I&EC research
Industrial & Engineering Chemistry Research

Article

Multiperiod Planning and Scheduling of Multiproduct Batch Plants under Demand Uncertainty

Spas B. Petkov, and Costas D. Maranas

Ind. Eng. Chem. Res., **1997**, 36 (11), 4864-4881• DOI: 10.1021/ie970259z • Publication Date (Web): 03 November 1997

Multiperiod Planning and Scheduling of Multiproduct Batch Plants under Demand Uncertainty

Spas B. Petkov and Costas D. Maranas*

Department of Chemical Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802

In this paper the multiperiod planning and scheduling of multiproduct plants under demand uncertainty is addressed. The proposed stochastic model, allowing for uncertain product demand correlations, is an extension of the deterministic model introduced by Birewar and Grossmann (*Ind. Eng. Chem. Res.* **1990**, *29*, 570). The stochastic model involves the maximization of the expected profit subject to the satisfaction of single or multiple product demands with prespecified probability levels (chance-constraints). The stochastic elements of the model are expressed with equivalent deterministic forms, eliminating the need for discretization or sampling techniques. This implies that problems with a large number of possibly correlated uncertain product demands can be efficiently handled. The resulting equivalent deterministic optimization models are MINLP's with convex continuous parts. An example problem involving 20 correlated uncertain product demands is addressed. A sequence of different models is considered which highlight different modeling features and their effect on computational performance and obtained results.

1. Introduction

In recent years there has been an increased interest in the design, planning, and scheduling of batch chemical plants. This has been catalyzed by the emergence of industrial interest in fine and specialty chemicals, as well as by changes in producer customer relations. These relations are now characterized by an increased demand for customized specifications, which favor batch processing as a production mode. In a competitive and changing environment the need to plan new output levels and production mixes is likely to arise much more frequently than the need to design new batch plants (Rippin, 1993). Given the unwillingness of large chemical companies to commit to large investments in new plants, the more efficient planning and operation of existing facilities becomes paramount. Therefore, increased emphasis is currently placed on simultaneously improving conflicting objectives such as manufacturing flexibility, customer responsiveness, lower operating costs, and reduced investments in inventory (McDonald and Karimi, 1996). In the presence of significant demand fluctuations, efficient use of the available equipment and a flexible inventory system targeted at customer satisfaction over a multiperiod horizon can be ensured through simultaneous planning and scheduling. An overview of scheduling and planning in batch plants can be found in the literature (Reklaitis, 1992; Rippin, 1993; Pantelides, 1994).

Deterministic models for process planning and scheduling assume that product demands are known with certainty. However, in medium- and long-term planning, product demands fluctuate. Failure to properly account for product demand fluctuations may lead to either unsatisfied customer demands and loss of market share or excessive inventory costs. A number of approaches have been proposed in the chemical engineering literature for the quantitative treatment of uncertainty in the design, planning, and scheduling of batch process plants with an emphasis on the design. These approaches have contributed to a better understanding of how uncertainty affects their performance. A classification of different areas of uncertainty is suggested by Subrahmanyam *et al.* (1994) including uncertainty in prices and demand, equipment reliability, and manufacturing uncertainty.

The most popular one so far has been the scenario-based approach which attempts to forecast and account for all possible future outcomes through the use of scenarios. The scenario approach was pioneered by Reinhart and Rippin (1986, 1987) and later adopted by Shah and Pantelides (1992) and Subrahmanyam *et al.* (1994) for batch plant design under uncertainty. Scenario-based approaches provide a straightforward way to implicitly account for uncertainty (see also the discussion in Liu and Sahinidis, 1996). Their main drawback is that they typically rely on either the *a priori* forecasting of all possible outcomes or the discretization of a continuous multivariate probability distribution resulting in an exponential number of scenarios. For example, the discretization of only 10 uncertain variables with 5 discretization points yields $5^{10} \approx 10^6$ scenarios.

A key concept in quantitatively measuring the effect of uncertainty is the stochastic flexibility index pioneered by Straub and Grossman (1990) and Pistikopoulos and Mazzuchi (1990) which measures the probability of feasible operation of a process design under stochastic uncertainty (see also Pistikopoulos, 1995). Evaluation of the stochastic flexibility index is a very computationally demanding task because it requires the integration of multivariate continuous probability functions (Rippin, 1993). Gaussian quadrature is a popular method in the chemical engineering literature for approximating multivariate probability integrals. The advantage of Gaussian quadrature integration is that it is largely unaffected by the type of employed continuous probability distribution and the location of discretization (quadrature) points is selected through the optimization process. The shortcoming of quadrature integration is that a large number of extra variables accounting for the quadrature points must typically be introduced to the optimization model. In general, this limits the applicability to problems with only a few uncertain parameters. By utilizing Gaussian quadrature, Straub

* Author to whom all correspondence should be addressed. E-mail: cdm8@psu.edu. Phone: 814-863-9958. Fax: 814-865-7846.

S0888-5885(97)00259-5 CCC: $14.00

and Grossman (1992), Ierapetritou and Pistikopoulos (1994, 1996), and Harding and Floudas (1997) addressed the design of different types of batch plants under various types of uncertainty.

An alternative to Gaussian quadrature integration for the approximation of multivariate probability integrals is the use of Monte Carlo sampling. The basic idea of Monte Carlo methods is to generate a large enough number of random variates distributed according to the evaluated multivariate probability function and approximate the multivariate probability integral as the ratio of the number of points within the integration region divided by the total number of points (Tong, 1990). More sophisticated Monte Carlo adaptations have been proposed by Deak (1988), Diwekar and Kalagnanam (1996), and Liu and Sahinidis (1996). The main advantage of Monte Carlo sampling methods is that for a given precision target the number of required function evaluations does not scale exponentially with the total number of correlated uncertain parameters. The application of Monte Carlo methods to optimization has been limited so far because not only the value of the probability integral but also its derivatives must be evaluated using simulation at each step of the optimization algorithm (Watanabe and Ellis, 1994).

So far the solution methods for stochastic models of batch process planning and scheduling have been much more computationally intensive than those for deterministic models. This is due to the fact that they rely on explicit (scenario-based approaches) or implicit (Gaussian quadrature) discretizations. Additionally, Monte Carlo sampling based approaches require multiple function evaluations to estimate the objective function, constraints, and their gradients at every iteration of the optimization algorithm. It is the objective of this paper to introduce a methodology for the direct deterministic equivalent representation of a stochastic model for planning and scheduling, circumventing any need for explicit/implicit discretization or sampling. The deterministic planning and scheduling model of multiproduct batch plants proposed by Birewar and Grossmann (1990) serves as the starting point for the development and solution procedure of the stochastic model presented herein. In this model, the planning and scheduling problems are embedded in a single optimization problem. The formulation accounts for inventory costs and enables inventory transfer to satisfy future demands. The planning and scheduling phases are connected through the cycle-time. The scheduling check during the planning phase ensures that the planned production levels can be met within the available cycle-time. Updated schedules can be later employed after the product demands are known. The following scheduling policy checks are considered: zero-wait (ZW) and unlimited intermediate storage (UIS) for single-product campaign (SPC) or multiple-product campaign (MPC) plants. Feasibility of the planning policy after invoking the most restrictive ZW scheduling policy check implies that any other scheduling policy will also be feasible. On the other hand, infeasibility with the least restrictive UIS schedule means that any other scheduling policy will yield an infeasible schedule.

The paper is organized as follows: The specifics of the problem are discussed in section 2. The proposed stochastic formulation based on the deterministic model of Birewar and Grossman (1990) is briefly summarized in section 3. In section 4, the conceptual stochastic formulation of the planning and scheduling problem under demand uncertainty is introduced. This formulation involves the maximization of the expected profit subject to product demand satisfaction for a single product or multiple products with a given probability level. The deterministic equivalent representation of the objective function and the demand satisfaction constraints are addressed in sections 5−7. Section 8 deals with the problem of revising and updating the scheduling and planning policy upon the realization of the random product demands. The solution procedure for the resulting convex MINLP problem is discussed in section 9, and a test problem involving 20 correlated random product demands is solved in section 10, highlighting various modeling and algorithmic issues. Section 11 summarizes the work and provides some concluding remarks.

2. Problem Definition

Given is a multiproduct batch plant with defined production lines, equipment sizes, and a set of products with given recipes. The demands for different products are uncertain and possibly correlated, reflecting changing market conditions and periodic variation in customer orders. The problem to be addressed is as follows:

Obtain an optimal planning policy and a corresponding feasible schedule such that the expected profit is maximized while single- and/or multiple-product demands are satisfied with at least a prespecified probability level.

The proposed stochastic model involves the following features and assumptions:

1. The product demands are modeled as multivariate normally distributed random variables. The normality assumption has been widely invoked in the literature because it captures the essential features of demand uncertainty and it is convenient to use. The use of more “complex” probability distributions is hindered by the fact that statistical information apart from mean and covariance estimates of product demands is rarely available. A theoretical justification of the normality assumption can be argued on the basis of the central limit theorem considering that product demands are typically affected by a large number of stochastic events.

2. Product demand correlation is included in the problem formulation. This enables handling correlation of demands for different products in the same time period and demand correlation for the same product in different time periods. For example, if two products are predominantly used as raw materials in another process, then their demands are going to be positively correlated in each time period. Alternatively, unusually high demand for a product in one time period more often than not is followed by lower than normal demand in the next period, implying negative correlation. Taking into account such information, whenever it is available, enables a more efficient allocation of production capacity to maximize profit and meet certain marketing objectives.

3. The following choices for scheduling policies are considered: SPC or MPC with ZW or UIS. This is accomplished by including a horizon constraint (scheduling check) which guarantees that the production goals can be achieved with the corresponding scheduling policy.

4. The unit production cost is assumed independent of capacity output (linearity assumption). More complex production cost policies can be readily incorporated in the model at the expense of introducing nonlinearities (see Birewar and Grossmann, 1990).

5. Transfer of inventory from the present to future time period is allowed and planned for. The inventory cost is assumed to be proportional to the arithmetic mean of the initial and final inventories for each product in every time period.

6. The penalty for production shortfalls is proportional to the amount of underproduction. The employed proportionality constant varies between zero and values higher than 100% of the profit margin (unit prices minus unit production cost).

3. Deterministic Model

The multiperiod planning/scheduling model for multiproduct batch plants, as introduced by Birewar and Grossmann (1990), serves as the starting point for the proposed stochastic framework. The following notation is used:

Sets:

$i = 1, ..., N$ products

$j = 1, ..., M$ stages

$l = 1, ..., L$ production lines

$t = 1, ..., T$ time periods

I_l = set of products i which are produced on line l

L_i = set of lines l which can produce product i

Parameters:

H_t = length of period t

QD_{it} = demand for product i in period t

P_{it} = market price of product i in time period t

C_{it} = cost of producing a unit of product i in time period t

γ_{it} = storage cost of product i in time period t

δ_{it} = penalty for production shortfalls

V_{jl} = volume of unit in stage j and production line l

S_{ijl} = size factor of product i at stage j on line l

t_{ijl} = processing time of product i at stage j on line l

SL_{ikj} = slack times for MPC with ZW scheduling policy

Variables:

QT_{it} = total quantity of product i produced in period t

QS_{it} = amount of product i planned for sale in period t

Q_{itl} = quantity of product i produced in period t on line l

IB_{it} = inventory of product i at the beginning of period t

IE_{it} = inventory of product i at the end of period t

n_{itl} = number of batches of product i produced in period t on line l

$NPRS_{iktl}$ = number of batches of product i followed by product k on line l and period t

The multiperiod planning and scheduling problem formulation (MPS) is as follows (see Birewar and Grossmann (1990) for details):

$$\max \sum_{i=1}^{N}\sum_{t=1}^{T}\left(QS_{it}P_{it} - QT_{it}C_{it} - \gamma_{it}\frac{IB_{it} + IE_{it}}{2} - \delta_{it}(P_{it} - C_{it})\max(0, QD_{it} - QS_{it})\right) \quad \text{(MPS)}$$

subject to

$$Q_{itl}S_{ijl} \le V_{jl}n_{itl}, \quad i \in I_l, \quad j = 1, ..., M, \quad l \in L_i, \quad t = 1, ..., T$$

$$\sum_{l \in L_i} Q_{itl} = QT_{it}, \quad i = 1, ..., N, \quad t = 1, ..., T$$

$$QS_{it} \le QD_{it}, \quad i = 1, ..., N, \quad t = 1, ..., T$$

$$IE_{it} = IB_{it} + QT_{it}, \quad i = 1, ..., N, \quad t = 1, ..., T$$

$$IB_{it+1} = IE_{it} - QS_{it}, \quad i = 1, ..., N, \quad t = 1, ..., T$$

$$g_{tl}(n_{itl}) \le 0, \quad t = 1, ..., T, \quad l \in L_i$$

$$Q_{itl}, QS_{it}, QT_{it}, IE_{it}, IB_{it} \ge 0$$

$$n_{itl} \in \{0, 1, 2, ...\}$$

where $g_{tl}(n_{itl}) \le 0$ represents the horizon constraints whose form depends on the type of scheduling policy:

1. SPC with ZW.

$$\sum_{i \in I_l} n_{itl}T_{L_{il}} \le H_t \text{ where } T_{L_{il}} = \max_j t_{ijl}$$

2. MPC with ZW.

$$\sum_{i \in I_l} n_{itl}t_{ijl} + \sum_{i \in I_l}\sum_{k \in I_l} NPRS_{iktl}SL_{ikj} \le H_t$$

$$\sum_{k \in I_l} NPRS_{iktl} = n_{itl}$$

$$\sum_{i \in I_l} NPRS_{iktl} = n_{ktl}$$

Above, the values of the slack times, SL_{ikj}, are parameters determined by the procedure outlined in Appendix B of Birewar and Grossmann (1990).

