldots, M$$

$$\sum_{r=N_j^L}^{N_j^U} y_{jr} = 1, \quad \sum_{i=1}^{N} x_i = 1, \quad x_i, y_{jr} \in \{0,1\}$$

The solution strategy for this MINLP problem is motivated by the following observation: *For a fixed* $K \le 0$, *implying that* $\alpha \ge 0.5$, *the above formulation is a convex MINLP.*

This observation redefines the task at hand to the solution of a single-parameter convex MINLP problem assuming that the mean cycle-time is less than the available horizon ($\alpha \ge 0.5$) at the optimal solution. This can be accomplished by iteratively solving the above convex MINLP for different values of $K \le 0$ and constructing the tradeoff curve between the optimum expected DCFR and α. The convex MINLP problems are solved to global optimality by utilizing the outer approximation (OA) algorithm of Duran and Grossmann. The maximum of the tradeoff curve (see examples section) provides the batch plant design with the optimum expected DCFR and probability of meeting product demands α. While for most realistic problems, only solutions with $\alpha \ge 0.5$ are of interest, for some cases it is worth analyzing the $\alpha \le 0.5$ regime. The presence of nonlinear equality constraints can be handled with the equality relaxation outer approximation the ER/OA algorithm (Kocis and Grossmann, 1988) implemented into DICOPT (Kocis and Grossmann, 1989). While the latter cannot guarantee convergence to the global optimum, computational experience indicates that in most cases it performs well after careful initialization.

Variable Bounds

A significant factor affecting the CPU requirements for solving MINLP problems with the OA algorithm is the tightness of the LP relaxation of the MILP master subproblems. Tight LP relaxations are aided by providing the tightest possible lower and upper variable bounds.

A collection of tight bounds for the original variables v_j, t_{Li}, and b_i can be found in Biegler et al. (1997) and are as follows

$$\ln\left(V_j^L\right) \le v_j \le \ln\left(V_j^U\right)$$

$$\max_{j=1,\ldots,M} \ln\left(\frac{t_{ij}}{N_j^U}\right) \le t_{Li} \le \max_{j=1,\ldots,M} \ln\left(\frac{t_{ij}}{N_j^L}\right)$$

$$\min_{j=1,\ldots,M} \ln\left(\frac{V_j^L}{S_{ij}}\right) \le b_i \le \min_{j=1,\ldots,M} \ln\left(\frac{V_j^U}{S_{ij}}\right)$$

Based on the above relations, the development of bounds for the supplementary variables a_i, σ_{ct}, $r_{ii'}$ and w_i, which are functions of the original variables v_j, t_{Li}, and b_i, is straightforward. In addition, three extra constraints are developed to improve the MILP relaxation:

(1) From the problem definition (Biegler et al., 1997), we have $V_j \ge S_{ij} B_i$ and $T_{Li} \ge t_{ij}/N_j$. Because a_i is equal to T_{Li}/B_i, it follows that

$$a_i \ge \frac{t_{ij} S_{ij}}{N_j V_j}$$

Substituting the exponentially transformed expressions for N_j and V_j above yields the following convex lower bounding expression for a_i

$$a_i \ge t_{ij} S_{ij} \exp\left(-v_j - \sum_{r=N_j^L}^{N_j^U} y_{jr} \ln(r)\right), \qquad i = 1, \ldots, N; \; j = 1, \ldots, M$$

(2) Next, an upper bounding constraint for $r_{ii'}$ is derived. For $i = i^*$ we have

$$\frac{P_{i'}}{a_{i'}} \ge \frac{P_i}{a_i}, \quad i' = 1, \ldots, N; \; i = i^*$$

Because $r_{ii'}$ is equal to $a_{i'}/a_i$, we can write

$$r_{ii'} \le \frac{P_{i'}}{P_i}, \quad i' = 1, \ldots, N; \; i = i^*$$

Utilizing the binary variable x_i to model the i^* index, we obtain the following upper bound for $r_{ii'}$

$$r_{ii'} \le \frac{P_{i'}}{P_i} + \left(r_{ii'}^U - \frac{P_{i'}}{P_i}\right)(1 - x_i), \quad i, i' = 1, \ldots, N$$

The last inequality is active when $i = i^*$, and inactive otherwise.

(3) Finally, a bounding expression for w_i is derived. From the definition of i^* we have

$$P_{i'} w_{i'} \ge P_i w_i, \quad i' = 1, \ldots, N; \; i = i^*$$

The utilization of the binary variable x_i in a fashion similar to the previous constraint yields

$$P_{i'} w_{i'} \ge P_i w_i - (1 - x_i)(P_i w_i - P_{i'} w_{i'}^L), \quad i, i' = 1, \ldots, N$$

This expression can be written as the following linear cut

$$P_{i'} w_{i'} \ge P_i z_i + P_{i'} w_{i'}^L (1 - x_i), \quad i, i' = 1, \ldots, N$$

after replacing the binary-continuous product $x_i w_i$ with z_i.

