Optimal Procurement Contract Selection with Price Optimization under Uncertainty for Process Networks

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Abstract

In this work, we propose extending the production planning decisions of a chemical process network to include optimal contract selection under uncertainty with suppliers and product selling price optimization. We use three quantity-based contract models: discount after a certain purchased amount, bulk discount, and fixed duration contracts. We propose the use of general regression models to describe the relationship between selling price, demand, and possibly other predictors, such as economic indicators. For illustration purposes, we consider three demand-response models (i.e., selling price as a function of demand) that are typically encountered in the literature: linear, constant-elasticity, and logit. We develop a mixed-integer nonlinear two-stage stochastic programming that accounts for uncertainty in both supply (e.g., raw material spot market price) and demand (random nature of the residuals of the regression models) for the planning of the process network. The proposed method is illustrated with two numerical examples of chemical process networks.

Keywords: Optimal Contract Selection, Price Optimization, Uncertainty, Process Network Production Planning
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1. Introduction

Manufacturing enterprises deal with uncertainty from both internal and external sources. Internally, production variability due to unplanned events may prevent the company to achieve its demand-driven production targets. Externally, fluctuations in supply and demand as well as market economic conditions pose challenges to efficient operation of the supply chain. One way to reduce the level of uncertainty on both the supply and the customer sides, and that is typically used by companies, is by making contractual agreements. In the context of this paper, a contract is a binding agreement in which the seller provides the specified product and the buyer pays for it under specific terms and conditions.

A different approach to managing uncertainty is pricing analytics, also known as price optimization. In formulating such a problem, selling prices become decision variables, and the demand of a product is modeled as a function of its price. Nonetheless, this still typically

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does not completely eliminate uncertainty, since stochastic environmental, economic, and market conditions remain uncontrollable by the manufacturing company.

In this paper, we combine the aforementioned uncertainty management strategies in a two-stage stochastic optimization model for multi-period, multi-site tactical production planning. Uncertain parameters include raw material and finished product price and availability/demand. We propose a manufacturer-centric approach in which the purchase contract structures are set by suppliers, and it is the manufacturer's decision to select which contract, if any, to sign. In addition, the manufacturer sets the selling price of its main products that may be used to design sales contracts with its customers. However, it is the customer's decision to select the sales contracts, if any, designed by the manufacturer. The contract design problem is not addressed in this paper, but is discussed as a future work. We demonstrate how different pricing models, linear and nonlinear, can be used within the proposed optimization framework. Throughout this paper, we refer to price as *unit* price (e.g., \$/kg, \$/t, etc.).

The paper is organized as follows. Section 2 provides a literature review of contract modeling and selection and price optimization. Section 3 defines the problem under investigation and states the model assumptions. Section 4 describes the deterministic production planning model, the contract selection and price optimization elements of the planning model, and the stochastic optimization model. Two numerical examples are discussed in Section 5 followed by a discussion on reformulations. Finally, conclusions and suggested extensions of the proposed approach are presented in Section 6.

2. Literature Review

2.1. Contract Modeling and Selection

Tsay et al. (1999) provide a literature review on contracts from a modeling perspective. The authors classify the literature on contracts in the context of Supply Chain Management (SCM) by eight contract clauses: (a) specification of decision rights, (b) pricing, (c) minimum purchase commitments, (d) quantity flexibility, (e) buyback or returns policies, (f) allocation rules, (g) lead time, and (h) quality. Moreover, Höhn (2010) discusses some model extensions and other contract types based on finance theories, such as auction and real options.

Even though the modeling of contracts has been addressed by different communities, including operations research and management science, economics, and finance, the optimal selection of contracts has received relatively less attention in the literature. The contract selection problem can be defined as follows: given the structure (price and quantity or volume) of the different contract types, the multi-period optimization model has to select which contracts to use. We present some specific examples of this problem that are relevant to the Process Systems Engineering (PSE) community.

Park et al. (2006) used disjunctive programming to model three types of quantity-based contracts that a company may sign with suppliers and customers. The production planning and capacity expansion decisions are augmented by the selection of contracts. The disjunctions are reformulated resulting in a tight Mixed-Integer Linear Programming (MILP) formulation. Bansal et al. (2007) modeled quantity- and price-based contracts and coupled their selection with a multi-period optimization model for the minimization of total procurement costs of a multinational company (buyer). Khalilpour and Karimi (2011) developed a multi-period optimization model to minimize total procurement cost applied to liquefied natural gas (LNG) value chain. The model selects LNG contracts that are modeled with price formulations, flexibility, duration, quality, quantity, commitment, discount, and other terms and conditions. We note that the aforementioned works have only considered deterministic formulations.

Some authors, however, have considered uncertainty in the contract selection problem. For instance, Rodríguez and Vecchietti (2009) addressed the delivery and purchase optimization in a supply chain under provision uncertainty. Quantity-based contracts were modeled with disjunctions and logic restrictions, and the uncertain amount delivered by the suppliers is modeled with a decision tree approach that represents supplier failure discrete probability distributions. Rodríguez and Vecchietti (2012) proposed a mid-term planning model with sales contracts. Piece-wise linear price-response models were used to model demand as a function of selling price. If no sales contract is signed, then safety stock is considered to deal with demand uncertainty. Feng et al. (2013) developed a two-stage stochastic programming model with fixed recourse to coordinate contract selection and capacity allocation in a three-tier manufacturing supply chain in the oriented strand board industry. The uncertain parameters include price and quantity (availability and demand) of materials.

2.2. Pricing Analytics

Pricing decisions have been discussed in the revenue management literature and constitute one set of demand-management decisions that can be made by a firm (Talluri and van Ryzin, 2005). Some examples of pricing decisions include setting posted prices, individual-offer prices, and reserve prices (in auctions), pricing across product categories, pricing over time, and discounting over the product lifetime.

By treating selling price as an additional degree of freedom, a company can adjust its prices in order to maximize its overall profitability. The typical modeling approach reported in the literature is the use of a price-response model $d(p)$, which specifies demand d for the product of a single seller as a function of the price p offered by that seller (Phillips, 2005; Bodea and Ferguson, 2014). More details on pricing models are given in Subsection 4.3.

Several papers address pricing problems whose optimization model only contains continuous decision variables, and is sometimes unconstrained (e.g., maximization of profit). For such problems, analytical expressions for the optimal pricing scheme can be derived (Chong and Cheng, 1975; Pasche, 1998; Lobo and Boyd, 2003; Thiele, 2005). Some counterexamples include the following works. Kaplan et al. (2011) used a constant price elasticity model in a multi-period, multi-echelon supply chain optimization model. Such pricing model results in a nonlinear, but concave, objective function, and the authors proposed a reformulation to account for unbounded derivatives. Lin and Wu (2014) formulated a two-stage stochastic programming model and used a linear pricing model. The authors observed that as the variance of the demand distribution increases, the manufacturer will increase its inventory to levels that are greater than the anticipated demand to prevent the potential loss of sales and will simultaneously raise product prices to obtain a greater profit. Gjerdrum et al. (2001) developed a mixed-integer nonlinear programming (MINLP) model to for the optimal calculation of *transfer prices* for the supply chain optimization involving multiple enterprises. The authors used game theoretical Nash-type models to obtain a fair, optimized profit distribution between members of multienterprise supply chains.

Based on the review of previous work, it is clear that integrating contract selection and price optimization with general pricing models in the optimization of process networks under uncertainty has not been addressed before.

3. Problem Statement

The supply chain structure considered in this paper is shown in Figure 1. The manufacturer owns one or multiple production sites that may be situated at different geographic locations. The key decisions of the manufacturing company include: (1) selection of procurement contracts, and (2) set selling product prices. The manufacturer-centric approach taken in this work means that the contract structure (prices and quantity thresholds) are specified, and it is ultimately the manufacturer's decision to sign or not a particular type of contract for a raw material. Moreover, the manufacturer can use price- or demand-response models to set the price of its finished products.

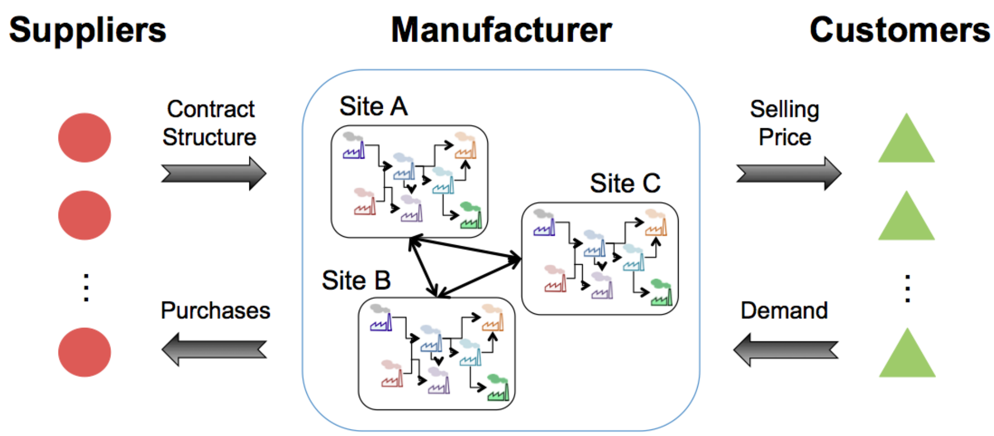


Figure 1: Supply chain structure considered in this work.