3. MPC with UIS. This case involves the same constraints as MPC with ZW, but the slack times are all set equal to zero.

The introduced scheduling constraints guarantee that the process cycle-time, necessary to achieve the production goals based on the chosen scheduling policy, does not exceed the available time horizon. Note that in the SPC production mode the exact ordering of the different product campaigns does not affect the cycle-time. In the case of the MPC production mode, a valid schedule can be recovered after applying the graph enumeration procedure of Birewar and Grossmann (1989) for the values of the $NPRS_{iktl}$ variables found above. However, the resulting feasible schedule does not always involve the minimum process makespan. To obtain the most efficient schedule for the set production goals, once the number of batches n_{itl} are determined, the makespan

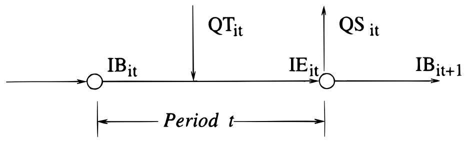

Figure 1. Inventory balance for the deterministic model.

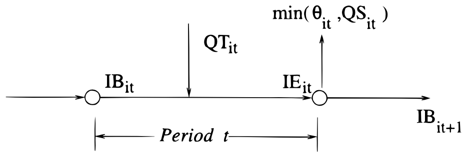

Figure 2. Inventory balance for the stochastic model.

minimization problem (Birewar and Grossmann, 1990) must be considered. This will be discussed further in section 9.

The objective function of MPS accounts for revenues, production costs, inventory costs, and production shortfall penalties. The first two constraints relate the production requirements with the available equipment. The third constraint restricts the sales to the available demands. The next two inventory constraints relate the inventory at the beginning and end of a time period with the production rate and sales. This inventory transfer allows the utilization of unused plant capacity to manufacture a product at an earlier period, anticipating an elevated future demand at a later period. A graphical representation of the inventory balance is given in Figure 1.

4. Stochastic Formulation

The probabilistic description of demand uncertainty renders the planning and scheduling model stochastic. The proposed stochastic model attempts to (i) maximize the expected profit; (ii) avoid overproduction which leads to unnecessarily high production and inventory costs; (iii) safeguard against underproduction which results in missed sales; and (iv) uphold a targeted market share.

While in the deterministic model the planned sales QS_{it} are always realized, this is not always true in the stochastic case. If a particular product demand realization θ_{it} is higher than QS_{it}, then the entire quantity QS_{it} planned for sale can be sold. However, if θ_{it} is less than QS_{it}, then only up to θ_{it} of product i can be sold in period t. This implies that the amount of product i sold in period t is the minimum between θ_{it} and QS_{it}:

$$\min(\theta_{it},QS_{it})$$

The updated inventory balance for the stochastic case is illustrated in Figure 2. The inventory balance constraints are modified to

$$\left.\begin{aligned} IE_{it} &= IB_{it} + QT_{it} \\ IB_{it+1} &= IE_{it} - \min(\theta_{it},QS_{it}) \end{aligned}\right\} i = 1, ..., N, \quad t = 1, ..., T$$

The above expressions imply that, apart from the inventory at the beginning of the first period IB_{i1} which is known, the inventories at the beginning and end of all subsequent periods are functions of the uncertain product demands θ_{it} and thus are stochastic. By resolving the recursion defined by the above expressions, the following expression is obtained for the inventory at the beginning of a period:

$$IB_{it} = IB_{i1} + \sum_{t'=1}^{t-1} QT_{it'} - \sum_{t'=1}^{t-1} \min(\theta_{it'},QS_{it'}), \quad t = 2, ..., T$$

Clearly, for a feasible inventory policy, $IB_{it} \geq 0$, $\forall t = 2, ..., T$. Note that positivity of IE_{it} is guaranteed if $IB_{it} \geq 0$ because $IE_{it} = IB_{it} + QT_{it}$ and $QT_{it} \geq 0$. Because $\min(\theta_{it},QS_{it})$ is always less than QS_{it}, positivity of IB_{it} and thus of IE_{it} is maintained if

$$IB_{i1} + \sum_{t'=1}^{t-1} QT_{it'} - \sum_{t'=1}^{t-1} QS_{it'} \geq 0, \qquad t = 2, ..., T$$

Addition of this constraint in the stochastic model maintains feasibility of the inventory policy.

The objective function of MPS involves the maximization of the expected revenue minus the inventory, underproduction, and production costs

$$E[RE_{it}(\theta_{it}) - IC_{it}(\theta_{it}) - UP_{it}(\theta_{it})] - PC_{it}$$

where E is the expectation operator. While the production cost

$$PC_{it} = C_{it} QT_{it}$$

remains deterministic, the remaining terms must be redefined to reflect that in the stochastic case the product sales are equal to $\min(\theta_{it},QS_{it})$ and not simply QS_{it}. Thus, the revenue from the sales of product i in period t is equal to

$$RE_{it}(\theta_{it}) = P_{it} \min(\theta_{it},QS_{it})$$

The inventory costs are equal to

$$IC_{it}(\theta_{it}) = \gamma_{it}\left(\frac{IB_{it} + IE_{it}}{2}\right)$$

After substituting $IE_{it} = IB_{it} + QT_{it}$ and invoking the recursive expression for IB_{it}, the relation for the inventory cost becomes

$$IC_{it}(\theta_{it}) = \gamma_{it}\left[IB_{i1} + \sum_{t'=1}^{t-1} QT_{it'} - \sum_{t'=1}^{t-1} \min(\theta_{it'},QS_{it'}) + \frac{QT_{it}}{2}\right]$$

The underproduction cost measures the loss of profit due to unrealized sales forced by the unavailability of a product,

$$UP_{it} = \delta_{it}(P_{it} - C_{it})\begin{cases} \theta_{it} - QS_{it}, & \text{if } \theta_{it} \geq QS_{it} \\ 0, & \text{if } \theta_{it} \leq QS_{it} \end{cases} = \delta_{it}(P_{it} - C_{it}) \max(0,\theta_{it} - QS_{it})$$

For $\delta_{it} = 1$ the underproduction cost is exactly equal to the profit lost due to the unsatisfied demand. Higher or lower values of the parameter δ_{it} impose stricter or more relaxed safeguards against underproduction.

The maximization of the objective function, as defined above, establishes the production and planned sales policy which most appropriately balances profits with inventory costs and underproduction shortfalls. A product demand satisfaction level is not explicitly imposed, but rather it is the outcome of the maximization of the profit function. While higher values of the parameter δ_{it} conceptually increase the probability of demand satisfaction, this strategy may still lead to unacceptably low probabilities of satisfying certain product demands (see examples). Therefore, the setting of explicit probability targets on product demand satisfaction is much more desirable. A systematic way to accomplish this is to impose explicit lower bounds on the probabilities of satisfying a single product demand or groups of product demands. This requirement for product i in period t assumes the following form:

$$\Pr\,[QS_{it} \geq \theta_{it}] \geq \beta_{it}$$

This constraint, known as a *chance-constraint*, imposes a lower bound β_{it} on the probability that the planned sales QS_{it} for product i in period t will be greater than the demand realization θ_{it}. In some cases a probability target is desired for the demand satisfaction of a group of products at a given period or for the demand satisfaction of a given product over a number of periods. This gives rise to *joint chance-constraints*

$$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \geq \beta_p, \qquad p = 1, ..., P$$

where I_p is the set of product−period (i, t) combinations whose simultaneous demand satisfaction with probability of at least β_p is sought and $p = 1, ..., P$ is the set of all joint chance-constraints.

Based on this analysis the stochastic multiperiod planning and scheduling model (SMPS) is as follows:

$$\max\ E[\sum_i\sum_t RE_{it}(\theta_{it}) - IC_{it}(\theta_{it}) - UP_{it}(\theta_{it})] - \sum_i\sum_t PC_{it} \quad \text{(SMPS)}$$

where

$$\left.\begin{aligned} PC_{it} &= C_{it}QT_{it} \\ RE_{it}(\theta_{it}) &= P_{it}\min(\theta_{it},QS_{it}) \\ IC_{it}(\theta_{it}) &= \gamma_{it}[IB_{i1} + \sum_{t'=1}^{t-1} QT_{it'} - \\ &\qquad \sum_{t'=1}^{t-1}\min(\theta_{it'},QS_{it'}) + \frac{QT_{it}}{2}] \\ UP_{it}(\theta_{it}) &= \delta_{it}\max(0,\theta_{it}-QS_{it})(P_{it} - C_{it}) \end{aligned}\right\} \begin{aligned} i &= 1, ..., N \\ t &= 1, ..., T \end{aligned}$$

subject to

$$\Pr\,[QS_{it} \geq \theta_{it}] \geq \beta_{it}, \qquad i = 1, ..., N, \quad t = 1, ..., T$$

$$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \geq \beta_p, \qquad p = 1, ..., P$$

$$Q_{itl}S_{ijl} \leq V_{jl}n_{itl}, \qquad i \in I_l, \quad j = 1, ..., M, \quad l \in L_i, \quad t = 1, ..., T$$

$$\sum_{l\in L_i} Q_{itl} = QT_{it}, \qquad i = 1, ..., N, \quad t = 1, ..., T$$

$$IB_{i1} + \sum_{t'=1}^{t-1} QT_{it'} - \sum_{t'=1}^{t-1} QS_{it'} \geq 0, \qquad t = 2, ..., T, \quad i = 1, ..., N$$

$$g_{tl}(n_{itl}) \leq 0, \qquad l = 1, ..., L, \quad t = 1, ..., T$$

$$Q_{itl},\ QT_{it},\ QS_{it} \geq 0$$

$$n_{itl} \in \{0, 1, 2, ...\}$$

The solution of SMPS defines a production QT_{it} and planned sales QS_{it} policy which maximizes the expected profit while satisfying single or joint product demands with probabilities β_{it} and β_p, respectively. By solving SMPS for different values of β_{it} and β_p, trade-offs between profit maximization and demand satisfaction can be established. The constraint ensuring positivity of the inventory throughout the period imposes a conservative estimate for the inventory level because it does not account for the inventory transfer of the amount $\max(0,QS_{it}-\theta_{it})$ whenever it is available. This leads to conservative estimates for the expectation of the profit and the probabilities of demand satisfaction. The excess inventory, however, can be accounted for based on the revision of planning and scheduling procedure described in section 8.

The proposed stochastic formulation involves the following types of stochastic expressions:

(1) $$E[\sum_i\sum_t (RE_{it} - IC_{it} - UP_{it})]$$

(2) $$\Pr\,[QS_{it} \geq \theta_{it}] \geq \beta_{it}$$

(3) $$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \geq \beta_p$$

Each one of these requires a different course of action for transforming it into an equivalent deterministic form (see also Appendix D of Wellons and Reklaitis (1989), Maranas (1997), and Petkov and Maranas (1997)). The deterministic equivalent representation of the expectation of the objective function (1) is examined in the next section.

5. Expectations of the Stochastic Objective Function

The expectation of the sum of a number of stochastic terms is equal to the sum of the expectations of the individual terms (Wilks, 1962). Therefore,

(1) $$E[\sum_i\sum_t (RE_{it} - IC_{it} - UP_{it})] = \sum_i\sum_t (E[RE_{it}] - E[IC_{it}] - E[UP_{it}])$$

This decomposes the task of identifying the expectation of the objective function into identifying the expectations of the revenue, inventory, and underproduction costs, respectively.

5.1. Expectation of Revenue. The revenue from product i in period t is equal to

$$RE_{it}(\theta_{it}) = P_{it}\min(\theta_{it},QS_{it}) = \begin{cases} P_{it}\theta_{it} & \text{if } \theta_{it} \leq QS_{it} \\ P_{it}QS_{it} & \text{if } \theta_{it} \geq QS_{it} \end{cases}$$

This representation implies that RE_{it} is a random variable which is not normally distributed. Inside the interval $(-\infty,P_{it}QS_{it}]$, RE_{it} is stochastic and equal to $P_{it}\theta_{it}$, but inside $[P_{it}QS_{it},-\infty]$, it is deterministic with a value of $P_{it}QS_{it}$.