Application of the derived bounds and binding constraints to the large-scale example in the example section yields more than 30% savings in CPU time because of the smaller number of iterations for the OA algorithm.

Formulation with Penalty for Production Shortfalls

The use of penalty functions in the objective function for stochastic models was pioneered by Evers (1967) as a way of accounting for losses due to infeasibility. In the context of designing chemical batch plants under uncertain demands, a penalty term in the objective function is employed to quantify the effect of missed revenues and loss of customer confidence. It typically assumes the following form

$$-\gamma \sum_{i=1}^{N} P_i \max[0,(\theta_i - Q_i)]$$

where γ is the penalty coefficient whose value determines the relative weight attributed to production shortfalls as a fraction of the profit margins (Wellons and Reklaitis, 1989; Birewar and Grossmann, 1990a; Ierapetritou and Pistikopoulos, 1996).

The introduction of the penalty for production shortfalls term augments the inner problem formulation as follows

$$\max_{Q_i} \sum_{i=1}^{N} P_i Q_i - \gamma \sum_{i=1}^{N} P_i(\theta_i - Q_i)$$

subject to

$$Q_i \le \theta_i, \quad i = 1, \ldots, N$$

$$\sum_{i=1}^{N} Q_i \exp(t_{Li} - b_i) \le H$$

Grouping of the common terms in the objective function yields

$$\max_{Q_i} \sum_{i=1}^{N} (1+\gamma) P_i Q_i - \gamma \sum_{i=1}^{N} P_i \theta_i$$

Note that the new production level Q_i coefficients are all multiplied by the same quantity $1+\gamma$. This means that the new optimal production levels Q_i^{opt} are the same as those identified earlier. This implies that the presence of a penalty for the production shortfalls term does not impact the optimal operating policy for a given plant design.

The expected value of the optimal solution for the new inner problem is thus related to that without the γ term as follows

$$E\left[f_{\text{inner},\gamma}^{\text{opt}}\right] = (1+\gamma) E[f_{\text{inner}}^{\text{opt}}] - \gamma \sum_{i=1}^{N} P_i \hat{\theta}_i$$

After substituting the expression for $E[f_{\text{inner}}^{\text{opt}}]$ we obtain

$$E\left[f_{\text{inner},\gamma}^{\text{opt}}\right] = \sum_{i=1}^{N} P_i \hat{\theta}_i - (1+\gamma) \frac{P_{i^*}}{a_{i^*}} \sigma_{ct}[K\Phi(K) + f(K)]$$

Substitution of the solution of the inner problem in the outer problem formulation gives rise to a one-parameter convex MINLP for $K \le 0$. The solution strategy is identical to the one discussed in the previous section, (iterative solution of a single-parameter MINLP for different values of K).

Higher values of γ penalize production shortfalls more heavily giving rise to higher probabilities α of satisfying all product demands at the optimal solution. This implies that changes on either parameter γ or α have the same qualitative effect on the optimal solution. This observation motivates the following question: *Is the optimal design obtained for a given value of the penalty parameter γ the same as those obtained without using the penalty term γ but rather selecting a high enough value for α?*

A formal proof is necessary because the γ formulation is similar, but not the same with the mathematically identical penalty representation (by penalizing $K \le K_0$) of the α formulation. A proof of equivalence between the γ and the α formulations is presented in the Appendix. This equivalence gives rise to (α, γ) pairs for which the optimal batch plant designs are identical. This is a powerful result, because it demonstrates that when one of the two formulations is solved an optimal solution is also obtained for the other.

Computational Results

A small illustrative, a medium and a large-scale example are next considered to highlight the proposed solution strategy and obtain results for different problem sizes. Each example is solved iteratively for different values of K ($\alpha \ge 0.5$). The obtained results are then used to construct the tradeoff curve between the expected DCFR and probability of meeting all product demands α. The outer approximation (OA) algorithm of Duran and Grossmann (1986a,b) is implemented in GAMS (Brooke et al., 1988) to solve the resulting convex MINLP. CPLEX 4.0 and MINOS 5.4 are used as MILP and NLP solvers, respectively. The stopping criterion on OA is crossover of the lower and upper bounds, which guarantees global optimality of the solution for convex MINLP problems. Additionally, the nonconvex formulations arising when K is not fixed or K is fixed at a positive value are solved using DICOPT which implements the outer approximation with equality relaxation (Kocis and Grossmann, 1987, 1988, 1989). All reported CPU times are in seconds on an IBM RS6000 43P-133 workstation.