The following assumptions are considered:

- The contract structure is given and fixed (see Subsection 4.2), i.e., no negotiation between supplier and manufacturer is allowed;
- Operating, inventory, and inter-site transfer costs are given and deterministic;
- A price- or demand-response model (see Subsection 4.3) is given. A price-response model expresses demand as function of price (i.e., $d(p)$), whereas a demand-response model provides the inverse relationship (i.e., $p(d)$).

4. Production Planning Model

4.1. Deterministic Model

We begin by describing the deterministic multi-period, multi-site production planning model is described as follows. It extends the short-term planning model described in Park et al. (2006) by accounting for multiple sites. The procurement contract and pricing models are described in Subsection 4.2 and Subsection 4.3. Lastly, the stochastic programming model is discussed is Subsection 4.4.

Nomenclature

Indices

i Process or chemical plant

j Chemical

s Site

t Time period

Sets

IS_s Set of processes that belong to site s

JM_i Set of main products of process i

JP Set of products

JR Set of raw materials

I Set of processes or chemical plants

I_j Set of processes that consume chemical j

J_i Set of chemicals involved in process i

O_j Set of processes that produce chemical j

ST Set of sites

T Set of time periods

Parameters

$\alpha_{j,s,t}^{\mathrm{spot}}$ Spot market price of raw material j to site s at time period t

$\delta_{i,s,t}$ Operating cost of process i in site s at time period t

$\eta_{j,s,s',t}$ Inter-site transfer cost of chemical j from site s to site s' at time period t

$\mu_{i,j,s}$ Mass factor of product j in process i in site s

$\xi_{j,s,t}$ Inventory cost of chemical j in site s at time period t

$a_{j,s,t}^{\mathrm{L}}$, $a_{j,s,t}^{\mathrm{U}}$ Lower and upper bounds on availability of raw material j to site s at time period t

$F_{j,s,s',t}^{\mathrm{U}}$ Upper bound on inter-site transfer of chemical j from site s to site s' at time period t

$Q_{i,s,t}$ Production capacity of process i in site s at time period t

$V^{\mathrm{U}}_{j,s,t}$ Upper bound on inventory of chemical j in site s at time period t

Variables

$\mathrm{COST}^{c}_{j,s,t}$ Procurement cost for raw material j in site s at time period t and contract type c

$\mathrm{COST}_{j,t}$ Purchase costs of raw material j in time period t

PROFIT Objective function variable representing the profit of the production planning model

$\mathrm{SALES}_{j,t}$ Sales of product j in time period t

$F_{j,s,s',t}$ Inter-site transfer amount of product j from site s to site s' at time t

$P_{j,s,t}$ Purchase amount of raw material j by site s at time period t

$P^{\mathrm{spot}}_{j,s,t}$ Spot market component of purchase amounts of raw material j by site s in time period t

$P^{c}_{j,s,t}$ Contract component of purchase amounts of raw material j by site s in time period t and contract type c

$S_{j,t}$ Aggregated sales amount of product j for all sites at time t

$SS_{j,s,t}$ Sales amount of product j from site s at time t

$V_{j,s,t}$ Inventory level of chemical j in site s at time t

$W_{i,j,s,t}$ Amount of chemical j consumed or produced in process i in site s at time t

The objective function to be maximized is the profit of the overall production planning decisions as given in equation (1). The first term is the revenue obtained from sales for all products j and time periods t. The second term is the overall purchase costs from the spot market and/or contracts. These two terms will be defined later. The third term accounts for the operating costs of plant i in each site s. The fourth term is the total inventory cost. The final term accounts for the inter-site transfer costs.

$$\begin{aligned}\mathrm{PROFIT} = &\sum_{j\in\mathrm{JP}}\sum_{t\in T}\mathrm{SALES}_{j,t} - \sum_{j\in\mathrm{JR}}\sum_{t\in T}\mathrm{COST}_{j,t} - \sum_{s\in ST}\sum_{i\in\mathrm{IS}_s}\sum_{j\in\mathrm{JM}_i}\sum_{t\in T}\delta_{i,s,t}W_{i,j,s,t} \\ &- \sum_{j\in J}\sum_{s\in ST}\sum_{t\in T}\xi_{j,s,t}V_{j,s,t} - \sum_{s\in ST}\sum_{\substack{s'\in ST\\ s'\neq s}}\sum_{j\in J}\sum_{t\in T}\eta_{j,s,s',t}F_{j,s,s',t} \end{aligned} \tag{1}$$

A simple input-output relationship is used to model the chemical processes as shown in equation (2). The mass factor $\mu_{i,j,s}$ (positive for inputs, negative for outputs) is defined for the main products j of process i. The process capacity is enforced in equation (3).

$$W_{i,j,s,t} = |\mu_{i,j,s}|W_{i,j',s,t} \qquad \forall\ s\in ST,\ i\in\mathrm{IS}_s,\ j\in J_i,\ j'\in\mathrm{JM}_i,\ t\in T \tag{2}$$

$$W_{i,j,s,t} \leq Q_{i,s,t} \qquad \forall\ s\in ST,\ i\in\mathrm{IS}_s,\ j\in\mathrm{JM}_i,\ t\in T \tag{3}$$

Raw material availability is represented by equation (4).

$$a^{\mathrm{L}}_{j,s,t} \le P_{j,s,t} \le a^{\mathrm{U}}_{j,s,t} \qquad \forall\, s \in ST,\ j \in \mathrm{JR},\ t \in T \tag{4}$$

A material balance for each chemical j in every site s at time period t is given by equation (5). The sales amount for each site, $SS_{j,s,t}$, is aggregated to all sites in equation (6).

$$V_{j,s,t-1} + \sum_{i \in O_j} W_{i,j,s,t} + P_{j,s,t} = V_{j,s,t} + \sum_{i \in I_j} W_{i,j,s,t} + \sum_{\substack{s' \in ST \\ s' \neq s}} F_{j,s,s',t} + SS_{j,s,t} \quad \forall\, s \in ST,\ j \in J,\ t \in T \tag{5}$$

$$S_{j,t} = \sum_{s \in ST} SS_{j,s,t} \qquad \forall\, j \in J,\ t \in T \tag{6}$$

Upper bounds on inventory levels and inter-site transfers are represented by equations (7) and (8).

$$V_{j,s,t} \le V^{\mathrm{U}}_{j,s,t} \qquad \forall\, s \in ST,\ j \in J,\ t \in T \tag{7}$$

$$F_{j,s,s',t} \le F^{\mathrm{U}}_{j,s,s',t} \qquad \forall\, (s, s') \in ST,\ s \neq s',\ j \in J,\ t \in T \tag{8}$$

The purchase cost term in the objective function, $\mathrm{COST}_{j,t}$, is defined in the next subsection.

4.2. Procurement Contract Models

We use the same three contract types described in Park et al. (2006): discount after a certain purchased amount, bulk discount, and fixed duration contracts. These contract types are modeled with disjunctions and reformulated using the convex hull approach as mixed-integer linear programming (MILP) constraints. In this work, we employ the same reformulated constraints presented in the original paper with the only difference being that all variables have an additional index s for sites (see AppendixA). Figure 2 illustrates the three contract types considered in this work.

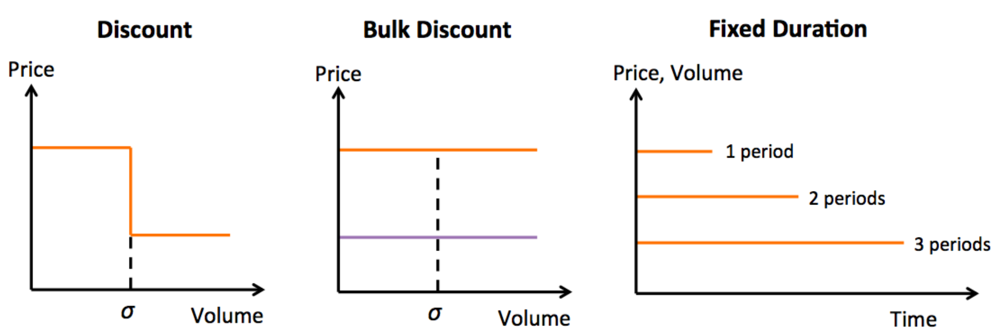


Figure 2: Schematic of contract types. **Discount**: pay higher price for quantity up to threshold value σ, and pay discounted price for any amount beyond σ. **Bulk Discount**: if purchased amount exceeds threshold value σ, then pay discounted price; otherwise, pay higher price. **Fixed Duration**: pay discounted price according to contract term duration.