To facilitate the calculation of the expectation on RE_{it}, the standardization of the normally distributed variables θ_{it} and deterministic variables QS_{it} is first performed. Normal random variables can be recast into the standardized normal form, with a mean of zero and a variance of 1, by subtracting their mean and dividing by their standard deviation (square root of variance). This defines the standardized normal variables

$$x_{it} = \frac{\theta_{it} - \hat{\theta}_{it}}{\sigma_{it}}$$

where $\hat{\theta}_{it}$ denotes the mean of θ_{it} and σ_{it} the square root of its variance. In the same spirit, the "standardization" of the deterministic variables QS_{it} defines

$$K_{it} = \frac{QS_{it} - \hat{\theta}_{it}}{\sigma_{it}}$$

Using this notation, the probability that $\theta_{it} \leq QS_{it}$ is the same as the probability that $x_{it} \leq K_{it}$ which is equal to $\Phi(K_{it})$, where Φ denotes the cumulative probability function of a standard normal random variable. This implies that the probability that $QS_{it} \leq \theta_{it}$ is equal to $(1 - \Phi(K_{it}))$.

The expectation of the revenue RE_{it} is obtained by applying the probability-scaled additive property of the expectation operation:

$$E[RE_{it}] = \Phi(K_{it})\ E[RE_{it}|\theta_{it} \leq QS_{it}] + (1 - \Phi(K_{it}))E[RE_{it}|\theta_{it} \geq QS_{it}]$$

After subtracting $\hat{\theta}_{it}$ from the inequalities defining the conditional probabilities and dividing by σ_{it}, we have

$$E[RE_{it}] = \Phi(K_{it})\ E\left[P_{it}\theta_{it}\left|\frac{\theta_{it} - \hat{\theta}_{it}}{\sigma_{it}} \leq \frac{QS_{it} - \hat{\theta}_{it}}{\sigma_{it}}\right.\right] + (1 - \Phi(K_{it}))E\left[P_{it}QS_{it}\left|\frac{\theta_{it} - \hat{\theta}_{it}}{\sigma_{it}} \geq \frac{QS_{it} - \hat{\theta}_{it}}{\sigma_{it}}\right.\right]$$

The substitution of the standardized variables x_{it}, K_{it} for θ_{it}, QS_{it}, respectively, yields

$$E[RE_{it}] = P_{it}\hat{\theta}_{it} + P_{it}\sigma_{it}\{\Phi(K_{it})\ E[x_{it}|x_{it} \leq K_{it}] + (1 - \Phi(K_{it}))E[K_{it}|K_{it} \leq x_{it}]\}$$

The conditional expectation of a deterministic variable is equal to itself:

$$E[K_{it}|K_{it} \leq x_{it}] = K_{it}$$

By applying the definition of the expectation of a standard normal distribution truncated at $x_{it} = K_{it}$, we have

$$E[x_{it}|x_{it} \leq K_{it}] = \frac{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{K_{it}} x_{it} \exp\left(-\frac{1}{2}x_{it}^2\right) \mathrm{d}x_{it}}{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{K_{it}} \exp\left(-\frac{1}{2}x_{it}^2\right) \mathrm{d}x_{it}} = \frac{-1}{\Phi(K_{it})}\frac{\exp\left(-\frac{1}{2}K_{it}^2\right)}{\sqrt{2\pi}} = -\frac{f(K_{it})}{\Phi(K_{it})}$$

where f is the standardized normal distribution function. The substitution of the last two expressions into the relation for the revenue yields

$$E[RE_{it}] = P_{it}\hat{\theta}_{it} + P_{it}\sigma_{it}[-f(K_{it}) + (1 - \Phi(K_{it}))K_{it}]$$

This means that the expectation of the revenue is equal to the unit price times the mean of the uncertain product demand augmented by an expression which is a function of K_{it} and scaled by σ_{it}. After "standardizing" the expression for the revenue expectation, we have

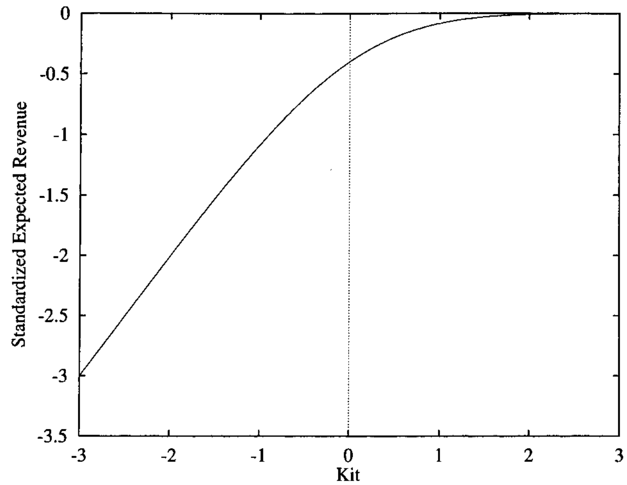

Figure 3. Plot of the standardized expected revenue.

$$\frac{E[RE_{it}] - P_{it}\hat{\theta}_{it}}{P_{it}\sigma_{it}} = -f(K_{it}) + (1 - \Phi(K_{it}))K_{it}$$

which measures the deviation of the variance-scaled expected revenue from the revenue for a deterministic product demand equal to $\hat{\theta}_{it}$. Figure 3 pictorially shows the standardized expected revenue as a function of K_{it}. As K_{it} goes to infinity ($QS_{it} \gg \hat{\theta}_{it}$), the standardized expected revenue goes to zero:

$$\lim_{K_{it}\to+\infty} E[RE_{it}] = P_{it}\hat{\theta}_{it}$$

Alternatively, as K_{it} goes to minus infinity, the standardized expected revenue becomes equal to K_{it}:

$$\lim_{K_{it}\to-\infty} E[RE_{it}] = P_{it}QS_{it}$$

Furthermore, for $K_{it} = 0$ ($QS_{it} = \hat{\theta}_{it}$), we have

$$E[RE_{it}] = P_{it}\left(\hat{\theta}_{it} - \frac{\sigma_{it}}{\sqrt{2\pi}}\right)$$

The standardized expected revenue is a concave function of K_{it} because the second-order derivative of $E[RE_{it}]$ with respect to K_{it} is always negative:

$$\frac{\mathrm{d}^2E[RE_{it}]}{\mathrm{d}K_{it}^{\ 2}} = -P_{it}\sigma_{it}f(K_{it}) \leq 0, \qquad \forall K_{it} \in R$$

5.2. Expectation of Inventory Cost. The inventory cost is equal to

$$IC_{it} = \gamma_{it}\left(\frac{IB_{it} + IE_{it}}{2}\right) = \gamma_{it}\left[IB_{i1} + \sum_{t'=1}^{t-1}QT_{it'} - \sum_{t'=1}^{t-1}\min(\theta_{it'},QS_{it'}) + \frac{QT_{it}}{2}\right]$$

After substituting the expression

$$E[\min(\theta_{it},QS_{it})] = \hat{\theta}_{it} + \sigma_{it}[-f(K_{it}) + (1 - \Phi(K_{it}))K_{it}]$$

derived in the previous subsection into the one for the expectation of the inventory cost, we obtain

$$E[IC_{i1}] = \frac{\gamma_{i1}}{2}(2IB_{i1} + QT_{i1}) \qquad \text{for } t = 1$$

$$E[IC_{it}] = \gamma_{it}\left\{IB_{i1} + \sum_{t'=1}^{t-1} QT_{it'} + \frac{QT_{it}}{2} - \sum_{t'=1}^{t-1}[\hat{\theta}_{it'} + \sigma_{it'}(-f(K_{it'}) + (1 - \Phi(K_{it'}))K_{it'})]\right\} \qquad \text{for } t \geq 2$$

The expectation of the inventory cost is a linear function of the production levels QT_{it}, and a convex function in terms of K_{it} (or QS_{it}). Unlike the expectation of the revenue, the expectation of the inventory cost depends on variables referring to all previous periods.

5.3. Expectation of Penalty of Underproduction. An underproduction penalty term UP_{it} for product i in period t is introduced, as explained in section 4, to quantify the cost of losing market share due to failure to satisfy a product demand (see also Birewar and Grossmann, 1990; Ierapetritou and Pistikopoulos, 1996):

$$UP_{it} = \delta_{it}(P_{it} - C_{it}) \max(0,\theta_{it} - QS_{it})$$
$$= -\delta_{it}(P_{it} - C_{it}) \min(0,QS_{it} - \theta_{it})$$
$$= -\delta_{it}(P_{it} - C_{it})[\min(\theta_{it},QS_{it}) - \theta_{it}]$$

Therefore, the expectation of UP_{it} is equal to

$$E[UP_{it}] = -\delta_{it}(P_{it} - C_{it})\{E[\min(\theta_{it},QS_{it})] - \hat{\theta}_{it}\}$$
$$= -\delta_{it}(P_{it} - C_{it})\sigma_{it}[-f(K_{it}) + (1 - \Phi(K_{it}))K_{it}]$$

which is a convex function of K_{it}.

Summarizing the expectation of the profit is rigorously transformed into a deterministic expression without introducing additional variables. Furthermore, based on the concavity/convexity results of the individual terms, it can be deduced that the expected profit is a concave function of QS_{it} and linear in QT_{it}. Therefore, the maximization of the expected profit involves a *single* solution. This result is important in optimization studies.

6. Probabilistic Bounds on Individual Product Demand Satisfaction

The second type of stochastic terms impose a lower bound on the probability of the demand satisfaction of a single product i in period t:

$$\Pr\,[QS_{it} \geq \theta_{it}] \geq \beta_{it} \tag{2}$$

This expression defines a chance-constraint whose deterministic equivalent representation can be obtained based on the concepts introduced by Charnes and Cooper (1962).

Specifically, by subtracting the mean and dividing by the standard deviation of θ_{it}, the chance-constraint can equivalently be written as

$$\Pr\left[\frac{QS_{it} - \hat{\theta}_{it}}{\sigma_{it}} \geq \frac{\theta_{it} - \hat{\theta}_{it}}{\sigma_{it}}\right] \geq \beta_{it} \quad \text{or}$$
$$\Pr\,[K_{it} \geq x_{it}] \geq \beta_{it}$$

The right-hand side of the inequality within the probability sign is a normally distributed random variable with a mean of zero and a variance of 1 (standardized form). This implies that the chance-constraint can be replaced with the following deterministic equivalent expression:

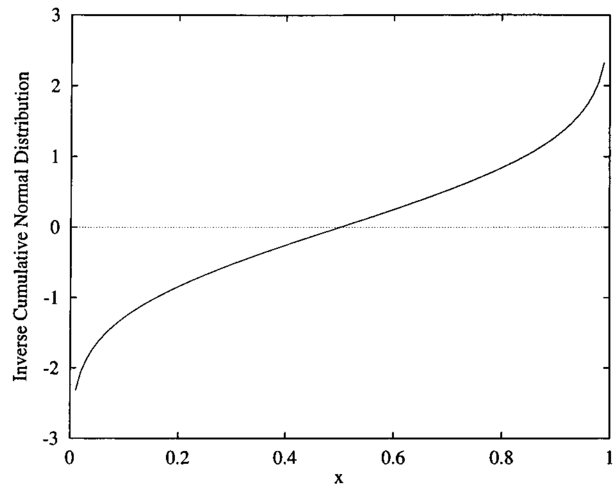

Figure 4. Inverse normal cumulative distribution.

$$\Phi(K_{it}) \geq \beta_{it}$$

The application of the inverse of the normal cumulative distribution function Φ^{-1}, which is a monotonically increasing function, yields

$$K_{it} \geq \Phi^{-1}(\beta_{it})$$

or equivalently

$$\hat{\theta}_{it} - QS_{it} + \sigma_{it}\Phi^{-1}(\beta_{it}) \leq 0$$

Inspection of the deterministic equivalent constraint reveals that it is *linear in the deterministic variables* QS_{it} and composed of the mean of the original constraint augmented by the squared root of its variance times $\Phi^{-1}(\beta_{it})$. The plot of Φ^{-1} is given in Figure 4. Typically, β_{it} is greater than 0.5 and thus $\Phi^{-1}(\beta_{it}) \geq 0$. This implies that the variance term penalizes the deterministic equivalent constraint, making it more restrictive than the mean of the original constraint. In fact, the higher the imposed probability β_{it}, the stricter (tighter) the constraint becomes. While a normality assumption is imposed for θ_{it}, the above-described deterministic equivalent representation can be accomplished for any *stable* (Allen *et al.*, 1974) up to two-parameter probability distribution (e.g., Poisson, χ^2, binomial, etc.).