Illustrative Example

This example was first addressed by Grossmann and Sargent (1979). It involves the design of a batch which produces only two products. Each product recipe involves three production stages with only one piece of equipment allotted per stage. The time horizon is 8,000 h and the stage capacities vary between 500 and 4,500 units. The annualized investment cost coefficient δ is equal to 0.3. The uncertain product demands are modeled as the normally distributed variables $N(200,10)$ and $N(100,10)$, respectively. The size factors and processing times are given in Table 1. The investment cost coefficients and profit margins are given in Table 2. The resulting convex MINLP formulation involves two binary variables, 82 continuous variables, and 43 constraints.

Figure 4 plots the optimal expected DCFR for different values of α. The maximum expected profit occurs at $\alpha = 0.81$. The optimal batch plant design for $\alpha = 0.81$ involves an objective value of $1{,}266.87 \times 10^3$ and optimal equipment vol-

Table 1. Processing Data for the Illustrative Example

	Size Factors, S_{ij}			Processing Times, t_{ij}		
Product	Stage 1	Stage 2	Stage 3	Stage 1	Stage 2	Stage 3
1	2	3	4	8	20	8
2	4	6	3	16	4	4

Table 2. Cost and Profit Margin Data for the Illustrative Example

Investment Cost Coeff.			Price Data	
Stage	α_j (\$/L)	β_j	Product	Profit Margin, P_i (\$/kg)
1	5,000	0.6	1	5.5
2	5,000	0.6	2	7.5
3	5.000	0.6		

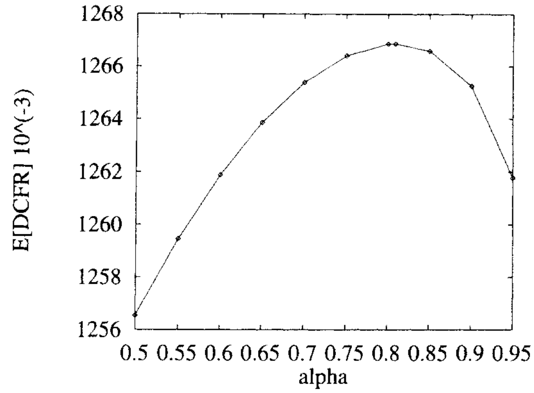

Figure 4. Optimal expected DCFR vs. α for the illustrative example.

umes of $V_1 = 1{,}882$, $V_2 = 2{,}824$ and $V_3 = 3{,}765$. Table 3 summarizes the optimal expected DCFR, equipment volumes, and batch sizes at different probabilities α. Equipment volumes and batch sizes increase with α as a result of higher production levels. In this example, the product with the smallest profit rate (P_i/a_i) is product 2 at all probability levels α. The CPU requirements associated with this problem are between 0.10 and 0.20 s per point. For comparison, the same problem is solved using discretization of the uncertain parameters and Gaussian quadrature integration of the expected objective value using 5, 10, 15, and 24 quadrature points per uncertain demand, respectively. The obtained results, CPU requirements, and number of variables and constraints are listed in Table 4. These results indicate that while for only a few quadrature points the solution times are relatively small, the obtained accuracy is questionable. A larger number of quadrature points improve accuracy at the expense of a significant increase in the CPU requirements even when only two uncertain product demands are present.

Next, the relation between the probability of meeting all product demands α and the penalty parameter γ is investigated. The nonconvex formulation, without fixing the K variable, is solved using DICOPT for a range of γ values between 0 and 6. The corresponding probabilities α of meeting all product demands are then calculated using the relationship $\alpha = 1 - \Phi(K)$. Examination of the results validates the theoretical developments by revealing a one-to-one correspondence between the optimal solutions obtained using the γ penalty parameter and the optimal solutions obtained after fixing α at the calculated value. The pairs of γ and α for which the batch plant optimal designs match are plotted in Figure 5. This plot establishes a way of relating the value of the penalty parameter, whose *a priori* selection is difficult, to the well defined parameter α.

Medium-Scale Example

This example involves the design of a batch plant producing five different products (Biegler et al., 1997; Harding and Floudas, 1997). Each product recipe requires six production stages with up to five identical units per stage. The unit capacities are allowed to vary between 500 and 3,000 L. The time horizon is 6,000 h per year, and the annualized investment cost coefficient is 0.3. The data for processing times, size factors, and profit margins are given in Tables 5, 6, and 7, respectively. The mean annual demands for the five products are 250, 150, 180, 160 and 120 ton, respectively. The uncertainty in the demands is quantified by selecting standard deviations which are 20% of the mean product demand values. The description of this problem as an MINLP requires five binary variables identifying i^*, 30 binary variables modeling the number of units per stage (six stages $\times$ up to five units), 529 continuous variables, and 191 constraints. The problem is iteratively solved for fixed values of K corresponding to probabilities α between 0.1 and 0.999 of meeting all product demands. The expected DCFR values are plotted as a function of the probability levels in Figure 6. This plot