Let $c \in C$ denote a contract type. The total purchased amount and total procurement cost have two components, market (spot) and contract with supplier. The former is subject to uncertainty as will be discussed later. Equations (9) and (10) are used to calculate these two quantities, respectively.

$$P_{j,s,t} = P^{\text{spot}}_{j,s,t} + \sum_{c\in C} P^{c}_{j,s,t} \qquad \forall\, s\in ST,\ j\in \text{JR},\ t\in T \tag{9}$$

$$\text{COST}_{j,t} = \sum_{s\in ST}\left[\alpha^{\text{spot}}_{j,s,t}P^{\text{spot}}_{j,s,t} + \sum_{c\in C}\text{COST}^{c}_{j,s,t}\right] \qquad \forall\, j\in \text{JR},\ t\in T \tag{10}$$

where $\text{COST}^{c}_{j,s,t}$ is the procurement cost of contract type c for raw material j in site s at time period t. Expressions for $\text{COST}^{c}_{j,s,t}$ for each contract type c are given in Park et al. (2006) and can be found in AppendixA.

4.3. Price Optimization Models

As mentioned in the literature review (Subsection 2.2), the main goal in price optimization is for a company to set and adjust its prices to maximize profitability. Pricing decisions rely on price-response models (PRMs) usually denoted by $d(p)$, where p is the price of a product and d is the expected demand for that product and its given price. As commonly treated in the literature, we use demand and sales interchangeably as we assume that the manufacturer has enough capacity to meet its customer demand. Three PRMs typically encountered in the literature are given in Table 1.

Table 1: Typical price-response models (PRMs).

Model	**Equation**
Linear	$d(p) = \beta_0 - \beta_1 p$
Constant-Elasticity	$d(p) = \beta_2 p^{-E_d}$
Logit	$d(p) = \dfrac{\beta_3 e^{-(\beta_4+\beta_5 p)}}{1+e^{-(\beta_4+\beta_5 p)}}$

The different βs are estimated parameters (e.g., from a regression analysis), and E_d is the price elasticity of demand, which is a measure used in economics to show the responsiveness, or elasticity, of the quantity demanded of a good or service to a change in its price. Using the definition of point elasticity, $E_d(p) = -d'(p)p/d(p)$, for $p > 0$, one can relate the βs with the elasticity (see Phillips (2005)). Note that the maximum demand (at $p = 0$) predicted by each PRM in Table 1 is given as follows: linear, $d(0) = \beta_0$; constant-elasticity, $d(0) \to \infty$ for the vast majority of goods ($E_d \geq 0$); logit, $d(0) = \frac{\beta_3 e^{-\beta_4}}{1+e^{-\beta_4}}$.

We note that for typical production planning models, the sales flow decision variable appears in both constraints and objective function. Therefore, the choice of a nonlinear PRM results in nonlinear terms in both constraints (e.g., equation (5)) and objective function (in the form of selling price $\times$ sales). In order to restrict nonlinear terms to the objective function, it may be advantageous to use demand-response models (DRMs), i.e., $p(d)$. The PRMs described in Table 1 can be inverted to DRMs as shown in Table 2.

Table 2: Typical demand-response models (DRMs).

Model	Equation
Linear	$p(d) = \beta_0' - \beta_1' d$
Constant-Elasticity	$p(d) = \beta_2' d^{-1/E_d}$
Logit	$p(d) = \dfrac{1}{\beta_5}\left[\ln\left(\dfrac{\beta_3 - d}{d}\right) - \beta_4\right]$

The following relationships hold: $\beta_0' = \frac{\beta_0}{\beta_1}$, $\beta_1' = \frac{1}{\beta_1}$, and $\beta_2' = \beta_2^{1/E_d}$. Note that, in the logit DRM case, the maximum demand must be less than β_3 in order to avoid violating the domain of the logarithm function. For implementation purposes, we set the upper bound of the demand (or sales) variable to $\min\left\{0.99\beta_3, \frac{\beta_3 e^{-\beta_4}}{1+e^{-\beta_4}}\right\}$, where the second argument of the min operator is numerically equal to $d(0)$.

Therefore, the sales term (selling price $\times$ sales flow, i.e., $p(d) \times d$) in the objective function in equation (1) for each DRM (linear, constant-elasticity, and logit) is given in equations (11)–(13).

$$\text{SALES}_{j,t} = \beta_0' S_{j,t} - \beta_1' S_{j,t}^2 \qquad \forall\, j \in \text{JP},\ t \in T \tag{11}$$

$$\text{SALES}_{j,t} = \beta_2' S_{j,t}^{1-1/E_j} \qquad \forall\, j \in \text{JP},\ t \in T \tag{12}$$

$$\text{SALES}_{j,t} = \frac{1}{\beta_5}\left[\ln\left(\frac{\beta_3 - S_{j,t}}{S_{j,t}}\right) - \beta_4\right] S_{j,t} \qquad \forall\, j \in \text{JP},\ t \in T \tag{13}$$

We note that the linear DRM yields a concave quadratic term in the objective function, the constant-elasticity DRM results in a nonlinear, but concave term for $E_j > 1$ (elastic products) and nonlinear, nonconvex term for $0 < E_j < 1$ (inelastic products), and the logit DRM yields, in principle, a general nonlinear, nonconvex term. We show in AppendixB that the logit DRM results in a concave term for specific conditions on its parameters.

Remark. Even though the PRMs (DRMs) listed in Table 1 (Table 2) are typically used in the literature, we argue that general, and likely more complex regression models can be employed to model the relationship between selling price, demand, and possibly additional predictors. For instance, a more general, multiple linear PRM is given in equation (14),

$$d(X) = \beta_0 + \sum_{i=1}^{m} \beta_i X_i \tag{14}$$

where the βs are parameters to be estimated, and X_i, $i = 1, \ldots m$, are predictors (or regressors). Examples of predictors in addition to the selling price p may include raw material prices, economic indicators (e.g., gross domestic product), crude oil and other product prices as well as their time-lagged values. Note that the multiple linear PRM can also be inverted to a multiple linear DRM generally denoted by $p(X)$.

Nonlinear PRMs or DRMs may capture more accurately the relationship between predictors and the response variable at the expense of yielding a (mixed-integer) nonlinear production planning model. General parametric, semi-parametric, or nonparametric nonlinear models can be employed. An alternative to pre-specifying regression models is Symbolic Regression (also known as Genetic Programming) (Koza, 1992), which is a technique to generate general regression models from data via evolutionary programming concepts.

4.4. Stochastic Programming Model

The previous two subsections presented ways to anticipate the uncertainty in the production planning decision-making process. However, the uncertainty in the market remains regardless if the manufacturer signs contracts with suppliers (and/or customers). Moreover, the predictive accuracy of demand-response models (DRMs) is not guaranteed to be perfect. In this subsection, we extend the deterministic optimization model presented in Subsection 4.1 by including sources of uncertainty in both supply and demand sides.

We propose a scenario-based two-stage stochastic programming framework (Birge and Louveaux, 2011) to explicitly account for uncertainty in spot market prices of raw materials and the predictability of DRMs. More specifically, we describe a multi-period, two-stage stochastic programming model whose first-stage decisions are the selection of contracts (discrete decisions) and the selling prices (which determine sales flows), and second-stage decisions include the remaining flows and inventory levels in the network.

Let $k \in K$ represent the index and discrete set of scenarios used to approximate the possible realizations of the uncertain parameters. From equations (9) and (10), the total purchase amount and cost may have two contributions: spot market and signed contracts. Contractual agreements are considered deterministic and fixed, and must be honored if selected. The volatility in the market is then represented by raw material prices. Therefore, the corresponding scenario-based constraints are given by

$$P_{j,s,t,k} = P^{\text{spot}}_{j,s,t,k} + \sum_{c \in C} P^{c}_{j,s,t} \qquad \forall\, s \in ST,\ j \in \text{JR},\ t \in T,\ k \in K \tag{15}$$

$$\text{COST}_{j,t,k} = \sum_{s \in ST} \left[\alpha^{\text{spot}}_{j,s,t,k} P^{\text{spot}}_{j,s,t,k} + \sum_{c \in C} \text{COST}^{c}_{j,s,t} \right] \qquad \forall\, j \in \text{JR},\ t \in T,\ k \in K \tag{16}$$

Spot market prices of raw material are typically predicted using time series models. The literature on time series analysis is extensive and includes linear, nonlinear, parametric, semi-parametric, and nonparametric models (Brockwell and Davis, 2002; Fan and Yao, 2002; Box et al., 2008). Figure 3 illustrates the simulation of time series models that can be used to generate scenarios.