7. Probabilistic Bounds on Multiple-Product Demand Satisfaction

Joint chance-constraints impose a probability target of *simultaneously* satisfying the demands for a group of products in different periods:

$$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \geq \beta_p \tag{3}$$

In this case, β_p can be thought of as the stochastic flexibility index of the batch plant (see for definition Pistikopoulos and Mazzuchi (1990)). This description is useful when a probability target for a set of products rather than individual ones must be imposed; for example, when only up to 10% unsatisfied product demand can be tolerated throughout the entire horizon

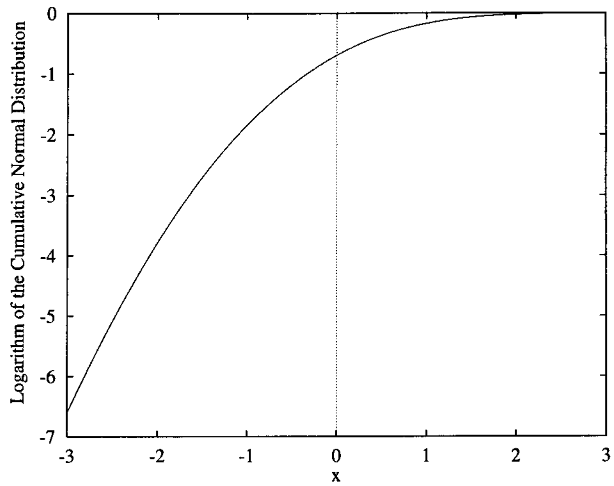

Figure 5. Logarithm of the normal cumulative distribution.

without distinguishing between different products. While single-product chance-constraints are unaffected by correlations between product demands, this is not always the case for joint chance-constraints. In the next subsection, first the uncorrelated demand case will be examined followed by the general case of arbitrarily correlated demands.

7.1. Uncorrelated Product Demands. When the demands are independent (uncorrelated) random variates, then the joint chance-constraint can be decomposed into the product of the constituting chance-constraints.

$$\prod_{(i,t)\in I_p} \Pr\,[QS_{it} \geq \theta_{it}] \geq \beta_p$$

Because, as shown earlier, $\Pr[QS_{it} \geq \theta_{it}] = \Phi(K_{it})$, we have

$$\prod_{(i,t)\in I_p} \Phi(K_{it}) \geq \beta_p$$

Note that the product on the left-hand side is neither convex nor concave (Miller and Wagner, 1964). However, upon its logarithmic transformation,

$$\sum_{(i,t)\in I_p} \ln(\Phi(K_{it})) \geq \ln(\beta_p)$$

it defines a convex constraint. Figure 5 pictorially illustrates that the logarithm of the cumulative normal distribution is a concave function. This is rigorously shown in Appendix A.

7.2. Joint Chance-Constraints with Correlated Random Demands. Correlation between the uncertain demands θ_{it} implies that cross-product, cross-period correlation parameters are needed to fully describe the statistics of the uncertain demands. These elements constitute a symmetric, positive definite $(N\cdot T \times N\cdot T)$ variance-covariance matrix $\mathbf{\Sigma}$. The diagonal elements of $\mathbf{\Sigma}$ are the variances of the uncertain demands:

$$Var(\theta_{it}) = \sigma_{it}^{\;2}, \qquad i = 1, ..., N, \quad t = 1, ..., T$$

The off-diagonal elements are the covariances between different uncertain parameters θ_{it} and $\theta_{i't'}$:

$$Cov(\theta_{it},\theta_{i't'}), \qquad i, i' = 1, ..., N, \quad t, t' = 1, ..., T$$

In general, for correlated uncertain demands the joint probabilities cannot be decoupled. This complicates the calculation of the probability and requires the simultaneous integration of multivariate probability distributions. Several methods have been suggested for accomplishing this task. The earliest practical approach for calculating multivariate probability functions is the tetrachoric series expansion by Kendall (1941). Though the series is widely used, Harris and Soms (1980) showed that convergence of the series cannot always be attained. Other analytical approaches involve dimension reductions based on Plackett's identity (Plackett, 1954; Tong, 1980, 1990; Iyengar, 1993). In general, the application of tetrachoric series and dimension reduction techniques involves a practical upper limit of 5 or 6 random variables (Deak, 1988). Gaussian quadrature has been extensively used for approximate multidimensional integration in the area of chemical engineering, but its accuracy and computational performance is adversely affected by the number of uncertain parameters. For higher dimensional integrals Monte Carlo type sampling methods provide a promising alternative (Deak, 1988).

In this paper, a new approach is examined for handling multivariate probability integrals. This approach, denoted as ΣA, is based on the approximation of the variance–covariance matrix.

7.3. The Σ*A* Approach. The basic idea of Σ*A* is to approximate the original variance–covariance matrix $\mathbf{\Sigma}$ with a new one $\mathbf{\Sigma}'$ (which is as close to $\mathbf{\Sigma}$ as possible) such that (1) $\Pr_{\Sigma'}[\cap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}]$ is "easy" to evaluate and (2) $\Pr_{\Sigma}[\cap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \cong \Pr_{\Sigma'}[\cap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}]$.

A variance–covariance matrix $\mathbf{\Sigma}'$ of special structure, for which (i) the multivariate probability integration is tractable and (ii) it can adequately approximate arbitrary variance–covariance matrices, is one which has off-diagonal elements of the following form:

$$Cov(\theta_{it},\theta_{i't'}) = \sigma_{it}\sigma_{i't'}\lambda_{it}\lambda_{i't'}$$

where

$$\lambda_{it}, \lambda_{i't'} \in R$$

This defines the set Ω of variance–covariance matrices whose covariance elements conform to the above-described functionality. A variance–covariance matrix $\mathbf{\Sigma}'$ belongs to Ω if and only if there exists λ_{it} such that all off-diagonal elements of $\mathbf{\Sigma}'$ can be recast in the above-described form. For example, the following standardized variance–covariance matrix:

$$\begin{pmatrix} 1 & -1/6 & 3/8 \\ -1/6 & 1 & -1/4 \\ 3/8 & -1/4 & 1 \end{pmatrix}$$

belongs to Ω with

$$\begin{pmatrix} \lambda_1 = 1/2 \\ \lambda_2 = -1/3 \\ \lambda_3 = 3/4 \end{pmatrix}$$

For any set of product demands I_p whose variance–covariance matrix $\mathbf{\Sigma}$ belongs to Ω the joint chance-constraint is rigorously equal to the following 1D integral:

$$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] = \int_{-\infty}^{+\infty} \prod_{(i,t)\in I_p} \left[\Phi\left(\frac{K_{it} - \lambda_{it} z}{\sqrt{1 - \lambda_{it}^{\;2}}}\right)\right] f(z)\, dz$$

Proof of this property can be found in Appendix B. Note that for uncorrelated demands the expression derived in subsection 7.1 is recovered after selecting $\lambda_{it} = 0$. The expression $(1 - \lambda_{it}^2)^{1/2}$ in the denominator of the 1D integral implies that the argument of Φ remains a real number only if $\lambda_{it} \in [-1, 1]$. A discussion on probability integration with complex numbers is included in Appendix C.

Prekopa (1995) has shown that the joint chance-constraint upon logarithmic transformation yields a convex constraint. Therefore, the following deterministic constraint is an exact convex representation of the original joint chance-constraint:

$$\ln\left\{\int_{-\infty}^{+\infty} \prod_{(i,t)\in I_p} \left[\Phi\left(\frac{K_{it} - \lambda_{it} z}{\sqrt{1 - \lambda_{it}^2}}\right)\right] f(z)\,\mathrm{d}z\right\} \geq \ln(\beta_p)$$

assuming that $\mathbf{\Sigma} \in \Omega$. Note that evaluation of this constraint requires one-dimensional integration rather than N-dimensional integration, avoiding exponential complexity in the uncertain parameters. The 1D integral can be efficiently calculated using any of many available numerical techniques (e.g., Gaussian quadrature, trapezoidal, Simpson's rule, etc.).

When the variance–covariance matrix $\mathbf{\Sigma}$ under consideration does not belong to Ω, then a variance–covariance matrix $\mathbf{\Sigma}'$ is sought which is as "close" to $\mathbf{\Sigma}$ as possible. This objective is quantified by selecting the parameters λ_{it} so that the sum of the squared differences between the off-diagonal elements of $\mathbf{\Sigma}$ and $\mathbf{\Sigma}'$ is minimized. Note that this does not necessarily find the "best" $\mathbf{\Sigma}'$ but rather a reasonable estimate by solving the following optimization problem:

$$\min_{\lambda_{it}} \sum_{(i,t)} \sum_{(i',t')\neq(i,t)} \left(\lambda_{it}\lambda_{i't'} - \frac{Cov(\theta_{it},\theta_{i't'})}{\sigma_{it}\sigma_{i't'}}\right)^2$$

subject to

$$-1 \leq \lambda_{it} \leq 1, \qquad i = 1, ..., N, \quad t = 1, ..., T$$

The above minimization model is a nonconvex problem, and therefore it may involve multiple local optima which were, in fact, observed in practice. Therefore, a multistart procedure is employed to locate the global minimum. Guidelines on how to globally solve problems of this type can be found elsewhere (Maranas and Floudas, 1995; Androulakis *et al.*, 1995).

The ΣA approach for approximating the multivariate probability integral involves a number of important properties.

Property 1. If all off-diagonal elements of $\mathbf{\Sigma}'$ are less than those of $\mathbf{\Sigma}$, then the ΣA approximation provides a rigorous lower bound (Slepain inequality (Slepain, 1962)):

$$\Pr_{\mathbf{\Sigma}} [\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \geq \Pr_{\mathbf{\Sigma}'} [\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}]$$

This condition can be met if instead of solving the least-squares minimization problem the λ_{it}'s are selected by considering the following alternative formulation:

$$\min_{\lambda_{it}, s\geq 0} s$$

subject to

$$Cov(\theta_{it},\theta_{i't'}) - (\sigma_{it}\sigma_{i't'})\lambda_{it}\lambda_{i't'} \leq s, \qquad \forall (i,t) \text{ and } (i',t') \neq (i,t)$$

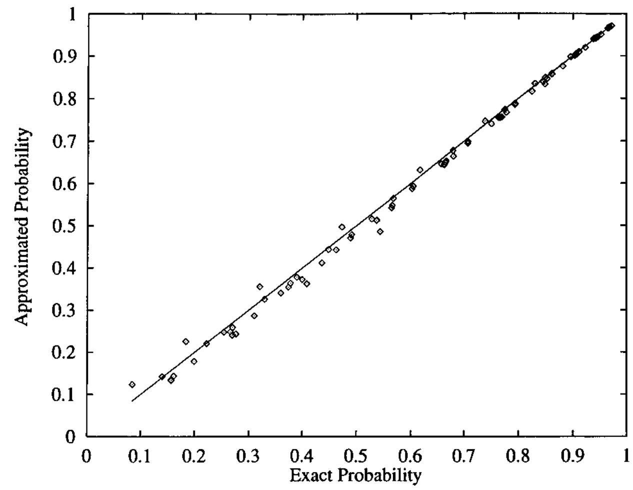

Figure 6. Comparison of exact joint probability values with the results obtained with the ΣA procedure.

and

$$-1 \leq \lambda_{it} \leq 1, \qquad i = 1, ..., N, \quad t = 1, ..., T$$

This formulation provides tight lower bounds, in particular for positively correlated demands.

Property 2. If the variance–covariance matrix $\mathbf{\Sigma}$ is *equicorrelated,*

$$\frac{Cov(\theta_{it},\theta_{i't'})}{\sigma_{it}\sigma_{i't'}} = \rho \text{ (constant)}$$

then the ΣA approximation is *exact*. This can be shown by selecting $\lambda_{\mathrm{it}} = \sqrt{\rho}$.

Property 3. For probability integrals involving up to three uncertain parameters, the ΣA procedure provides *exact* results (see Appendix C for proof).

The performance of the ΣA approximation was empirically verified. Ten different correlation matrices of dimension 10×10 were considered (zero sparsity). For each of the matrices the least-squares minimization problem was solved using multiple runs with different starting points to identify the best approximating matrix belonging to the set Ω. For a set of ten hyper-rectangular regions of different sizes the joint probabilities, calculated with the ΣA procedure, were compared with the exact joint probabilities obtained with Monte Carlo sampling (Tong, 1990) on the original variance–covariance matrix. Figure 6 illustrates the good agreement between the probability estimates obtained with ΣA and the exact results obtained with Monte Carlo simulation especially in the range of high probability values most important in practice. Note that the ΣA approximation results are obtained with 2–3 orders of magnitude less CPU time compared with the ones obtained with Monte Carlo simulation (tens of seconds). It is interesting also that in most cases the obtained approximations are lower bounds of the exact probabilities.

The independence assumption for the random variables is verified to ensure that the observed tightness of the ΣA approximation is not due to the fact that covariances do not contribute significantly in the joint probabilities. The same probability evaluations were carried out, assuming independence between the random variables, and the results are plotted in Figure 7. These results indicate that ignoring correlations may indeed lead to significant errors in the estimation of the joint probabilities. Specifically, the independence assumption leads to the same estimates for the joint

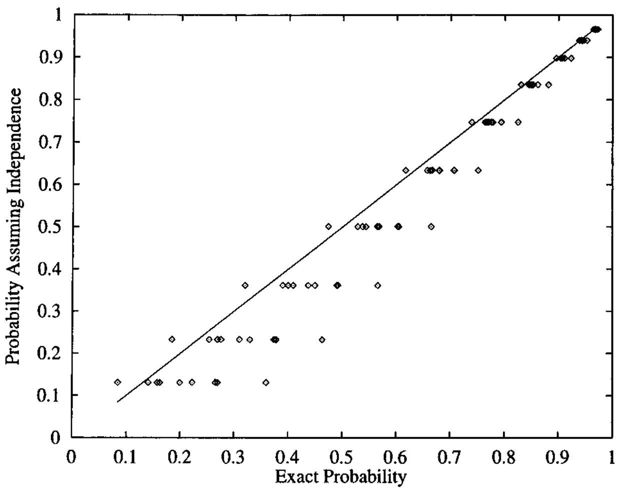

Figure 7. Comparison of exact joint probability values with the ones obtained after ignoring product demand correlations.

probabilities even when different values for the covariance elements are selected. This is pictorially demonstrated in Figure 7.