Table 3. Optimal Expected DCFR and Corresponding Equipment Volumes (L) and Batch Sizes (kg) at Different Probability Levels α

α	E [DCFR]$\times 10^{-3}$	V_1	V_2	V_3	B_1	B_2
0.579	1,260.93	1,818.87	2,728.30	3,637.74	909.43	454.72
0.655	1,264.05	1,837.74	2,756.60	3,675.47	918.87	459.43
0.726	1,265.97	1,856.60	2,784.91	3,713.21	928.30	464.15
0.788	1,266.81	1,875.47	2,813.21	3,750.94	937.74	468.87
0.809	1,266.87	1,882.46	2,823.69	3,764.92	941.23	470.62
0.841	1,266.70	1,894.34	2,841.51	3,788.68	947.17	473.58
0.885	1,265.80	1,913.21	2,869.81	3,826.42	956.60	478.30
0.919	1,264.28	1,932.08	2,898.11	3,864.15	966.04	483.02
0.945	1,262.27	1,950.94	2,926.42	3,901.89	975.47	487.74
0.964	1,259.91	1,969.81	2,954.72	3,939.62	984.91	492.45
0.977	1,257.30	1,988.68	2,983.02	3,977.36	994.34	497.17

Table 4. Solution of Illustrative Example Based on Gaussian Quadrature

Q Points	E [DCFR]$\times 10^{-3}$	V_1	V_2	V_3	CPU (s)	Constr.	Var.
5	1,489.71	1,800	2,700	3,600	0.27	94	228
10	1,267.17	1,877	2,816	3,754	1.26	319	828
15	1,266.63	1,879	2,818	3,758	2.91	456	1,828
24	1,266.66	1,884	2,825	3,767	9.61	1747	4,636

reveals the presence of an optimum probability level for which the expected DCFR value is maximized. Levels of α below or above 0.69 result in smaller expected DCFR values due to loss of sale profits or excessive investment cost, respectively. The tradeoff curve is relatively flat around the optimal solution indicating the insensitivity of the optimal expected DCFR to small changes in the design variables. The obtained tradeoff curve exhibits a number of important features which are the manifestation of changes in the optimal batch plant design at different levels of α. Discontinuities indicate the transition points of the optimal batch plant configuration described by N_j, $j=1,\ldots,M$. These transitions involve either the addition of a new parallel unit or the reallocation of a processing unit to a different stage. Discontinuities in the slope of the tradeoff curve typically imply the emergence of a new product i^* with the smallest profit rate due to changes in the design. Table 8 summarizes the optimal batch plant designs at different probabilities α. Entries shown in bold indicate changes in the plant configuration. For example at $\alpha=0.183$ i^* switches from product four to product one, at $\alpha=0.46$ a third unit is added in the third stage, and at $\alpha=0.69$ the expected DCFR is maximized. The most drastic drop in the tradeoff curve occurs at $\alpha=0.802$, where a second unit is added to the fifth production stage. The computational requirements consistently decrease as α increases. This trend is due to the decrease in the relative magnitude of the "uncertainty-induced" penalty term in the objective function.

Summarizing, this medium-scale example demonstrated how complex are the relations between maximum expected profit, plant configuration, and probability of meeting product demands. These relations are shown with the tradeoff curve. Construction of the tradeoff curve is possible only because of significant computational savings stemming from the derived MINLP respresentation. For comparison, the formulation of this model based on Gaussian quadrature using only five quadrature points results in 15,636 variables, 3,155 constraints (containing 15,625 nonconvex terms), and requires more than 1,000 s to obtain a single point on the tradeoff curve.

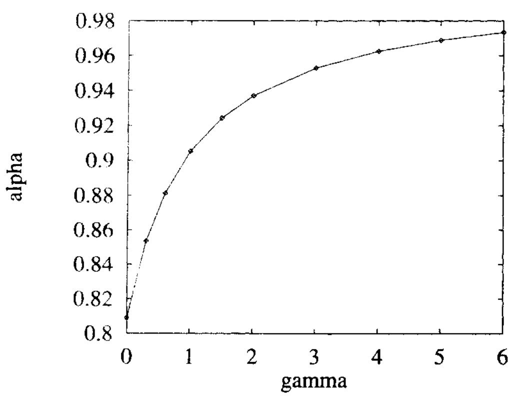

Figure 5. Matching curve between γ and α values.