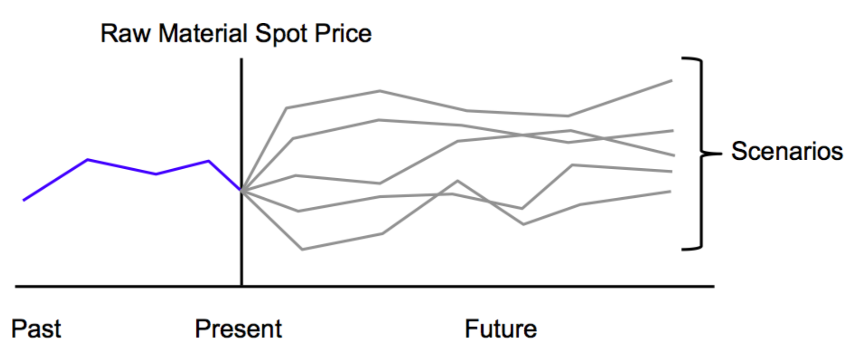


Figure 3: Time series model simulation for scenario generation.

For the demand side, the uncertainty in demand or selling price can be quantified by the distribution of residuals of the regression models as illustrated in Figure 4. By construction, the residuals must be independent and identically distributed (i.i.d.), have zero mean and constant variance, and be uncorrelated with each other. Additional assumptions are typically used, e.g., the residuals follow a normal distribution with zero mean and known variance σ^2.

$$p(d) = \underbrace{f(d)}_{\text{Deterministic}} + \underbrace{\epsilon}_{\text{Stochastic}}$$

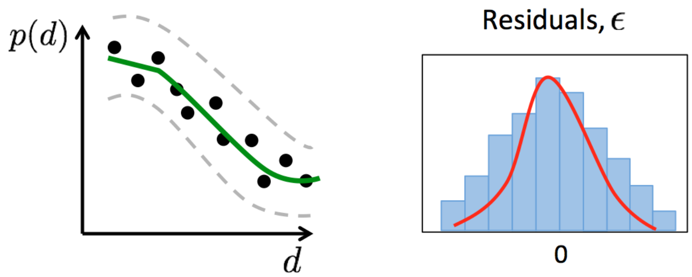


Figure 4: Deterministic and stochastic components of a regression-based demand-response model (DRM). The region delimited by the dashed lines on the left plot represents possible realizations of price values according to the probabilistic nature of the residuals, ϵ. The distribution of the residuals can be sampled to generate scenarios.

A scenario-based version of a general DRM can be written for a particular realization of the residuals (scenario k) as follows:

$$p(d) = f(d) + \epsilon_k$$

Therefore, the scenario-based version of the sales term in the objective function (equation (1)) of each DRM listed in Table 2 is given as follows:

- Linear:

$$\text{SALES}_{j,t,k} = (\beta_0' - \beta_1' S_{j,t} + \epsilon_k) S_{j,t} = \beta_0' S_{j,t} - \beta_1' S_{j,t}^2 + S_{j,t}\epsilon_k \tag{17}$$

- Constant-Elasticity:

$$\text{SALES}_{j,t,k} = (\beta_2' S_{j,t}^{-1/E_j} + \epsilon_k) S_{j,t} = \beta_2' S_{j,t}^{1-1/E_j} + S_{j,t}\epsilon_k \tag{18}$$

- Logit:

$$\text{SALES}_{j,t,k} = \left\{ \frac{1}{\beta_5} \left[\ln\left(\frac{\beta_3 - S_{j,t}}{S_{j,t}} \right) - \beta_4 \right] + \epsilon_k \right\} S_{j,t} = \frac{1}{\beta_5} \left[\ln\left(\frac{\beta_3 - S_{j,t}}{S_{j,t}} \right) - \beta_4 \right] S_{j,t} + S_{j,t}\epsilon_k \tag{19}$$

As mentioned in the remark at the end of the previous subsection, when using a general (and possibly nonlinear) DRM denoted by $p(X)$, where X is a vector of predictors including $S_{j,t}$ and potentially others, the sales term can be written similarly as for the three special cases considered in this paper. That is, a sample of the residual distribution, ϵ_k, is added to the deterministic part of the model $p(X)$ and the result is multiplied by $S_{j,t}$.

Both deterministic and stochastic models are mixed-integer programming (MIP) problems. For linear DRMs, they are concave MIQP models, and for constant-elasticity and logit DRMs, they are concave and separable MINLP models depending on the values of the parameters in the DRMs. The complete deterministic equivalent model for the stochastic formulation is given by the following general MINLP model:

$$\max \mathbb{E}\,[\text{PROFIT}] = \sum_{k \in K} \pi_k \Bigg[\sum_{j \in \text{JP}} \sum_{t \in T} \text{SALES}_{j,t,k} - \sum_{j \in \text{JR}} \sum_{t \in T} \text{COST}_{j,t,k} - \sum_{s \in ST} \sum_{i \in \text{IS}_s} \sum_{j \in \text{JM}_i} \sum_{t \in T} \delta_{i,s,t} W_{i,j,s,t,k} - \sum_{j \in J} \sum_{s \in ST} \sum_{t \in T} \xi_{j,s,t} V_{j,s,t,k} - \sum_{s \in ST} \sum_{\substack{s' \in ST \\ s' \neq s}} \sum_{j \in J} \sum_{t \in T} \eta_{j,s,s',t} F_{j,s,s',t,k} \Bigg] \tag{20}$$

subject to

$$W_{i,j,s,t,k} = |\mu_{i,j,s}| W_{i,j',s,t,k} \qquad \forall\, s \in ST,\ i \in \text{IS}_s,\ j \in J_i,\ j' \in \text{JM}_i,\ t \in T,\ k \in K \tag{21}$$

$$W_{i,j,s,t,k} \leq Q_{i,s,t} \qquad \forall\, s \in ST,\ i \in \text{IS}_s,\ j \in \text{JM}_i,\ t \in T,\ k \in K \tag{22}$$

$$a^{\text{L}}_{j,s,t} \leq P_{j,s,t,k} \leq a^{\text{U}}_{j,s,t} \qquad \forall\, s \in ST,\ j \in \text{JR},\ t \in T,\ k \in K \tag{23}$$

$$V_{j,s,t-1,k} + \sum_{i \in O_j} W_{i,j,s,t,k} + P_{j,s,t,k} = V_{j,s,t,k} + \sum_{i \in I_j} W_{i,j,s,t,k} + \sum_{\substack{s' \in ST \\ s' \neq s}} F_{j,s,s',t,k} + SS_{j,s,t} \qquad \forall\, s \in ST,\ j \in J,\ t \in T,\ k \in K \tag{24}$$

$$P_{j,s,t,k} = P^{\text{spot}}_{j,s,t,k} + \sum_{c \in C} P^{c}_{j,s,t} \qquad \forall\, s \in ST,\ j \in \text{JR},\ t \in T,\ k \in K \tag{25}$$

$$\text{COST}_{j,t,k} = \sum_{s \in ST} \left[\alpha^{\text{spot}}_{j,s,t,k} P^{\text{spot}}_{j,s,t,k} + \sum_{c \in C} \text{COST}^{c}_{j,s,t} \right] \qquad \forall\, j \in \text{JR},\ t \in T,\ k \in K \tag{26}$$

$$S_{j,t} = \sum_{s \in ST} SS_{j,s,t} \qquad \forall\, j \in J,\ t \in T \tag{27}$$

$$V_{j,s,t,k} \leq V^{\text{U}}_{j,s,t} \qquad \forall\, s \in ST,\ j \in J,\ t \in T,\ k \in K \tag{28}$$

$$F_{j,s,s',t,k} \leq F^{\mathrm{U}}_{j,s,s',t} \qquad \forall\, (s,s') \in ST,\ s \neq s',\ j \in J,\ t \in T,\ k \in K \tag{29}$$

Contract selection constraints: Equations (A.1) to (A.18) (see AppendixA)

$$W_{i,j,s,t,k}, V_{j,s,t,k}, F_{j,s,s',t,k}, P_{j,s,t,k}, S_{j,t}, SS_{j,s,t} \geq 0$$
$$y^c_{j,s,t} = \{0,1\}$$

where π_k is the probability of scenario k, $\mathrm{SALES}_{j,t,k}$ which involves nonlinear terms, is given by equation (17), (18), or (19), and $y^c_{j,s,t}$ represent the binary variables for the selection of contracts (AppendixA). For illustration purposes, we will assume in the numerical examples that all scenarios have the same probability. Data-based scenario tree generation techniques can be used to calculate not only the probabilities of scenarios, but also the values of the outcomes in order to match statistical properties of historical and forecast data (Calfa et al., 2014).