8. Update of the Planning and Scheduling Policy

As discussed in section 4, the proposed SMPS formulation employs conservative estimates of the inventory levels as it does not account for the transfer of the amount $\max(0,QS_{it}-\theta_{it})$. This amount will be available if the planned sales exceed the demand realizations in a given period. To remedy this conservative feature of the model, it is proposed to revise the planning policy and update the corresponding schedule at the end of each time period based on the realized sales. After the solution of the planning/scheduling problem (SMPS), only the decision variables associated with the immediately following period may be taken as final. The decision variables referring to successive periods can be used for planning and activities related to the plant operation (e.g., raw material ordering and purchase, labor force planning, etc.).

The update of the planning policy and schedule at the end of period t is described in the following steps:

1. Update future demand statistics based on present and previous product demand realizations.

2. Calculate the inventory IB_{it+1} at the beginning of period $t + 1$:

$$IB_{it+1} = IE_{it} - \min(QS_{it},\theta_{it})$$

3. Resolve the planning/scheduling problem for $t' = t + 1, ..., T$.

4. Set $t \leftarrow t + 1$. If $t \leq T$, return to step 1.

The first step allows the use of updated demand forecasting information. If no new demand forecasts are available, the conditional multivariate probability density function based on the realizations of the demands in previous periods can be utilized. The procedure for finding the conditional distribution function is outlined below. The second step accounts for any unsold product amount. Step 3 involves the solution of the SMPS formulation, which, in turn, determines the new planning and scheduling policies.

The derivation of the conditional probability distribution based on the realization of previous random variables can be accomplished as follows. First, the random variables, θ_{it}, are partitioned into two sets. The first set

$$P = \{\theta_{it'}:\quad 1 \leq t' \leq t,\quad i = 1, ..., N\}$$

contains the product demands realized in the past periods $t' = 1, ..., t$. The second set

$$F = \{\theta_{it'}:\quad t + 1 \leq t' \leq T,\quad i = 1, ..., N\}$$

contains the uncertain product demands for the future periods. Based on this partitioning, the variance–covariance matrix can be expressed as follows:

$$\mathbf{\Sigma} = \begin{pmatrix} \Sigma_{PP} & \Sigma_{PF} \\ \Sigma_{FP} & \Sigma_{FF} \end{pmatrix}$$

where Σ_{PP} and Σ_{FF} are the variance–covariance submatrices of the product demands belonging to the sets P and F, respectively. The elements of submatrices $\Sigma_{PF} = (\mathbf{\Sigma}_{FP})^{\mathrm{T}}$ are the covariances between the elements of P and F. Let

$$\Xi = (\xi_{i1}, \xi_{i2}, ..., \xi_{it})$$

denote the realizations (outcomes) of the product demands of set P associated with past periods. The conditional means of the uncertain future product demands, included in F, are then given by

$$\mu_{F|P} = \mu_F + \mathbf{\Sigma}_{FP}\mathbf{\Sigma}_{PP}^{-1}(\Xi - \mu_P)$$

where $\mu_{F|P}$ denotes the conditional demand expectations and μ_P and μ_F are the past and future mean values. The new (conditional) variance–covariance matrix is equal to

$$\mathbf{\Sigma}_{F|A} = \mathbf{\Sigma}_{FF} - \mathbf{\Sigma}_{FP}\mathbf{\Sigma}_{PP}^{-1}\mathbf{\Sigma}_{FP}$$

A detailed treatise of conditional multivariate normal probability functions can be found in Tong, 1990. Note that while the conditional mean values, $\mu_{F|P}$, depend on the demand realizations in past periods, the conditional covariance matrix $\mathbf{\Sigma}_{F|A}$ is independent of the demand realizations Ξ. Updating the probability distribution at the end of each period "decreases" the uncertainty (variances) associated with the remaining random variables, thus increasing the predictive power of the stochastic model. This is observed in the example addressed in subsection 10.4.

9. Solution Procedure

The number of batches n_{itl} of product i in period t and on line l gives rise to a large number of discrete variables associated with the planning and scheduling problem. To limit the combinatorial complexity of the problem, Birewar and Grossmann (1990) proposed a simplifying procedure for the deterministic planning/scheduling problem which is based on treating the number of batches n_{itl} as continuous variables and approximating the makespan of the process with the cycle-time. This rounding-off of the number of batches leads to a suboptimal feasible (or near-feasible) solution because the cycle-time usually underestimates the process makespan. However, while this strategy works well for the deterministic formulation and the stochastic case under SPC scheduling policy, it typically results in violation of the probabilistic constraints in SMPS formulation when one of the MPC scheduling policies is implemented. Therefore, a variation of this procedure is utilized in this work. To ensure feasibility of the obtained solution, the process makespan under multiple-product campaigns is explicitly defined in the model through the constraints:

$$\sum_{i\in I_l} n_{itl}t_{ij} + \sum_{i\in I_l}\sum_{k\in I_l} NPRS_{iktl}SL_{ikj} + \sum_{i\in I_l}\sum_{k\in I_l}(\sum_{j'\le j} t_{ij'} + \sum_{j'\ge j} t_{ij'} - SL_{ikj})Y_{iktl} \le H$$

$$\sum_{k\in I_l} NPRS_{iktl} = n_{itl}$$

$$\sum_{i\in I_l} NPRS_{iktl} = n_{ktl}$$

$$\sum_{i\in I_l}\sum_{k\in I_l} Y_{iktl} = 1$$

This set of constraints ensures that the process makespan, equal to the cycle-time plus the "tail" times, does not exceed the time horizon. The binary variable Y_{iktl} determines where to "break" the production cycle for a feasible makespan, and the variable $NPRS_{iktl}$ identifies the number of product changeovers. In light of this, the solution procedure for SMPS is summarized in the following four steps:

Step 1: *Initialization*
Solve the continuous relaxation of the SMPS formulation having $0 \le Y_{iktl} \le 1$ and continuous batch sizes n_{itl}^{rlx}. The relaxed optimal solution provides good initial points for the continuous variables.

Step 2: *Domain Restriction*
Restrict the integer search domain as follows:

$$\lfloor n_{itl}^{rlx} \rfloor \le n_{itl} \le \lceil n_{itl}^{rlx} \rceil$$

Step 3: *MINLP Solution*
Solve the MINLP problem formulation (SMPS) in the defined search domain utilizing outer approximation (Duran and Grossmann, 1986a). If the problem does not have an integer solution, increase the integer domain bounds of step 2 by 1 and repeat step 3.

Step 4: *Optimal Schedule Recovery*
Fix the number of batches n_{itl} to the MINLP solution and solve the makespan minimization problem for each time period and line. This problem is described in Appendix 2 of Birewar and Grossmann (1990) and is formulated as follows:

$$\min MS_{tl}$$

subject to

$$MS_{tl} \ge \sum_{i\in I_l} n_{itl}t_{ij} + \sum_{i\in I_l}\sum_{k\in I_l} NPRS_{iktl}SL_{ikj} + \sum_{i\in I_l}\sum_{k\in I_l}(\sum_{j'\le j} t_{ij'} + \sum_{j'\ge j} t_{ij'} - SL_{ikj})Y_{iktl}$$

$$\sum_{k\in I_l} NPRS_{iktl} = n_{itl}$$

$$\sum_{i\in I_l} NPRS_{iktl} = n_{ktl}$$

$$\sum_{i\in I_l}\sum_{k\in I_l} Y_{iktl} = 1$$

$$Y_{iktl} \le NPRS_{iktl}$$

$$NPRS_{iktl} \ge 0$$

$$Y_{iktl} \in \{0, 1\}$$

Table 1. Volumes, V_{jl}

line	stage 1	stage 2	stage 3	stage 4
1	600	400	400	400
2	400	400	400	600
3	600	400	600	400

Table 2. Size Factors, S_{ij}

product	stage 1	stage 2	stage 3	stage 4
1	2	3	2	6
2	7	3	1	2
3	1	4	3	2
4	5	5	2	6
5	1	6	2	2

Table 3. Processing Times, t_{ij}

product	stage 1	stage 2	stage 3	stage 4
1	10	4	10	1
2	3	10	6	12
3	4	12	6	10
4	16	3	8	4
5	7	2	5	3

Table 4. Sale Prices, P_{it} ($/kg)

product	period 1	period 2	period 3	period 4
1	9.0	9.5	9.5	4.5
2	9.0	9.5	9.0	9.0
3	12.0	12.5	13.0	11.5
4	12.0	12.0	12.0	12.5
5	8.0	9.5	8.0	9.5

Table 5. Production Costs, C_{it} ($/kg)

product	period 1	period 2	period 3	period 4
1	4.5	4.5	4.5	4.5
2	4.5	4.5	4.5	4.5
3	6.0	6.0	6.0	6.0
4	6.0	6.0	6.0	6.0
5	4.0	4.0	4.0	4.0

The solution of the minimum makespan problem determines the optimal number of product changeovers $NPRS_{iktl}$. The exact scheduling sequence is then obtained based on the graph enumeration method of Birewar and Grossmann (1989).

This batch size relaxation results in very small integrality gaps (<0.01%), while the computational effort remains between tens to hundreds of seconds (see section 10). Infeasibility of the relaxed MINLP problem in step 1 implies that the imposed probability targets cannot be achieved with the available production resources and one must either relax the probability targets or introduce additional resources.

10. Example

The first example of Birewar and Grossmann (1990) with a modified description of the demand specifications is addressed. The plant has three defined production lines involving four production stages. Five different products are to be produced, and the time horizon of 6000 h is divided into four equal time periods. The stage volumes, size factors, processing times, sales prices, and production costs are given in Tables 1–5, respectively. The product demands in each period are described by normal multivariate probability distributions. The expected (mean) values of the demands are given in Table 6, and their standard deviation is assumed to be 5% of their mean values. This implies that 90% of their realizations will fall within $\pm 1.64 \times 5\% = 8.2\%$ from their mean values.

Three alternative model formulations, applied to the same example problem, are defined and solved using

Table 6. Mean Values of the Product Demand $\hat{\theta}_{it}$

period	product 1	product 2	product 3	product 4	product 5
1	2700	2100	13 600	5900	4000
2	5000	7600	15 000	5000	4500
3	4500	5400	17 200	6800	5500
4	3100	7300	13 100	7200	20400

the proposed solution procedure. Each one of these models includes some of the features of SMPS model as defined earlier.

Model 1:

$$\max E[\text{Profit}]$$

Model 1 maximizes the expectation function of the profit without setting any probabilistic demand satisfaction targets. Loss of profit due to underproduction is implicitly taken into account by utilizing a penalty for underproduction.

Model 2:

$$\max E[\text{Profit}]$$

subject to

$$\Pr\,[QS_{it} \geq \theta_{it}] \geq \beta_{it}$$

Model 2 also maximizes the expected profit, but additional probability targets are explicitly set for individual product demand satisfaction without utilizing a penalty for underproduction ($\delta_{it} = 0$).

Model 3:

$$\max E[\text{Profit}]$$

subject to

$$\Pr\,[QS_{it} \geq \theta_{it}] \geq \beta_{it}$$

$$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \geq \beta_p$$

Model 3 incorporates not only single but also joint chance-constraints for setting probability targets for the satisfaction of a group of products. First the uncorrelated case is addressed, and next the effect of correlation on the economic parameters and the optimal product mix is evaluated and discussed.

A customized implementation of the outer approximation algorithm (Duran and Grossmann, 1986a,b) utilizing the CONOPT and CPLEX 4.0 solvers, within GAMS (Brook *et al.*, 1988), is utilized to solve the above model formulations. The reported CPU times are on an IBM RS6000 43P-133 workstation.

10.1. Model 1: Penalty Approach for Cost of Underproduction. This model involves the maximization of the expectation of the stochastic profit function subject to production and inventory constraints and an MPC with UIS scheduling policy. The effect of the selection of the penalty parameter δ_{it} is examined by performing several runs with δ_{it} ranging from zero to 10 times the profit margin for each product. The results are summarized in Table 7. Note that the imposed integrality gap tolerance of 0.01% is met after only a few (always less than 10) iterations. The minimum and maximum probabilities of satisfying individual product demands as well as the joint probability of satisfying all product demands simultaneously are calculated for the planned sales production policy QS_{it} obtained for different values of δ_{it}. Even when the penalty for underproduction is as high as 10 times the profit margin, the joint probability of satisfying an individual demand target is only 16%. The results obtained from Model 1 demonstrate that by increasing the value of the penalty parameter δ_{it} the chances of satisfying the product demands are improved but the magnitude of the improvement cannot *a priori* be predicted and sometimes is not sufficient.