Table 5. Size Factors S_{ij} (L/kg) for the Medium-Scale Example

Product	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5	Stage 6
1	7.9	2.0	5.2	4.9	6.1	4.2
2	0.7	0.8	0.9	3.4	2.1	2.5
3	0.7	2.6	1.6	3.6	3.2	2.9
4	4.7	2.3	1.6	2.7	1.2	2.5
5	1.2	3.6	2.4	4.5	1.6	2.1

Table 6. Processing Times t_{ij} (h) for the Medium-Scale Example

Product	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5	Stage 6
1	6.4	4.7	8.3	3.9	2.1	1.2
2	6.8	6.4	6.5	4.4	2.3	3.2
3	1.0	6.3	5.4	11.9	5.7	6.2
4	3.2	3.0	3.5	3.3	2.8	3.4
5	2.1	2.5	4.2	3.6	3.7	2.2

Table 7. Equipment Cost and Profit Margin Data for the Medium-Scale Example

Investment Cost Coeff.			Price Data	
Stage	α_i (\$/L)	β_i	Product	P_i (\$/kg)
1	3,000	0.6	1	3.5
2	3,000	0.6	2	4.0
3	3,000	0.6	3	3.0
4	3,000	0.6	4	2.0
5	3,000	0.6	5	4.5
6	3,000	0.6		

Large-Scale Example

To investigate the computational performance of the proposed MINLP problem representation for large-scale problems, an example is constructed involving the design of a batch plant producing thirty products. Each product recipe requires

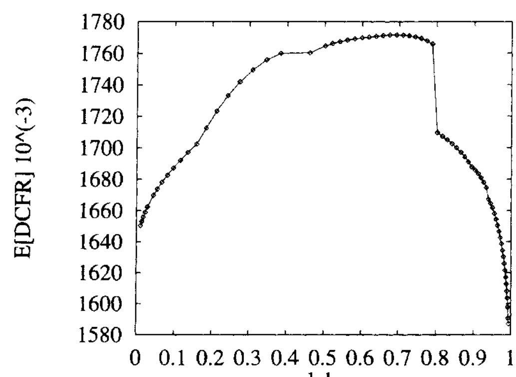

Figure 6. Optimal expected DCFR vs. α for the medium-scale example.

Table 8. Optimal Expected DCFR and Corresponding Number of Processing Units at Different Values of α for the Medium-Scale Example

α	E [DCFR]$\times 10^{-3}$	No. of Units per Stage						i^*	CPU (s)
0.104	1,687.26	2	2	2	2	1	1	4	97.3
0.136	1,697.22	2	2	2	2	1	1	4	59.8
0.159	1,702.43	2	2	2	2	1	1	4	72.4
0.183	1,712.53	2	2	2	2	1	1	1	70.7
0.212	1,723.44	2	2	2	2	1	1	1	58.4
0.382	1,759.94	2	2	2	2	1	1	1	15.4
0.462	1,760.32	2	2	**3**	2	1	1	3	18.1
0.500	1,764.68	2	2	3	2	1	1	3	9.3
0.579	1,769.24	2	2	3	2	1	1	3	22.8
0.655	1,771.24	2	2	3	2	1	1	4	9.1
0.691	1,771.64	2	2	3	2	1	1	4	8.3
0.726	1,771.06	2	2	3	2	1	1	4	8.4
0.802	1,709.67	2	2	3	2	**2**	1	4	10.6
0.816	1,707.37	2	2	3	2	2	1	3	16.2
0.829	1,705.07	2	2	3	2	2	1	4	15.7
0.841	1,702.63	2	2	3	2	2	1	4	12.4
0.894	1,687.94	**3**	2	3	2	**1**	1	4	12.4
0.911	1,683.55	3	2	3	2	1	1	4	10.9
0.939	1,667.39	**2**	2	3	2	**2**	**2**	3	7.7
0.950	1,661.82	2	2	3	2	2	2	3	4.5
0.991	1,603.62	2	2	3	2	2	2	1	6.6
0.992	1,597.88	2	2	3	**3**	2	2	1	7.0

ten production steps (stages), and a maximum of five identical units are allowed per stage. The horizon time is again 6,000 h and the annualized investment cost coefficient is equal to 0.3. The expected values of the product demands range between 10 and 60 ton per year, and their uncertainty is represented by standard deviations equal to 10% of their mean values. The processing unit volumes are allowed to vary between 2,000 and 5,000 L. The size-factors are selected to be between 1 and 4 L per kilogram of product and the processing times per stage assume values between 1 and 9 h. The detailed processing and cost data are given in Tables 9, 10, 11 and 12. This problem gives rise to an MINLP formulation involving 80 binary variables, 8,041 continuous variables, and 1,763 constraints.