5. Numerical Examples

To illustrate our proposed approach, we consider the two following examples. The first example involves a single site with three chemical plants, one raw material, one intermediate product, and two finished products. The same demand-response model (DRM) is used for both finished products. The second example considers a larger process network with 38 processes and 28 chemicals. In Subsection 5.3, we present a reformulation of the mixed-integer nonlinear programming (MINLP) models that decreases the solution times.

All optimization models were implemented in AIMMS 4.3 (Roelofs and Bisschop, 2014) and solved on a desktop computer with the following specifications: Dell Optiplex 990 with 4 Intel® Core™ i7-2600 CPUs at 3.40 GHz (total 8 threads), 8 GB of RAM, and running Windows 7 Enterprise. The mixed-integer quadratic (MIQP) solver used was GUROBI 6.0. The mixed-integer nonlinear programming (MINLP) models were solved using the convex AOA algorithm implemented in AIMMS. AOA stands for AIMMS Outer Approximation, which implements an outer approximation algorithm that alternates between the solution of a master problem (MILP) and a subproblem (NLP) (Duran and Grossmann, 1986). The MILP and NLP solvers used were GUROBI 6.0 and CONOPT 3.14V, respectively. The convex AOA algorithm is based on the work by Quesada and Grossmann (1992) and is described in Hunting (2012). The lower bound for the total sales variables, $S_{j,t}$, was set to 0.1. Time series analysis was performed in the `R` programming language (R Core Team, 2014) with the `forecast` package (Hyndman et al., 2014). We conclude this section by proposing a reformulation of the MINLP models that considerably reduces the solution times.

5.1. Example 1: Small Process Network

The process network for Example 1 is shown in Figure 5. It consists of raw material A, an intermediate product B, finished products C and D (only product D can be stored), and processes (plants) P1, P2, and P3. A time horizon consisting of 6 time periods (months) is considered. All data for this example can be found in AppendixC.

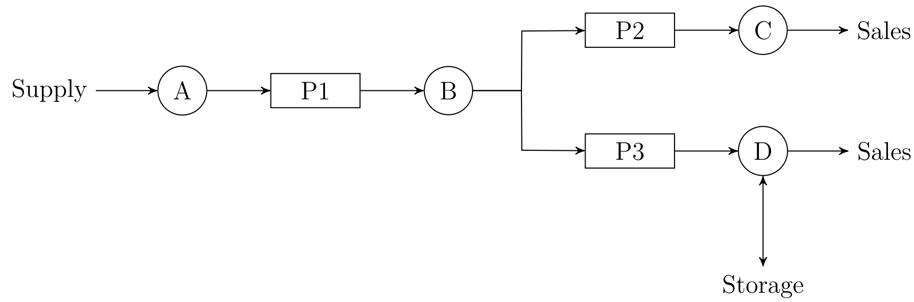


Figure 5: Process network for Example 1.

The stochastic programming model has ten scenarios and was solved using its deterministic equivalent formulation. The values of the spot market prices, $\alpha^{\text{spot}}_{j,s,t,k}$, for raw material A were generated from a simulation of a seasonal autoregressive integrated moving average (ARIMA) time series model, which is shown in Figure 6. In this figure, a forecasting model (solid line) was fitted to observed spot market prices (circles) of monthly data from 2011 to the fifth month of 2013. The predicted prices that compose the scenarios (red dotted lines) lie in the shaded regions (darker region means 80% prediction intervals, lighter region means 95% prediction intervals). Only three scenarios are displayed in order to illustrate the simulation results.

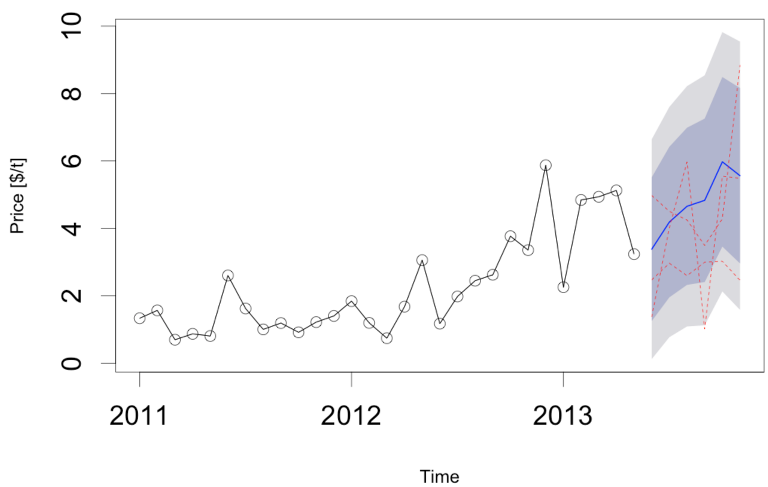
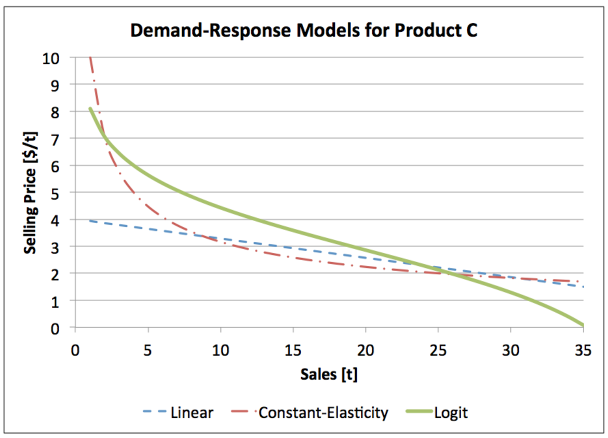


Figure 6: Simulated scenarios (red dotted lines in the shaded region) for the spot market prices of raw material A. Mean forecast is represented by blue solid line in the shaded region.

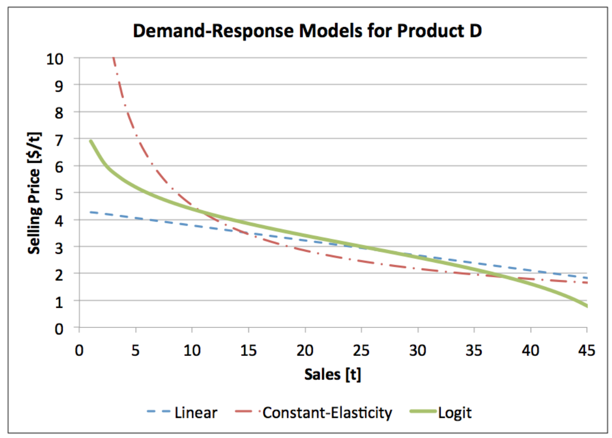
Three demand-response models (DRMs) were considered: linear, constant-elasticity, and logit. The parameters for each DRM are shown in Table 3, and the three DRMs are illustrated in Figure 7. The stochastic part of the DRMs for products C and D is assumed to be normally distributed, $\mathrm{N}(0,1)$ and $\mathrm{N}(0,2)$, respectively.

Table 3: Parameter values for the DRMs in Example 1.

DRM	Product C	Product D
Linear	$\beta_0' = 4.00\,\$/\mathrm{t}$ $\beta_1' = 0.07\,\$/\mathrm{t}^2$	$\beta_0' = 4.33\,\$/\mathrm{t}$ $\beta_1' = 0.06\,\$/\mathrm{t}^2$
Constant-Elasticity	$\beta_2' = 10.00\,\$/\mathrm{t}^{0.5}$ $E_C = 2$	$\beta_2' = 21.00\,\$/\mathrm{t}^{0.33}$ $E_D = 1.5$
Logit	$\beta_3 = 40.00\,\mathrm{t}$ $\beta_4 = -2.00$ $\beta_5 = 0.70\,\mathrm{t}/\$$	$\beta_3 = 50.00\,\mathrm{t}$ $\beta_4 = -3.00$ $\beta_5 = 1.00\,\mathrm{t}/\$$



(a)



(b)

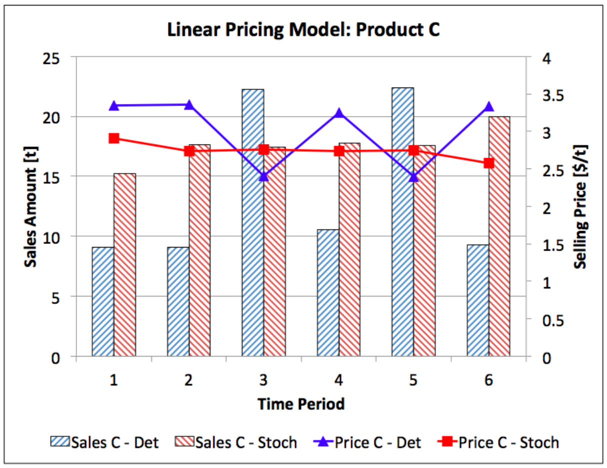
Figure 7: Illustration of DRMs for products C (a) and D (b).