10.2. Model 2: Single-Product Demand Probabilistic Constraints. Model 2 extends model 1 through the incorporation of individual product demand probability constraints. The resulting MINLP problem involves the same concave objective function (except for the penalty of underproduction term) and linear constraints of Model 1 plus a set of linear constraints representing the deterministic equivalent representation of the individual probability constraints. The results for β_{it} ranging from 0 to 0.95 are shown in Table 8. Note that for $\beta_{it} \leq 0.5$ the probability target constraints are not active, implying that the objective function maximization requires a probability greater than 0.5 for the satisfaction of individual product demands. For $\beta_{it} \geq 0.95$ the problem becomes infeasible, implying that available plant resources cannot guarantee probability targets greater than 0.95. Figure 8 shows the maximum expected profit for different probability target levels. The first trade-off curve refers to Model 1 and the second to Model 2. Model 2, which explicitly addresses probability target levels, involves a trade-off curve which is "above" the one of model 1. This is expected because model 1 only implicitly quantifies probability of demand satisfaction through an underproduction penalty. For the example at hand, Model 1 tracks reasonably well the Pareto optimum curve defined by the results of Model 2. The curves shown in Figure 8 provide a quantitative way to relate the value of the penalty of underproduction parameter δ_{it} with the probabilistic target β_{it}.

10.3. Model 3: Use of Joint Probability Constraints. Three separate cases are considered for Model 3 involving (i) uncorrelated, (ii) equicorrelated, and (iii) arbitrarily correlated product demands.

Table 7. Results of Model 1 (Integrality Gap = 0.01%)

δ_{it}	max. profit (with penalty)	max. profit (without penalty)	joint prob.	min prob.	max prob.	iter.	CPU (s)
0.0	833 910.31	833 910.31	0.000 003	0.447	0.5759	5	10.24
0.2	830 819.75	833 865.81	0.000 004	0.5000	0.5899	3	3.57
0.4	828 025.55	833 415.55	0.000 013	0.5000	0.6368	8	12.58
0.6	825 627.90	832 628.17	0.000 052	0.5845	0.6602	3	2.89
0.8	823 418.18	831 887.61	0.000 124	0.6006	0.6881	3	3.16
1.0	821 449.84	831 086.90	0.000 225	0.5975	0.7167	3	3.56
2.0	813 759.86	827 001.20	0.002 648	0.7218	0.7878	6	9.05
3.0	808 279.11	823 008.72	0.010 292	0.7705	0.8339	4	8.58
4.0	803 989.10	819 778.52	0.020 704	0.7699	0.8577	8	19.90
5.0	800 559.73	816 416.97	0.043 061	0.8449	0.8824	4	9.28
6.0	797 706.59	814 190.02	0.059 900	0.8530	0.8986	6	9.17
10.0	789 474.05	806 213.83	0.161 549	0.8896	0.9319	4	8.21

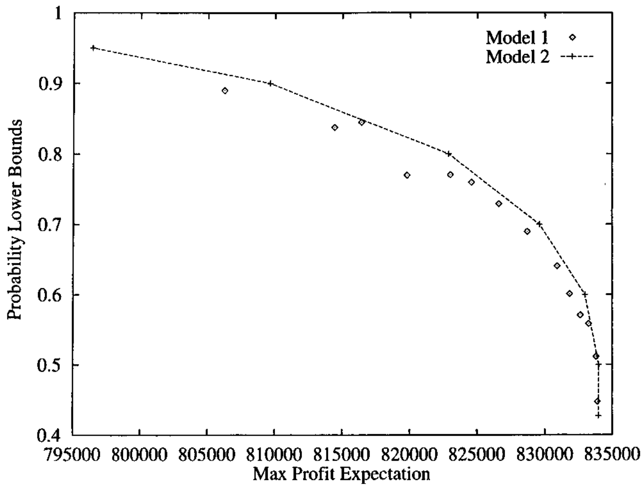

Figure 8. Plot of maximum expected profit vs the lower bound target on the probabilities for demand satisfaction for the results obtained for models 1 and 2.

Table 8. Results of Model 2 (Integrality Gap = 0.01%)

β_{it}	max profit	min prob.	max prob.	iter.	CPU (s)
0.4	833 969.47	0.427	0.5526	4	6.25
0.5	834 001.43	0.500	0.5526	2	1.41
0.6	832 967.15	0.600	0.6000	2	1.28
0.7	829 596.48	0.700	0.7000	2	9.80
0.8	822 882.99	0.800	0.8000	2	13.59
0.9	809 611.31	0.900	0.9000	2	2.50
0.95	796 394.99	0.950	0.9500	2	1.41

Table 9. Results of Model 3 with Uncorrelated Demands (Integrality Gap = 0.1%)

β_p	max profit	min prob.	max prob.	iter.	CPU (s)
0.0	833 969.47	0.4270	0.5526	4	6.25
0.1	814 714.31	0.7438	0.9759	2	4.64
0.2	808 670.28	0.8256	0.9826	2	4.31
0.3	803 277.27	0.8513	0.9914	2	4.49
0.4	798 160.49	0.8658	0.9933	2	4.09
0.5	793 620.73	0.9126	0.9930	2	5.02
0.6	788 089.87	0.9311	0.9965	5	7.75
0.7	782 091.97	0.9528	0.9965	2	5.82
0.8	773 949.73	0.9735	0.9981	2	6.25
0.9	762 261.52	0.9878	0.9989	3	7.57

10.3.1. Uncorrelated Case. For uncorrelated demands explicit convex deterministic equivalent relations can be obtained (see section 7) for the joint probabilities. Table 9 shows the values of the highest and lowest probability of satisfying the demand for each product in a single period. Note that the presence of nonlinear (convex) constraints in model 3 does not affect significantly the CPU requirements compared with model 2.

10.3.2. Equicorrelated Case. While correlations do not affect the results of models 1 or 2, the joint probability targets of model 3 are affected by possible demand correlation. This correlation affects the optimum expectation values of the stochastic economic parameters (profit, inventory costs, and penalty cost) as well as the optimum product-mix, production schedule, and planned sales. First, the magnitude of the effect of correlation is quantitatively examined. The same correlation coefficient ρ is selected for all product demands (equicorrelation), and ρ assumes values between 0 and 0.99, modeling various levels of demand correlation. Obviously, higher values of ρ imply stronger correlation. For the equicorrelated case it was shown in section 7 that the correlation matrix belongs to the set Ω with $\lambda_i = \sqrt{\rho}$. Therefore, the planning/scheduling problem can be solved exactly using model 3 and invoking the ΣA procedure (Table 10). The joint probability index, β, for the set of all 20 product demands is set to 80%, and the problem is solved for correlation coefficients varying between 0 and 0.99. For each value of β the optimal planning/scheduling policy is identified, and the profit expectation, production cost, and the expectation of the inventory cost are compared with those after ignoring demand correlation. The differences given in percentage deviations from the uncorrelated assumption are plotted in Figure 9. These results indicate that an increase in the profit expectation of more than 5% and a reduction of 20% in the inventory costs is possible if correlation between the product demands is properly accounted for. This expectation of the profit increase is a result of the fact that the joint probability target of 80% can be met with smaller production levels than the ones obtained after ignoring correlations.

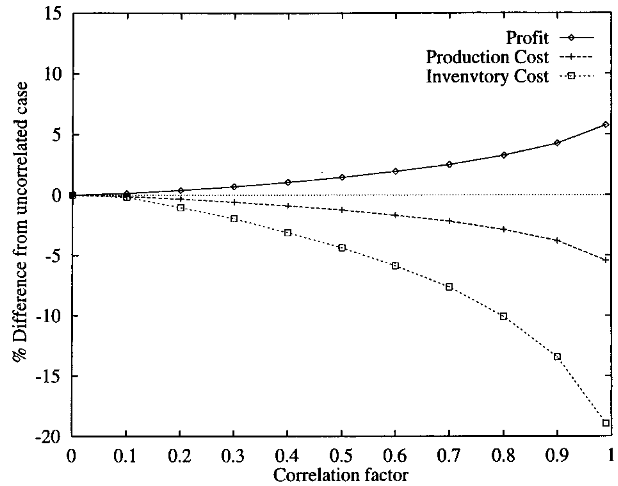

Figure 9. Effect of correlation on optimum expected profit.

Table 10. Results of Model 3 with Correlated Demands (Integrality Gap = 0.1%)

β_p	max profit	min prob.	max prob.	iter.	CPU (s)
0.0	833 969.47	0.427	0.5526	4	6.25
0.1	817 721.32	0.7247	0.9482	6	18.77
0.2	810 997.95	0.8162	0.9735	6	46.32
0.3	805 785.04	0.8511	0.9805	9	46.66
0.4	800 112.50	0.8882	0.9907	6	35.46
0.5	795 038.20	0.9096	0.9900	29	278.40
0.6	789 359.59	0.9405	0.9934	6	33.78
0.7	783 204.77	0.9496	0.9953	4	47.84
0.8	774 921.24	0.9721	0.9976	12	56.09
0.9	762 812.06	0.9879	0.9989	9	25.19

Table 11. Comparison of the Results Obtained by the ΣA Procedure, the Assumption of Ignoring Correlation, and Boole's Inequality

P_{target}	$P_{\Sigma A}$	$P_{Uncorr.}$	P_{Boole}
0.9	0.902	0.906	0.910
0.8	0.804	0.813	0.829
0.7	0.709	0.722	0.757
0.6	0.610	0.630	0.692
0.5	0.513	0.541	0.633
0.4	0.414	0.450	0.577
0.3	0.314	0.357	0.528
0.2	0.212	0.259	0.483
0.1	0.111	0.152	0.442

10.3.3. Correlated Case. The equicorrelated assumption utilized above provided the means to quantitatively assess the effect of different "magnitudes" of correlation in the planning/scheduling policy. However, realistic product demand correlations are not equicorrelated. A nonequicorrelated variance−covariance matrix is constructed and shown in Appendix D in its

Table 12. Employed Realizations of the Random Product Demands

product	period 1	period 2	period 3	period 4
1	2751	4690	4385	3038
2	2236	7945	5437	7046
3	14620	15124	17280	13507
4	5770	4819	6434	7785
5	4332	4257	5403	22011

standardized form. The latter has sparsity of 60%, and its off-diagonal elements vary between −0.3 and 0.6. The bias toward positive covariances is introduced to maintain semipositive−definiteness which is a property of all variance−covariance matrices.

The model 3 formulation is used to evaluate the performance of the (ΣA) approximation (see Table 11). The first column contains the targeted joint probability level, β, and the following columns list results obtained using (1) the ΣA approximation, (2) uncorrelated assumption, and (3) Boole inequality (lower bound)

$$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \geq \theta_{it}] \geq \sum_{(i,t)\in I_p} \Pr\,[QS_{it} \geq \theta_{it}] - (n-1)$$

These results demonstrate that especially for $\beta < 0.9$ both the independence assumption and the Boole inequality significantly underestimate the joint probability. The ΣA procedure provides a tight approximation of the joint probability over the entire range of probability targets with discrepancies which are always less than 2.5%. Next, the proposed update policy is applied on the example problem.

10.4. Revision of Planning Policy. The proposed revision of planning policy is next applied to the example problem at hand. To facilitate the study of the effect of updating the production and planned sales policies, only covariances between the demands of the same product in various time periods are considered. The following standardized correlation matrix is selected for each product:

$$\mathbf{\Sigma} = \begin{pmatrix} 1.00 & 0.40 & -0.24 & 0.48 \\ 0.40 & 1.00 & -0.15 & 0.30 \\ -0.24 & -0.15 & 1.00 & -0.18 \\ 0.48 & 0.30 & -0.18 & 1.00 \end{pmatrix}$$

Using this correlation matrix, a demand realization is randomly generated using the method presented by Tong (1990). The product demand realizations are given in Table 12, and when compared with the mean values (see Table 6), it is found that some of the demand realizations differ by as much as 1.66 times the standard deviation from the mean values. A joint probability target of 85% is set for the demand satisfaction of each product in all time periods. This introduces four joint probability constraints of the form

$$\Pr\,[\bigcap_t QS_{it} \geq \theta_{it}] \geq 0.85, \quad i = 1, ..., 5$$

in the model. The resulting optimization problem is solved in the entire time horizon. Next, based on (i) the demand realizations in the first period, (ii) the correlation matrix, (iii) the mean values of the remaining random demands, and (iv) the remaining inventory at the beginning of the second period, a new planning revision problem is solved for $t = 2-4$. This is repeated for all remaining time periods. The updated values of the mean vectors and standard deviations after each time period are given in Tables 13 and 14. After each revision, the elements of the variance−covariance matrix become smaller, which demonstrates that the planning revision reduces demand uncertainty (see Table 15).