Table 9. Size Factors S_{ij} (L/kg) for the Large-Scale Example

	Stages									
Product	1	2	3	4	5	6	7	8	9	10
1	1	2	2	3	2	1	2	3	2	1
2	3	3	2	3	4	2	2	3	2	1
3	1	1	2	1	1	2	2	1	1	2
4	2	2	1	2	1	3	2	3	2	1
5	4	4	4	3	4	3	2	1	1	2
6	1	2	2	3	2	1	2	1	1	2
7	3	3	2	3	4	2	4	3	4	3
8	1	1	2	1	1	2	2	3	2	1
9	2	2	1	2	1	3	2	1	1	2
10	4	4	4	3	4	3	4	3	4	3
11	1	2	2	3	2	1	2	3	2	1
12	3	3	2	3	4	2	2	3	2	1
13	1	1	2	1	1	2	2	1	1	2
14	2	2	1	2	1	3	2	1	1	2
15	4	4	4	3	4	3	2	3	2	1
16	1	2	2	3	2	1	2	3	2	1
17	3	3	2	3	4	2	2	3	4	2
18	1	1	2	1	1	2	1	2	1	3
19	2	2	1	2	1	3	1	2	1	3
20	4	4	4	3	4	3	1	2	1	3
21	1	2	2	3	2	1	2	1	1	2
22	3	3	2	3	4	2	2	1	1	2
23	1	1	2	1	1	2	2	3	4	2
24	2	2	1	2	1	3	2	1	1	2
25	4	4	4	3	4	3	2	1	1	2
26	1	2	2	3	2	1	2	1	1	2
27	3	3	2	3	4	2	2	1	1	2
28	1	1	2	1	1	2	2	3	4	2
29	2	2	1	2	1	3	2	1	1	2
30	4	4	4	3	4	3	2	1	1	2

Table 10. Production Times t_{ij} (h) for the Large-Scale Example

	Stages									
Product	1	2	3	4	5	6	7	8	9	10
1	5	6	3	3	5	7	7	6	6	5
2	5	6	6	5	6	7	5	5	4	3
3	3	3	3	3	2	1	5	1	3	2
4	3	2	2	2	1	5	5	3	2	2
5	2	3	4	3	4	7	8	6	9	1
6	5	6	3	3	5	7	7	6	6	5
7	5	6	6	5	6	7	5	5	4	3
8	3	3	3	3	2	1	5	1	3	2
9	3	2	2	2	1	5	5	3	2	2
10	2	3	4	3	4	7	8	6	9	1
11	5	6	3	3	5	7	7	6	6	5
12	5	6	6	5	6	7	5	5	4	3
13	3	3	3	3	2	1	5	1	3	2
14	3	2	2	2	1	5	5	3	2	2
15	2	3	4	3	4	7	8	6	9	1
16	5	6	3	3	5	7	7	6	6	5
17	5	6	6	5	6	7	5	5	4	3
18	3	3	3	3	2	1	5	1	3	2
19	3	2	2	2	1	5	5	3	2	2
20	2	3	4	3	4	7	8	6	9	1
21	4	6	3	3	5	7	7	6	6	5
22	5	6	6	5	6	7	5	5	4	3
23	3	3	3	3	2	1	5	1	3	2
24	3	2	2	2	1	5	5	3	2	2
25	2	3	4	3	4	7	8	6	9	1
26	5	6	3	3	5	7	7	6	6	5
27	5	6	6	5	6	7	5	5	4	3
28	3	3	3	3	2	1	5	1	3	2
29	3	2	2	2	1	5	5	3	2	2
30	2	3	4	3	4	7	8	6	9	1

Table 11. Profit Margins and Expected Demands for the Large-Scale Example

Product	1	2	3	4	5	6	7	8	9	10
P_i, ($/kg)	5	1	2	1	10	5	5	8	2	2
$\hat{\theta}_i$, (ton)	40	80	160	80	120	160	240	160	120	80
Product	11	12	13	14	15	16	17	18	19	20
P_i, ($/kg)	5	10	4	8	4	1	5	5	3	2
$\hat{\theta}_i$, (ton)	40	120	120	120	80	120	80	120	240	240
Product	21	22	23	24	25	26	27	28	29	30
P_i, ($/kg)	5	1	2	1	10	5	5	8	2	2
$\hat{\theta}_i$, (ton)	240	80	40	40	240	120	40	80	80	40

Table 12. Equipment Cost Coefficients for the Large-Scale Example

Stage	1	2	3	4	5	6	7	8	9	10
α_j (\$/L)	1,000	2,000	3,000	2,000	2,000	1,000	1,000	500	400	300
β_j	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6	0.6

The problem is solved for fixed negative K values corresponding to probability levels of α between 0.5 and 0.95. The values of the expected DCFR are plotted against the probability of meeting the demands (see Figure 7). For this example, no batch plant configuration changes are observed and the least profitable product is product 1 throughout the entire probability range. All optimal designs involve two units for stages one through five and ten, three units for stages six and eight, and four units for stages seven and nine. The expected DCFR is maximized for α of approximately equal to 0.6. Table 13 summarizes the required number of iterations of the OA algorithm, the total CPU time required, and the CPU time used for solving the master MILP problems. Note that most of the CPU time is spent on the MILP master problem due to the high number of binary variables present in the formulation. One of the ways to reduce the expense of the MILP master problem is to use the LP/NLP based branch and bound method proposed by Quesada and Grossmann (1992). Nevertheless, the CPU requirements per point do not exceed a few thousand seconds indicating that even larger problems can be addressed.