A total of six different optimization problems were solved: (i) deterministic with linear DRM, (ii) stochastic with linear DRM, (iii) deterministic with constant-elasticity DRM, (iv) stochastic with constant-elasticity, (v) deterministic with logit DRM, and (vi) stochastic with logit DRM. Problems (i) and (ii) are concave MIQPs, whereas problems (iii) – (vi) are concave MINLPs (maximization). Table 4 shows the computational results for all problems. All deterministic (stochastic) problems contain 60 (60) binary variables, 184 (725) continuous variables, and 264 (750) constraints.

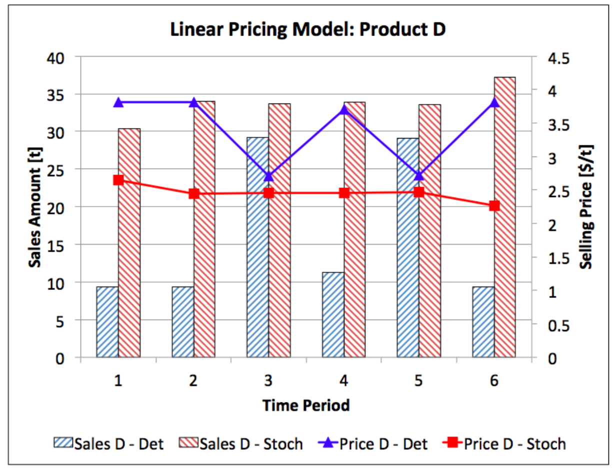
Table 4: Computational results for Example 1. C-E stands for Constant-Elasticity.

	Deterministic			**Stochastic**		
	Linear	*C-E*	*Logit*	*Linear*	*C-E*	*Logit*
MIQP/MILP Nodes	658	528	3,801	140	1,181	3,868
NLP Solves	–	34	114	–	55	224
Wall Time [s]	0.27	0.56	1.33	0.48	1.33	7.29

We restrict our analysis to the results of problems (i) and (ii) (i.e., with linear DRMs). In other words, we assess the impact of considering uncertainty in both raw material prices and the relationship between selling price and demand captured by linear DRMs. The profit of the deterministic problem is \$94.03, and the expected profit of the stochastic problem is \$259.69. The difference in profit values between the solutions is mainly attributed to the predominantly lower selling prices suggested by the stochastic model in comparison to the deterministic solution. Consequently, the lower prices obtained in the stochastic solution are correlated with more sales as shown in Figure 8, and higher overall profit.



(a)



(b)

Figure 8: Selling price and sales for products C (a) and D (b) in Example 1. "Det" and "Stoch" stand for deterministic and stochastic model solutions, respectively.

The amount of sales quantified by the DRM translates into the required purchase amounts. Figure 9 shows these purchases that include both contracts and spot market (average). According to the solution to the deterministic model, the manufacturer not only purchases raw material A from contracts with the supplier, but also from the spot market at certain time periods. The total average purchase amounts from the spot market represent 29% of total raw material purchases. However, the total purchase amount in the deterministic solution (155 t) is lower than what is required by the stochastic model (270 t). From the stochastic solution, the manufacturer does not use the spot market as a source of raw material. The reasons are two-fold: unfavorable market price variability and the need to increase the purchase amounts due to the increase in sales. Thus, the manufacturer opts for signing more contracts as a more cost-effective and less uncertain strategy. We note that similar trends occur in the other problems with the other two DRMs.

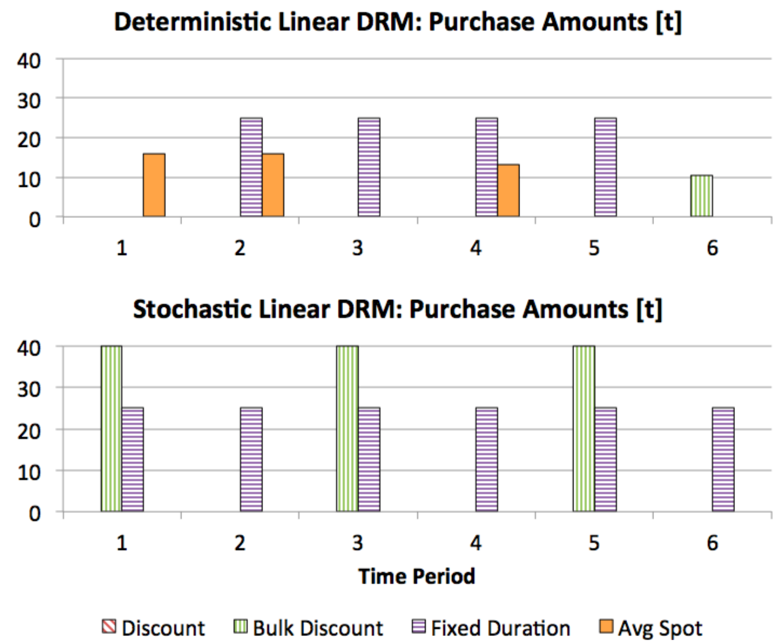


Figure 9: Purchase amounts from contracts and spot market (average) for the deterministic and stochastic problems in Example 1.

Even though the expected profit of the stochastic model is higher than the profit of the deterministic model, it is not appropriate to directly compare the objective function values of stochastic and deterministic solutions, since the latter only typically accounts for the average values of the uncertain parameters, and not the different possible outcomes considered by the former. A more meaningful comparison is performed through the calculation of the Value of the Stochastic Solution (VSS) as described in Birge and Louveaux (2011). The VSS is a metric to evaluate the performance of a deterministic solution in a stochastic environment. This is accomplished by solving the deterministic model with average values for the uncertain parameters, and then fixing the first-stage variables in the stochastic programming model to the values of the corresponding variables in the solution of the deterministic model. For a maximization problem, the VSS is calculated as follows:

$$VSS = RP - EV \tag{30}$$

where RP is the objective function value of the *recourse problem* (original stochastic model) and EV is the *expected value* solution (stochastic model with fixed first-stage decisions from deterministic model with average values for the uncertain parameters). In this motivating example, we have that $VSS = \$259.69 - \$190.47 = \$69.22$, which represents the additional expected profit from implementing the stochastic solution over the deterministic one, both with purchase contracts and pricing models. The VSS is approximately 27% of the solution obtained with the proposed method.

The calculation of the VSS can be modified to compare the solution of the proposed method with a *deterministic base case* model, which is typically used as a first approach in practical applications. The deterministic base case does not account for contract selection, and the demand and selling prices are fixed parameters. We call this modified metric a *restricted* VSS or RVSS. The formula is the same as in equation (30) with the difference being the meaning of the term EV, which now corresponds to the objective function value of the stochastic model with first-stage variables fixed to the solution of the deterministic base case. In this example, $RVSS = \$259.69 - \$134.10 = \$125.59$, i.e., the proposed method results in approximately 48% additional expected profits relative to the deterministic base case with no contracts and fixed demand and selling prices.

5.2. Example 2: Large Process Network

Example 2 is based on the process network shown in Figure 10 and discussed in Iyer and Grossmann (1998) (see the third example). The process network can be considered an integrated petrochemical site in which chemicals are produced in separate, dedicated production plants that are situated at the same geographic location due to economies of scale related to utility operations and supply chain cost advantages (Wassick, 2009). We do not include explicit data for this problem because of its size; however, this information is available from the authors upon request.