The inventory profile for product 4 is shown in Figure 10. The solid line denotes the inventory levels after the revision of the planning policy, and the dashed line denotes the inventory without employing any updating policy. Clearly, when the solution is updated, the planning policy is much more effective because overproduction is decreased. Examination of the demand profile for product 4 reveals that its high demand in the last period could not be fully satisfied by utilizing only the available resources of the last period. However, by transferring amounts produced in previous periods, through the inventory system, the satisfaction of the product demands with an overall probability of 85% is made possible.

11. Summary and Conclusions

In this paper, the multiperiod planning and scheduling of multiproduct plants under demand uncertainty was addressed. The following basic production/scheduling policies providing a check on the feasibility of the production levels identified in the planning phase were considered: SPC with ZW or MPC with ZW/UIS. A novel stochastic model, which extends the deterministic model proposed by Straub and Grossmann (1990), was introduced. This model involves the maximization of the expected profit subject to constraints for the satisfaction of single- and/or multiple-product demands with a prespecified level of probability (chance-constraints). The stochastic attributes of the model were expressed with equivalent deterministic forms, eliminating the need for discretization or sampling techniques at the expense of invoking the normality assumption. For the uncorrelated product demand case an exact deterministic representation was obtained. For the correlated case, the ΣA procedure was introduced for approximating joint probability integrals. The resulting equivalent deterministic optimization models are MINLP's with

Table 13. Updates of the Product Demand Expectations

time T	period	product 1	product 2	product 3	product 4	product 5
0	1	2700	2100	13600	5900	4000
	2	5000	7600	15000	5000	4500
	3	4500	5400	17200	6800	5500
	4	3100	7300	13100	7200	20400
1	2	5020	7654	15410	4948	4633
	3	4488	5367	16960	6831	5420
	4	3124	7365	13590	7138	20560
2	3	4509	5349	16970	6839	5445
	4	3082	7403	13550	7121	20510
3	4	3090	7397	13530	7149	20510

Table 14. Updates of the Product Demand Standard Deviations

time T	period	product 1	product 2	product 3	product 4	product 5
0	1	135	105	680	295	200
	2	250	380	750	250	225
	3	225	270	860	340	275
	4	155	365	655	360	1020
1	2	210	319	630	210	189
	3	212	227	722	320	259
	4	119	281	504	277	785
2	3	210	252	804	318	257
	4	117	276	495	272	771
3	4	117	274	493	271	767

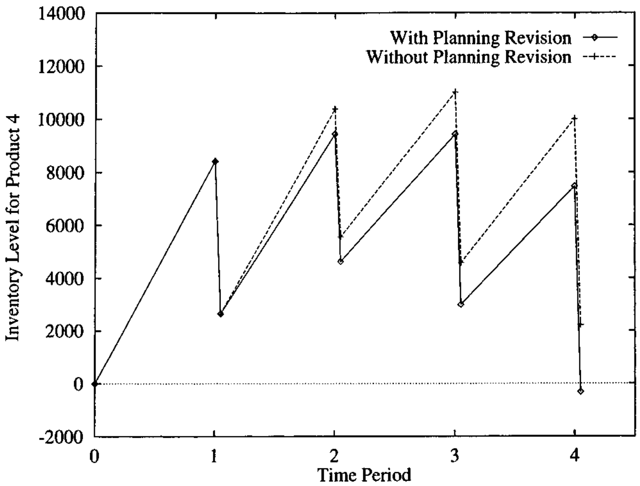

Figure 10. Inventory profile for product 4.

Table 15. Updates of the Product Demand Correlation Matrices

time T	period	1	2	3	4
0	1	1.00	0.40	−0.24	0.48
	2	0.40	1.00	−0.15	0.30
	3	−0.24	−0.15	1.00	−0.18
	4	0.48	0.30	−0.18	1.00
1	2		1.0	−0.06	0.14
	3		−0.06	1.0	−0.07
	4		0.14	−0.07	1.0
2	3			1.0	−0.054
	4			−0.054	1.0
3	4				1.0

convex continuous parts. A revision strategy for the planning policy and update of the corresponding schedule at the end of each time period based on the realized sales was also presented. This was accomplished by recalculating the conditional multivariate probability function given the demand realizations in previous periods. An example problem was also addressed, highlighting different features of the stochastic formulation.

Computational results demonstrate that the proposed stochastic formulation and solution strategies involve CPU requirements which are on the same order of magnitude as those in the deterministic case. The example considered involves 20 uncertain parameters, however, much larger problem sizes can be handled since no significant computational penalty exists for additional uncertain parameters. Comparison of the results of models 1 and 2 indicates that the inclusion of explicit probabilistic constraints for demand satisfaction provides a rigorous alternative to the use of the underproduction penalty whose *a priori* weight selection is sometimes difficult. Results from the equicorrelated case of model 3 demonstrate that the expected profit and in particular the corresponding planning policy and schedule are strongly affected by the presence of correlations. The results from the correlated case indicate that the ΣA approximation provides tight bounds for the joint probabilities which are significantly better than the ones obtained assuming independence or utilizing the Boole inequality. The proposed planning revision and scheduling updating policy by updating the probability distribution at the end of each period decreased uncertainty (variances) associated with the remaining random variables and thus increased the predictive power of the stochastic model for the subsequent periods.

Increased uncertainties in the product demands require on average higher inventory levels at the end of each period to guarantee the prespecified probability level of demand satisfaction. Thus, higher levels of uncertainty generally lead to longer process makespans. Computational experience demonstrated that increasing the probability of demand satisfaction also increases the required total processing time. So far, only simple scheduling policy checks involving SPC with ZW and MPC with UIS or ZW are considered at the planning stage. This is because once the production goals are set and their feasibility is checked for the basic scheduling policy which most realistically describes the available storage capacities and operation mode, detailed short-term scheduling can then be applied to revise the scheduling suggestions obtained at the planning phase. Examples of more complex scheduling rules include mixed-intermediate storage (MIS) and fixed-intermediate storage (FIS) (Kim *et al.*, 1996).

Acknowledgment

Financial support by the Du Pont Educational Aid Grant 1996/97 and the NSF Career Award CTS-97-01771 is gratefully acknowledged.

Appendix A: Concavity of ln(Φ(*K*))

The function ln(Φ(*K*)) is concave if its second derivative with respect to K is always nonpositive $\forall K \in R$. Consider the first and second derivatives of ln(Φ(*K*)):

$$\frac{\mathrm{d}\ln(\Phi(K))}{\mathrm{d}K} = \frac{f(K)}{\Phi(K)}$$

$$\frac{\mathrm{d}^2\ln(\Phi(K))}{\mathrm{d}K^2} = \frac{1}{\Phi^2(K)}\left[\frac{\mathrm{d}f(K)}{\mathrm{d}K}\Phi(K) - f^2(K)\right] = -\frac{f(K)}{\Phi^2(K)}[K\Phi(K) + f(K)]$$

where f(K) is the normal standardized probability function $f(K) = \mathrm{d}\Phi/(K)/\mathrm{d}K$. Because $f(K)$ and $\Phi(K)$ are always positive, it suffices to show that the term $K\Phi(K) + f(K)$ is always nonnegative.

For $K \geq 0$ it is clear that $K\Phi(K) + f(K)$ is always positive. For the case $K < 0$, the first derivative of

$K\Phi(K) + f(K)$ with respect to K is equal to:

$$\frac{d[K\Phi(K) + f(K)]}{dK} = \Phi(K)$$

This expression is always positive, implying that $K\Phi(K) + f(K)$ is strictly monotonically increasing. The limit of the latter when $K \to -\infty$ is

$$\lim_{K\to-\infty} [K\Phi(K) + f(K)] = \lim_{K\to-\infty} \left[\frac{K}{\sqrt{2\pi}}\int_{-\infty}^{K} e^{-x^2}\, dx + \frac{1}{\sqrt{2\pi}}e^{-K^2}\right] = 0$$

This implies that $K\Phi(K) + f(K)$ is nonnegative for any $K \in R$. Therefore, $\ln(\Phi(K))$ is a concave function of K for any $K \in R$.

Appendix B: Multivariate Probability Integration for $\Sigma \in \Omega$ Variance−Covariance Matrices

This proof follows the analysis of Tong (1990). Given is a vector $\mathbf{X}$ of normally distributed correlated random variates x_i, $i = 1, ..., N$, with standard deviations σ_i and covariance elements $Cov(x_i,x_j) = \lambda_i\lambda_j\sigma_i\sigma_j$. An alternative but equivalent representation of $\mathbf{X}$ is the vector of uncertain parameters

$$\mathbf{Y} = (\sigma_1(\sqrt{1 - \lambda_1^2}Z_1 + \lambda_1 Z_0) + \mu_1, ..., \sigma_n(\sqrt{1 - \lambda_n^2}Z_n + \lambda_n Z_0) + \mu_n)^T$$

where Z_0, Z_1, ..., Z_n are independent standardized normal random variables. This can be verified by calculating the mean, variance, and covariance elements of $\mathbf{Y}$

$$E[\sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i Z_0) + \mu_i] = \mu_i$$

$$Var[\sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i Z_0) + \mu_i] = \sigma_i^2$$

$$Cov[\sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i Z_0) + \mu_i, \sigma_j(\sqrt{1 - \lambda_j^2}Z_j + \lambda_j Z_0) + \mu_j] = \sigma_i\sigma_j\lambda_i\lambda_j$$

which are identical to the respective statistical parameters of the vector $\mathbf{X}$. This means that $\mathbf{Y} \equiv \mathbf{X}$ and thus

$$\Pr\,[\bigcap_i^n(a_i \le x_i \le b_i)] = \Pr\,\{\bigcap_i^n[a_i \le \sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i Z_0) + \mu_i \le b_i]\}$$

Note that Z_0 is the only common random variable shared by the elements of the $\mathbf{Y}$ vector and responsible for the covariances among them. Let z be a realization (outcome) of the random variable Z_0. Assuming that Z_0 realized the value z, then there is no statistical dependence (correlation) between the inequalities and thus

$$\Pr\,\{\bigcap_i^n[a_i \le \sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i z) + \mu_i \le b_i]\} = \prod_{i=1}^n \Pr\,[a_i \le \sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i z) + \mu_i \le b_i]$$

After probability averaging over all possible realizations z of Z_0, we have

$$\Pr\,[\bigcap_i^n(a_i \le x_i \le b_i)] = \Pr\,\{\bigcap_i^n[a_i \le \sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i Z_0) + \mu_i \le b_i]\} = \int_{-\infty}^{+\infty}\prod_{i=1}^n \Pr\,[a_i \le \sigma_i(\sqrt{1 - \lambda_i^2}Z_i + \lambda_i z) + \mu_i \le b_i]\, f(z)\, dz = \int_{-\infty}^{+\infty}\prod_{i=1}^n \Pr\left[\left(\frac{(a_i - \mu_i)/\sigma_i - \lambda_i z}{\sqrt{1 - \lambda_i^2}}\right) \le Z_i \le \left(\frac{(b_i - \mu_i)/\sigma_i - \lambda_i z}{\sqrt{1 - \lambda_i^2}}\right)\right] f(z)\, dz$$

where $f(z)$ is the standardized normal probability density. The deterministic equivalent recasting of the last expression yields

$$\Pr\,[\bigcap_i^n(a_i \le x_i \le b_i)] = \int_{-\infty}^{+\infty}\prod_{i=1}^n \left[\Phi\left(\frac{(b_i - \mu_i)/\sigma_i - \lambda_i z}{\sqrt{1 - \lambda_i^2}}\right) - \Phi\left(\frac{(a_i - \mu_i)/\sigma_i - \lambda_i z}{\sqrt{1 - \lambda_i^2}}\right)\right] f(z)\, dz$$

Note that no restriction on the λ_i's has been imposed; therefore, they can be real or complex numbers (see Appendix C). Switching back to the notation of section 7

$$(x_i \leftarrow \theta_{it},\ a_i \leftarrow -\infty,\ b_i \leftarrow QS_{it},\ \sigma_i \leftarrow \sigma_{it})$$

we recover

$$\Pr\,[\bigcap_{(i,t)\in I_p} QS_{it} \ge \theta_{it}] = \int_{-\infty}^{+\infty}\prod_{(i,t)\in I_p}\left[\Phi\left(\frac{K_{it} - \lambda_{it} z}{\sqrt{1 - \lambda_{it}^2}}\right)\right] f(z)\, dz \ \square$$

Appendix C: ΣA for up to Three Uncertain Parameters

Assuming that $n \le 3$, the joint probability $\Pr[\cap_{i=1}^n(a_i \le x_i \le b_i)]$ can be calculated exactly using the (ΣA) procedure. This is because the 3 × 3 variance−covariance matrix Σ can always be recast in a form which belongs to Ω. Specifically, the 3 × 3 variance−covariance matrix

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{pmatrix}$$

belongs in Ω if the following 3 × 3 system of nonlinear equations

$$\sigma_{12} = \lambda_1\lambda_2\sigma_{11}\sigma_{22}$$

$$\sigma_{13} = \lambda_1\lambda_3\sigma_{11}\sigma_{33}$$

$$\sigma_{23} = \lambda_2\lambda_3\sigma_{22}\sigma_{33}$$

has a solution. Solving for the λ_i's, we obtain

$$\lambda_1 = \frac{1}{\sigma_{11}}\sqrt{\frac{\sigma_{12}\sigma_{13}}{\sigma_{23}}}$$

$$\lambda_2 = \frac{1}{\sigma_{22}}\sqrt{\frac{\sigma_{12}\sigma_{23}}{\sigma_{13}}}$$

$$\lambda_3 = \frac{1}{\sigma_{33}}\sqrt{\frac{\sigma_{13}\sigma_{23}}{\sigma_{12}}}$$

These results demonstrate that when all the covariance elements are positive or when exactly two of the three covariance elements are negative, then the λ_i's are real numbers. However, there are two more cases which need to be considered:

1. One or more of the λ_i are greater than 1.
2. One or all of the three covariance elements are negative.

In the first case, the expression $(1 - \lambda_i^2)^{1/2}$ becomes an imaginary number. In the second case, the λ_i's are no longer real but they become imaginary numbers. However, the ΣA procedure can still be applied as long as the appropriate numerical algorithms are available for handling complex numbers.