Summary and Conclusions

A new approach for solving the design problem of multiproduct batch plants under SPC production mode involving normally distributed uncertain product demands was presented. By sacrificing some generality in terms of allowable production modes and probability distributions for the uncertain demands, the original two-stage stochastic program was transformed into an equivalent deterministic MINLP problem. This problem was shown to be convex for product demand satisifaction levels higher than 50%. The loss of profit due to inability to satisfy product demand was modeled with either the addition of a penalty of underproduction term or the explicit specification of the simultaneous product demand satisfaction probability. In particular, one-to-one correspondence between these two alternative formulations was revealed which obviates the need to solve both of them.

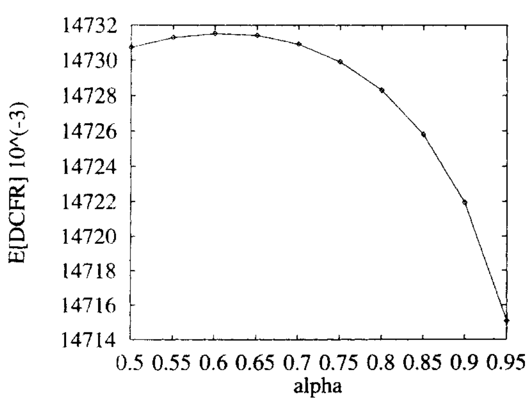

Figure 7. Optimal expected DCFR vs. α for the large-scale example.

Three example problems involving up to thirty uncertain product demands, ten production stages, and five identical units at each stage were included to highlight the proposed solution method and the results obtained for different problem sizes. The results revealed a surprising complexity in the shape and form of the constructed tradeoff curves between the probability of meeting all product demands and profit. These curves provided a systematic way for contrasting maximum profitability over demand satisfaction. In all examined cases, a single maximum was observed on the tradeoff curve implying the existence of a unique level of product demand satisfaction for maximum profit. The presence of discontinuities manifested ubiquitous transitions in the optimum batch plant configuration for different probability levels through the addition of new units or reallocation of existing ones. Slope discontinuities were indicative of the emergence of a new least profitable product. The proposed analytical solution of the inner problem and subsequent integration resulted in savings in the computational requirements of about two-orders of magnitude over existing methods (that is, Quadrature integration).

However, this computational advantage comes at the expense of restricted applicability to only the SPC production mode so far. Extensions to the multiproduct campaign (MPC) or multipurpose batch plants are complicated by the fact that more than one horizon constraint (one for each stage) must be present in the inner problem. Therefore, the solution of the inner problem and its subsequent integration over all feasible product demand realizations for an MPC batch plant are much more complicated to perform analytically. The feasibility of successively approximating MPC batch plants with SPC ones is currently under investigation. Nevertheless, results with the SPC production mode assumption provide valid lower bounds on the profit of MPC batch plants. In addition, the proposed model formulation and solution procedure are currently being extended to account for capacity expansions in a multiperiod framework so that plant capacity is optimally allocated not only between production stages but also over time.

Table 13. Optimal Expected DCFR and Computational Requirements for the Large-Scale Example

α	E [DCFR]$\times 10^{-3}$	OA Iter.	CPU_{Total}	CPU_{MIP}
0.50	14,730.74	8	4,306.46	4,268.41
0.55	14,731.30	7	3,078.06	3,034.85
0.60	14,731.53	5	1,289.88	1,253.70
0.65	14,731.43	5	1,354.27	1,326.81
0.70	14,730.93	5	1,227.76	1,197.43
0.75	14,729.92	5	951.66	920.84
0.80	14,728.30	5	1,103.84	1,069.19
0.85	14,725.81	5	983.51	955.11
0.90	14,721.93	4	655.17	628.93
0.95	14,715.08	4	510.42	477.29