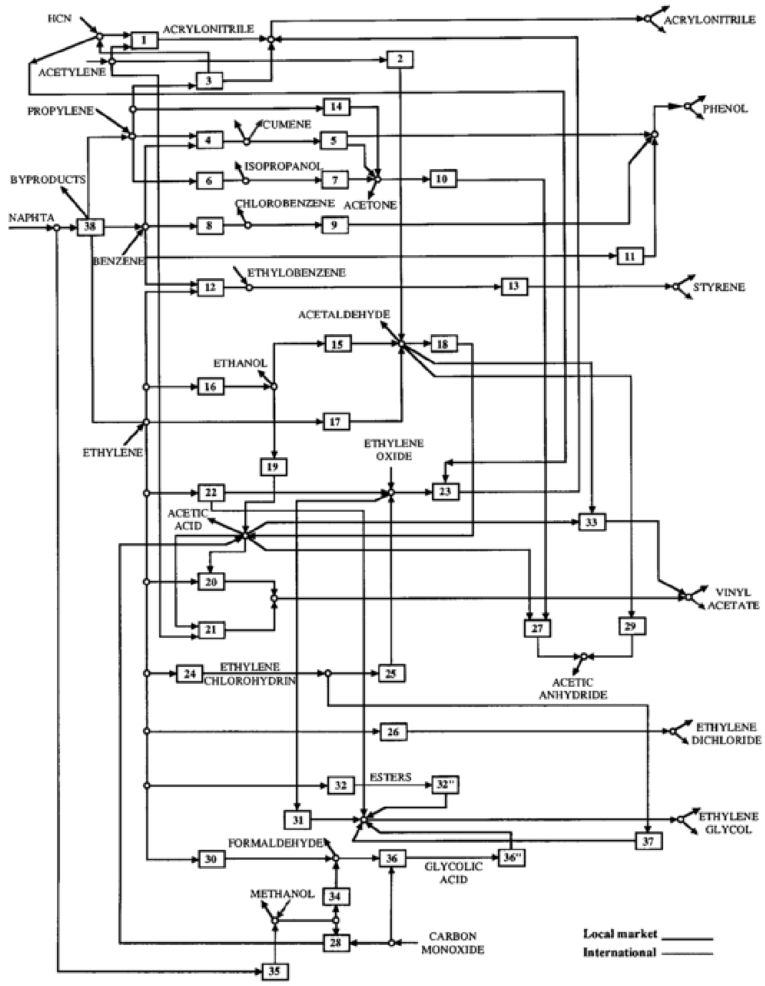


Figure 10: Process network in Example 2 (Iyer and Grossmann, 1998).

The process network has 38 processes (plants) and 28 chemicals, in which 17 are products and 11 are raw materials and intermediates. The time horizon is divided into 4 time periods that represent quarters in a year. Purchasing contracts are considered for all raw materials, and the three DRMs considered in this paper are used for all finished products. Similarly as in Example 1, 10 scenarios are considered. Each scenario contains spot market prices and samples of residuals of the DRMs. The spot market prices for the raw materials in each scenario were generated via simulation of ARIMA models, and for illustration purposes, the regression residuals of the DRMs are assumed to be normally distributed with given means and standard deviations.

Similarly as in Example 1, six different optimization problems were solved. They are the same models solved in Example 1, but with different data. Table 5 shows the computational results for all problems. All deterministic (stochastic) problems contain 400 (400) binary variables, 1,349 (6,777) continuous variables, and 2,383 (6,055) constraints. Note that, as the problem size increases relative to the previous example, the convex outer-approximation algorithm requires significantly more time, nodes in the solution of master MILP problems, and calls to the NLP subproblem. This is an indication that as the model size increases decomposition strategies should be required to reduce the computing time.

Table 5: Computational results for Example 2. C-E stands for Constant-Elasticity.

	Deterministic			**Stochastic**		
	Linear	*C-E*	*Logit*	*Linear*	*C-E*	*Logit*
MIQP/MILP Nodes	129	31,611	1,177,918	72	350	62,840
NLP Solves	–	220	1,571	–	31	366
Wall Time [s]	1.36	57.25	15,341	2.12	233.86	2,708

We restrict the analysis of the results to the deterministic and stochastic models with linear DRMs. The profit of the deterministic solution is \$33,783.48, and the expected profit of the stochastic solution is \$37,722.05. A key difference between the deterministic and stochastic solutions is the different types of contracts and the respective contracted amounts for certain products at each time period. The total sales influence the production rates, which in turn are connected to the total amount of purchases. Finally, the combined effect of these decisions and inventory considerations impact the overall profitability of the production plan under uncertain market conditions.

Proceeding as in the previous example, the calculated Value of the Stochastic Solution is $VSS = \$37,722.05 - \$34,076.98 = \$3,645.07$, which represents 10% of the solution obtained with the proposed method. However, when compared to the deterministic base case (i.e., no contracts and fixed demand and selling prices), the restricted VSS is $RVSS = \$37,722.05 - \$19,677.10 = \$18,044.95$, which amounts to 48% of the solution obtained with the proposed method. A summary of results for the two solutions with respect to total average purchase amounts, total average inventory levels, and individual scenario profit is shown in Figure 11. Note that the solution obtained with the proposed method (represented by the label RP) displays lower total average amounts for purchased raw materials (subfigure (a)) and inventory (subfigure (b)) than the expected value solution in all time periods. In fact, a slack variable had to be added to the right-hand side of the material and inventory balance constraint (equation (24)) and penalized in the objective function (equation (20)) in order to obtain a feasible solution. This indicates that the solution from the deterministic base case fails to balance inventory, production rates, and sales when subject to uncertainty in both supply and demand for certain chemicals. Note also that the profit of each scenario in the RP solution is always higher than in the EV solution (subfigure (c)).

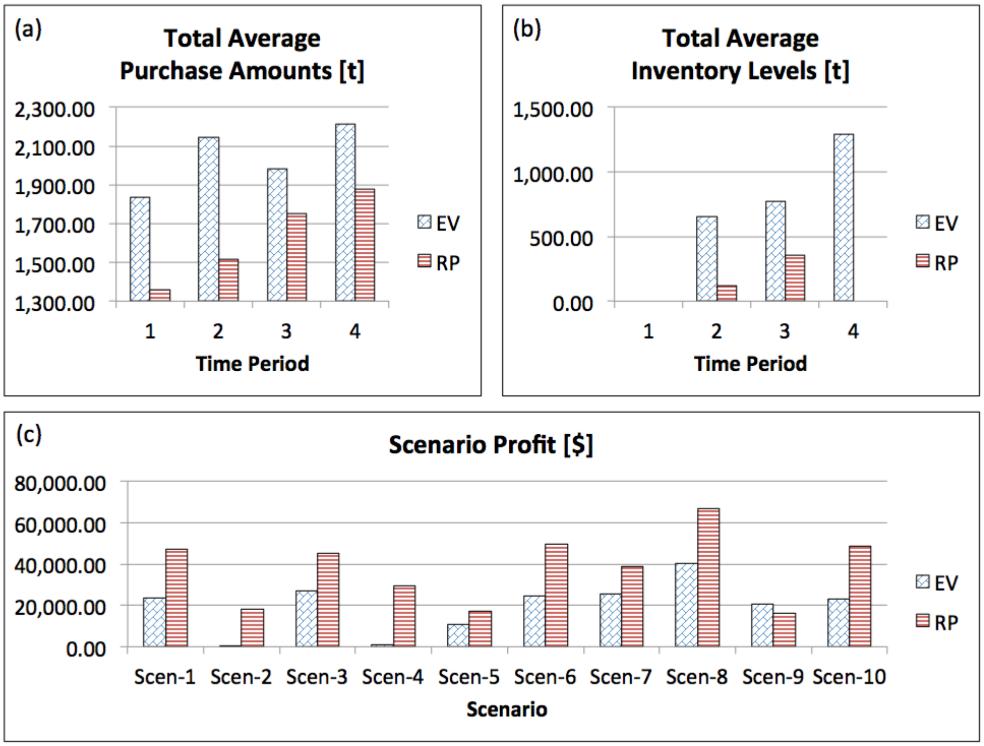
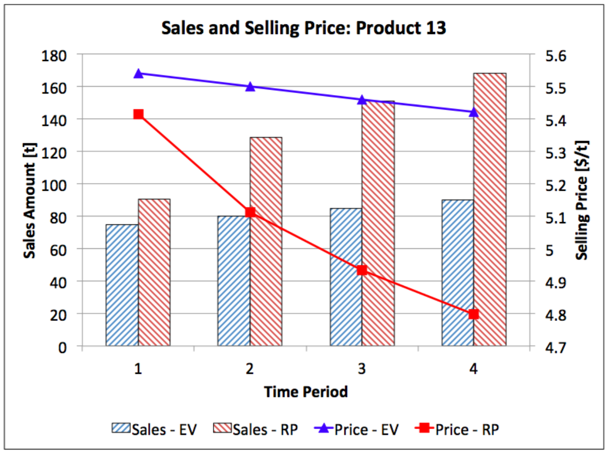
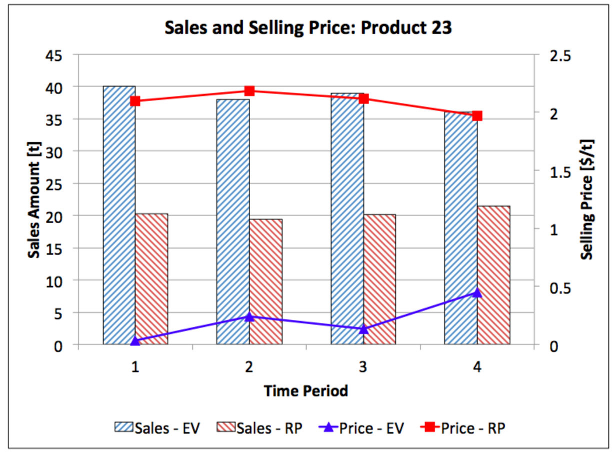


Figure 11: Summary of results in Example 2 (linear DRMs). RP and EV stand for recourse problem (proposed method) and expected value problem (stochastic model with first-stage decisions fixed to the solution of the deterministic base case).