For example, consider the vector **X** of three standard normally distributed random variables which are equicorrelated with a correlation coefficient $\rho = -0.2$. The corresponding λ_i are then imaginary numbers equal to $i\sqrt{0.2}$ where i is the complex unit. The joint probability

$$\Pr\left[\bigcap_{i=1,2,3} x_i \le 2\right]$$

is equal to 0.932 (estimated using Monte Carlo simulation). The value of the complex integral,

$$\int_{-\infty}^{+\infty}\prod_{i=1}^{3}\left[\Phi\left(\frac{2 - i\sqrt{0.2}z}{\sqrt{1 - (i\sqrt{0.2})^2}}\right)\right]f(z)\,\mathrm{d}z$$

corresponding to the ΣA procedure, yields the same result 0.93215.

Appendix D: Variance−Covariance Matrix

$$\begin{pmatrix}
1.0 & 0.0 & -0.2 & 0.2 & 0.0 & 0.3 & 0.0 & 0.0 & 0.0 & 0.3 & 0.0 & 0.1 & 0.2 & 0.4 & 0.0 & 0.2 & 0.0 & 0.0 & 0.2 & 0.0 \\
0.0 & 1.0 & 0.0 & 0.0 & 0.3 & 0.0 & 0.0 & 0.6 & 0.2 & 0.4 & 0.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.0 & 0.0 \\
-0.2 & 0.0 & 1.0 & 0.0 & 0.1 & 0.0 & 0.0 & 0.2 & 0.0 & 0.2 & 0.0 & 0.0 & -0.3 & -0.2 & 0.1 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.2 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.2 & 0.0 & 0.2 & 0.0 & 0.3 & 0.2 & 0.0 & 0.2 & 0.0 & 0.1 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.3 & 0.1 & 0.0 & 1.0 & 0.2 & 0.2 & 0.3 & 0.0 & 0.0 & 0.3 & 0.4 & 0.2 & 0.1 & 0.1 & 0.0 & 0.0 & 0.0 & 0.2 & 0.0 \\
0.3 & 0.0 & 0.0 & 0.0 & 0.2 & 1.0 & 0.0 & 0.2 & 0.1 & 0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.2 & 0.0 & 1.0 & 0.2 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.2 & 0.3 & 0.0 & 0.0 & 0.2 & 0.0 & 0.0 \\
0.0 & 0.6 & 0.2 & 0.2 & 0.3 & 0.2 & 0.2 & 1.0 & 0.0 & 0.4 & 0.3 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.1 & 0.2 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.1 & 0.0 & 0.1 & 0.4 & 0.3 & 0.0 & 0.0 & 0.0 \\
0.3 & 0.4 & 0.2 & 0.2 & 0.0 & 0.1 & 0.0 & 0.4 & 0.0 & 1.0 & 0.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.2 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.3 & 0.0 & 0.0 & 0.3 & 0.0 & 0.0 & 1.0 & 0.0 & 0.1 & 0.0 & 0.1 & 0.2 & 0.0 & 0.0 & 0.0 & 0.1 \\
0.1 & 0.2 & 0.0 & 0.3 & 0.4 & 0.0 & 0.0 & 0.0 & 0.0 & 0.2 & 0.0 & 1.0 & 0.1 & 0.0 & 0.0 & 0.0 & 0.3 & 0.0 & 0.0 & 0.0 \\
0.2 & 0.0 & -0.3 & 0.2 & 0.2 & 0.0 & 0.0 & 0.0 & 0.1 & 0.0 & 0.1 & 0.1 & 1.0 & 0.1 & 0.0 & 0.0 & 0.4 & 0.2 & 0.0 & 0.0 \\
0.4 & 0.0 & -0.2 & 0.0 & 0.1 & 0.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.1 & 1.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.1 \\
0.0 & 0.0 & 0.1 & 0.2 & 0.1 & 0.1 & 0.3 & 0.0 & 0.1 & 0.0 & 0.1 & 0.0 & 0.0 & 0.2 & 1.0 & 0.0 & 0.0 & 0.1 & 0.0 & 0.0 \\
0.2 & 0.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.4 & 0.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.2 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.3 & 0.0 & 0.0 & 0.3 & 0.4 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.4 & 0.0 & 0.0 & 0.0 & 0.0 & 0.2 & 0.0 & 0.0 & 0.2 & 0.0 & 0.0 & 0.2 & 0.0 & 0.1 & 0.2 & 0.0 & 1.0 & 0.0 & 0.0 \\
0.2 & 0.0 & 0.0 & 0.0 & 0.2 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.1 & 0.0 & 0.0 & 0.1 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0
\end{pmatrix}$$

Literature Cited

Allen, F. M.; Braswell, R. N.; Rao, P. V. Distribution-free approximations for chance constraints. *Oper. Res.* **1974**, *22*, 610.

Androulakis, I. P.; Maranas, C. D.; Floudas, C. A. αBB: a global optimization method for general constrained nonconvex problems. *J. Global Optim.* **1995**, *7*, 337.

Birewar, D. B.; Grossmann, I. E. Efficient Optimization Algorithms for Zero-Wait Scheduling of Multiproduct Batch Plants. *Ind. Eng. Chem. Res.* **1989**, *28*, 1333.

Birewar, D. B.; Grossmann, I. E. Simultaneous Production Planning and Scheduling in Multiproduct Batch Plants. *Ind. Eng. Chem. Res.* **1990**, *29*, 570.

Brooke, A.; Kendrick, D.; Meeraus, A. *GAMS: A User's Guide*. Scientific Press: Palo Alto, CA, 1988.

Charnes, A.; Cooper, W. W. Normal Deviates and Chance Constraints. *J. Am. Stat. Assoc.* **1962**, *52*, 134.

Deak, I. Multidimensional Integration and Stochastic Programming. In *Numerical Techniques for Stochastic Optimization*; Ermoliev, Y., Wets, J. B., Eds.; Springer-Verlag: New York, 1988.

Diwekar, U. M.; Kalagnanam, J. R. Robust Design Using an Efficient Sampling Technique. *Comput. Chem. Eng.* **1996**, *20* (Suppl. A), S389.

Duran, M. A.; Grossmann, I. E. An outer approximation algorithm for a class of mixed-integer nonlinear programs. *Math. Program.* **1986a**, *36*, 307.

Duran, M. A.; Grossmann, I. E. A mixed-integer nonlinear programming algorithm for process systems synthesis. *AIChE J.* **1986b**, *32*, 592.

Harding, S. T.; Floudas, C. A. Global Optimization in Multiproduct and Multipurpose Batch Design. *Ind. Eng. Chem. Res.* **1997**, *36*, 1644.

Harris, B.; Soms, A. The use of tetrachoric series for evaluating multivariate normal probabilities. *J. Multivar. Anal.* **1980**, *10*, 252.

Ierapetritou, M. G.; Pistikopoulos, E. N. Novel Optimization Approach of Stochastic Planning Models. *Ind. Eng. Chem. Res.* **1994**, *33*, 1930.

Ierapetritou, M. G.; Pistikopoulos, E. N. Batch Plant Design and Operations under Uncertainty. *Ind. Eng. Chem. Res.* **1996**, *35*, 772.

Iyengar, S. Plackett's Identity, Its Generalizations, and Their Uses. In *Multiple Comparisons, Selection, and Applications in Biometry*; Hoppe, F. M., Ed.; Marcel Dekker Inc.: New York, 1993.

Kendall, M. Proof of relations connected to the tetrachoric series and its generalization. *Biometrika* **1941**, *32*, 196.

Kim, M.; Jung, J. H.; Lee, I. Optimal Scheduling of Multiproduct Batch Processes for Various Intermediate Storage Policies. *Ind. Eng. Chem. Res.* **1996**, *35*, 4058.

Liu, M. L.; Sahinidis, N. V. Optimization of Process Planning Under Uncertainty. *Ind. Eng. Chem. Res.* **1996**, *35*, 4154.

Maranas, C. D. Molecular Design Under Property Prediction Uncertainty. *AIChE J.* **1997**, *5*, 1250.

Maranas, C. D.; Floudas, C. A. Finding All Solutions of Nonlinearly Constrained Systems of Equations. *J. Global Optim.* **1995**, *7*, 143.

McDonald, C. M.; Karimi, I. A. Planning and Scheduling of Parallel Semicontinuous processes—Part I: Production Planning. *Ind. Eng. Chem. Res.* **1996**, *36*, 2691.

Miller, B. L.; Wagner, H. M. Chance Constrained Programming with Joint Constraints. *Oper. Res.* **1964**, *13*, 930.

Pantelides, C. C. Unified frameworks for optimal process planning and scheduling. In *Foundations of Computer Aided Process Operations*; Rippin, D. W. T., Hale, J. C., Davis, J. F., Eds.; CACHE: Austin, TX, 1994.

Petkov, S. B.; Maranas, C. D. Quantitative Assessment of Uncertainty in the Optimization of Metabolic Pathways. *Biotechnol. Bioeng.* **1997**, in press.

Pistikopoulos, E. N. Uncertainty in Process Design and Operations. *Comput. Chem. Eng.* **1995**, *19S*, S553.

Pistikopoulos, E. N.; Mazzuchi, T. A. A Novel Flexibility Analysis Approach for Processes with Stochastic Parameters. *Comput. Chem. Eng.* **1990**, *14*, 991.

Plackett, R. Reduction formula for multivariate normal integrals. *Biometrika* **1954**, *41*, 351.

Prekopa, A. *Stochastic Programming*; Kluwer Academic Publishers: Norwell, MA, 1995.

Reinhart, H. J.; Rippin, D. W. T. The Design of Flexible Batch Plants. AIChE Annual Meeting, New Orleans, Nov 1986.

Reinhart, H. J.; Rippin, D. W. T. Design of flexible multi-product plants—a new procedure for optimal equipment sizing under uncertainty. AIChE Annual Meeting, New York, Nov 1987.

Reklaitis, G. V. Overview of scheduling and planning of batch process operations. In *Batchprocessing Systems Engineering*; NATO Advanced Study Institute, Antalya, Turkey, 1992.

Rippin, D. W. T. Batch Process Systems Engineering: A Retrospective and Prospective Review. *Comput. Chem. Eng.* **1993**, *17*, Suppl. S1.

Shah, N.; Pantelides, C. C. Design of Multipurpose Batch Plants with Uncertain Production Requirements. *Ind. Eng. Chem. Res.* **1992**, *31*, 1325.

Slepain, D. The one-sided barrier problem for Gaussian noise. *Bell Syst. Tech. J.* **1962**, *41*, 463.

Straub, D. A.; Grossmann, I. E. Integrated stochastic metric of flexibility for systems with discrete state and continuous parameter uncertainties. *Comput. Chem. Eng.* **1990**, *14*, 967.

Straub, D. A.; Grossmann, I. E. Evaluation and Optimization of Stochastic Flexibility in Multiproduct Batch Plants. *Comput. Chem. Eng.* **1992**, *16*, 69.

Subrahmanyam, S.; Pekny, J. F.; Reklaitis, G. V. Design of Batch Chemical Plants under Market Uncertainty. *Ind. Eng. Chem. Res.* **1994**, *33*, 2688.

Tong, Y. L. *Probability Inequalities for Multivariate Distributions*; Academic Press: New York, 1980.

Tong, Y. L. *The Multivariate Normal Distribution*; Springer-Verlag: New York, 1990.

Watanabe, T.; Ellis, H. A joint chance−constrained programming model with row dependence. *Eur. J. Oper. Res.* **1994**, *77*, 325.

Wellons, H. S.; Reklaitis, G. V. The design of multiproduct batch plants under uncertainty with staged expansion. *Comput. Chem. Eng.* **1989**, *13*, 115.

Wilks, S. S. *Mathematical Statistics*; John Wiley & Sons, Inc.: New York, 1962.

Received for review April 3, 1997
Revised manuscript received August 8, 1997
Accepted August 10, 1997[⊗]

IE970259Z

[⊗] Abstract published in *Advance ACS Abstracts,* October 1, 1997.