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Notation

b_i = exponentially transformed batch size for product i
B_i = batch size for product i
Cov = covariance operator
$f_{\text{inner}}^{\text{opt}}$ = optimum value of inner problem
$f_{\text{inner},\gamma}^{\text{opt}}$ = optimum value of inner problem including the penalty of underproduction term
j = stage: $j = 1, \ldots, M$
N_j = number of parallel units at stage j
N_j^L, N_j^U = lower and upper bounds on the allowable number of parallel equipment units at stage j
r = number of units
$r_{ii'}$ = ratio of the profit rates a_i, $a_{i'}$ of products i, i'
sign (K) = sign of K
t_{L_i} = exponentially transformed cycle time of product i
T_{Li} = cycle time of product i
v_j = exponentially transformed equipment size at stage j
V_j = equipment size at stage j
Var = variance operator
V_j^L, V_j^U = lower and upper bounds on capacity size of equipment at stage j
w_i = ratio of σ_{ct} over a_i
x = standardized normal variable N[0,1]
x_i = binary variable identifying the least profitable product i^*
y_{jr} = binary variable which is equal to one if there are r units at stage j
z_i = product of w_i times the binary x_i
α_j = preexponential coefficient for the investment cost of process equipment at stage j
β_j = exponent for the investment cost of process equipment at stage j
λ_{ai} = Lagrange multiplier of a_i defining constraint
λ_{K_o} = Lagrange multiplier of $K \leq K_o$ constraint
λ_{z_i} = Lagrange multiplier of z_i defining constraint
$\lambda_{\sigma_{ct}}$ = Lagrange multiplier of cycle-time defining constraint
$\hat{\theta}_i$ = mean of the demand for product i
Φ = standarized normal cumulative probability function

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Appendix: Proof of Equivalence for α and γ Formulations

To reveal the equivalence of the two problems, the different parts of the necessary optimality conditions between the two problems are isolated. The necessary optimality condi-

$$\alpha-\text{formulation} \qquad\qquad \gamma-\text{formulation}$$

$$-P_{i^*}z_{i^*}\Phi(K)+\lambda_K\sigma_{ct}-\lambda_{K0}=0 \qquad -(1+\gamma)P_{i^*}z_{i^*}\Phi(K)+\lambda'_K\sigma_{ct}=0$$

$$-P_{i^*}[K\phi(K)+f(K)]+\lambda_{z_i^*}=0 \qquad -(1+\gamma)P_{i^*}[K\Phi(K)+f(K)]+\lambda'_{z_i^*}=0$$

tions for the two problems are identical apart from those with respect to K and z_{i^*}. The differing elements of the two formulations and the corresponding multipliers contributing to the optimality conditions are

α – Formulation

$$\max \quad \ldots - P_{i^*}z_{i^*}[K\Phi(K)+f(K)] - \ldots$$

$$\text{subject to} \quad w_i-(1-x_i)w_i^U \le z_i,\ i=1,\ \ldots,\ N \leftarrow \lambda_{z_i}$$

$$K\sigma_{ct} \ge \sum_{i=1}^{N} a_i\hat{\theta}_i - H \leftarrow \lambda_K$$

$$K \le K_0 \leftarrow \lambda_{K_o}$$

γ-Formulation

$$\max \quad \ldots -(1+\gamma)P_{i^*}z_{i^*}[K\Phi(K)+f(K)] - \ldots$$

$$\text{subject to} \quad w_i-(1-x_i)w_i^U \le z_i,\ i=1,\ \ldots,\ N \leftarrow \lambda'_{z_i}$$

$$K\sigma_{ct} \ge \sum_{i=1}^{N} a_i\hat{\theta}_i - H \leftarrow \lambda'_K$$

Note that when $\gamma=0$ and K is not constrained by K_o, both formulations yield the same optimal solution. It will be shown that for any positive γ there always exists K_o such that both formulations have the same optimal solution. In the above excerpts of the formulations, the investment cost and the constraints which are not directly related to γ or K_o are omitted for clarity. Also, only the active constraint i^* from the sets of constraints defining z_i is included.

The necessary optimality conditions with respect to K and z_{i^*} are

The above optimality conditions yield the following two seemingly different expressions for γ as a function of the multipliers of the two problems

$$1+\gamma=\frac{\lambda'_K\sigma_{ct}}{\lambda_K\sigma_{ct}-\lambda_{K_o}}$$

$$1+\gamma=\frac{\lambda'_{z_i^*}}{\lambda_{z_i^*}}$$

However, after dividing by parts the above defined necessary optimality conditions yield

$$\frac{\lambda'_K\sigma_{ct}}{\lambda'_{z_i^*}}=\frac{\lambda_K\sigma_{ct}-\lambda_{K_o}}{\lambda^*_{z_i}}=\frac{z_{i^*}\Phi(K)}{[K\Phi(k)+f(K)]}$$

This means that,

$$\frac{\lambda'_K\sigma_{ct}}{\lambda_K\sigma_{ct}-\lambda_{K_o}}=\frac{\lambda'_{z_i^*}}{\lambda_{z_i^*}}$$

Therefore, a unique value for the penalty coefficient γ exists and is consistent with the necessary optimality conditions proving the equivalence of the two formulations.

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