The differences between the two solutions may be attributed to the total sales and selling prices. Figure 12 shows the optimal values for sales and selling prices for two products, 13 and 23 (acetone and ethylene dichloride, respectively, in the problem discussed in the original paper). Recall that the solution to the EV problem has fixed demand and selling prices. Note that, in RP solution, the sales of product 13 are always larger than in the EV solution, whereas the opposite is true for product 23. In addition, simple contract information with suppliers that imposes ranges of the demand can also be used. The design of customer contracts; however, is a more challenging problem, and some suggestions of extensions to the proposed method are given in the conclusion section. Notice that the results shown in the top subfigures of Figure 11 are *total* expected amounts, whereas Figure 12 shows results for two out of the twenty-eight chemicals.



(a)



(b)

Figure 12: Selling price and sales for products 13 (a) and 23 (b) in Example 2 (linear DRMs). RP and EV stand for recourse problem and expected value problem solutions, respectively.

5.3. Reformulation of MINLP Models

When using constant-elasticity or logit DRMs, the objective function contains nonlinear terms, which are concave (maximization) under certain conditions. We propose transferring the nonlinear terms in the objective function to the set of constraints by introducing non-negative auxiliary variables, $\text{SALES}^{\text{aux}}_{j,t}$. Specifically, for the two nonlinear DRMs considered in this work, the sales term of the objective function of the deterministic model in equation (1), $\text{SALES}_{j,t}$, is simply rewritten as $\text{SALES}^{\text{aux}}_{j,t}$, and equivalently in equation (20) of the stochastic model, the sales term $\text{SALES}_{j,t,k}$ becomes $\text{SALES}^{\text{aux}}_{j,t} + S_{j,t}\epsilon_k$. The additional set of constraints is given as follows:

- Constant-Elasticity:

$$\text{SALES}^{\text{aux}}_{j,t} \leq \beta_2' S_{j,t}^{1-1/E_j} \qquad \forall\, j \in J,\ t \in T \tag{31}$$

- Logit:

$$\text{SALES}^{\text{aux}}_{j,t} \leq \frac{1}{\beta_5}\left[\ln\left(\frac{\beta_3 - S_{j,t}}{S_{j,t}}\right) - \beta_4\right] S_{j,t} \qquad \forall\, j \in J,\ t \in T \tag{32}$$

The advantage of the reformulated model is that more cuts or inequalities (linearizations) are generated and added to the master MILP problem in an outer-approximation algorithm, since $|J| \times |T|$ cuts are generated (corresponding to the nonlinear constraints) as opposed to a single cut per NLP solve generated by restricting the nonlinear terms to the objective function. One potential disadvantage is the need to solve larger MILP models. However, the increased number of cuts generated in the reformulated model may provide tighter and more accurate outer-approximation of the feasible region, thus decreasing the solution time.

In Table 6, the computational results of the proposed reformulation are compared with the results of the original models (nonlinear terms in the objective function only) shown in Tables 4 and 5. Considerable speed-ups, and decrease in the number of MILP nodes and NLP solves were observed with the reformulated model. Even though the proposed reformulation significantly reduced solution times, decomposition approaches may be necessary as the problem instance increases in size and more general nonlinear DRMs are used.

6. Conclusions

In this paper, we have formulated a multi-period, multi-site stochastic programming production planning model that combines optimal procurement contract selection with selling price optimization under supply and demand uncertainty. The proposed approach is manufacturer-centric in the sense that it is the manufacturer's decision to sign or not contracts with suppliers in order to hedge against spot market supply uncertainty, and the manufacturer can set selling prices for its customers. The possible selection of sales contracts is considered to be the customer's decision, and was not addressed in this work. With regards to price optimization, the formulation of three price-response models that are typically encountered in the literature was discussed, even though we argued that general regression models can be used. The demand uncertainty is represented by samples from the distribution of regression residuals. We showed that it may be more advantageous to use demand-response models (DRMs), i.e., price as a function of demand, and we provided conditions on the parameters of the logit model that yield a concave revenue term in the objective function.

The proposed approach was illustrated with two numerical examples. In the first example (small process network), the stochastic model set the selling prices predominantly lower than the deterministic model, and had larger sales, and thereby an overall higher expected profit. The larger volume of sales in the stochastic solution relative to the deterministic solution translated into larger purchase amounts in the former, all of which was obtained through contracts (i.e., no purchases from the uncertain spot market). The computational results showed that the optimization models with logit DRMs were more computationally intensive than the models with linear and constant-elasticity DRMs due to the increase in complexity of the MINLP. Similar conclusions were drawn from the second example (large process network), in which the economic advantage of the stochastic solution over the deterministic one was measured by calculating the Value of the Stochastic Solution. The solution time increased considerably in the second example when using the original models. However, transferring the nonlinear terms from the objective function to the set of constraints demonstrated to significantly reduce solution times. Moreover, in both examples, the Value of the Stochastic Solution (VSS) showed a modest improvement of the proposed stochastic method over its deterministic solution; however, by comparing the proposed method with a deterministic base case (no contracts and fixed demand and selling price), the calculated restricted VSS showed that the proposed method exhibited significant improvement with regards to expected profitability when uncertainty in both supply and demand is considered.

Possible extensions of the proposed approach include: (1) design of sales contracts with customers, where the decision to sign or not these contracts are made by each customer in a bilevel programming framework (Shimizu et al., 1997; Bard, 1998); (2) approximate decomposition approaches when dealing with nonlinear DRMs, for example, via piece-wise linear functions (Taha, 2010).

Table 6: Computational results comparing original and reformulated MINLP models. C-E stands for Constant-Elasticity. Speed-Up is calculated as the ratio between CPU time of original and reformulated models.

			Original			**Reformulation**			
Example	*Problem*	*DRM*	*CPU [s]*	*MILP Nodes*	*NLP Solves*	*CPU [s]*	*MILP Nodes*	*NLP Solves*	*Speed-Up*
1	Deterministic	C-E	0.56	528	34	0.08	95	6	7x
		Logit	1.33	3,801	114	0.23	1,643	14	6x
	Stochastic	C-E	1.33	1,181	55	0.25	956	9	5x
		Logit	7.29	3,868	224	0.48	3,299	13	15x
2	Deterministic	C-E	57.25	31,611	220	3.28	2,362	24	18x
		Logit	15,341	1,1777,918	1,571	6.57	10,902	15	2,335x
	Stochastic	C-E	233.86	350	31	30.61	153	15	8x
		Logit	2,708	62,840	366	19.75	2,002	18	137x

Acknowledgment

The authors gratefully acknowledge financial support from The Dow Chemical Company.

AppendixA. Purchase Contract Mixed-Integer Linear Models

The models for the three contract types (discount, bulk, and fixed duration) are proposed in Park et al. (2006). In this section, we present the mixed-integer linear constraints obtained by reformulating the disjunctions using the convex hull approach. At most one contract type can be selected for a given raw material j, which is expressed as follows:

$$\sum_{c \in C} y^c_{j,s,t} \le 1 \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in t \tag{A.1}$$

where $C = \{d, b, l\}$.

AppendixA.1. Discount Contract

Contract type $c = d$ and two price schemes, d_1 and d_2.

$$\text{COST}^d_{j,s,t} = \varphi^{d_1}_{j,s,t} P^{d_1}_{j,s,t} + \varphi^{d_2}_{j,s,t} P^{d_2}_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.2}$$

$$P^d_{j,s,t} = P^{d_1}_{j,s,t} + P^{d_2}_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.3}$$

$$P^{d_1}_{j,s,t} = P^{d_{1,1}}_{j,s,t} + P^{d_{1,2}}_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.4}$$

$$0 \le P^{d_{1,1}}_{j,s,t} \le y^{d_1}_{j,s,t} \sigma^d_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.5}$$

$$P^{d_{1,2}}_{j,s,t} = y^{d_2}_{j,s,t} \sigma^d_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.6}$$

$$0 \le P^{d_2}_{j,s,t} \le y^{d_2}_{j,s,t} U^d_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.7}$$

$$y^{d_1}_{j,s,t} + y^{d_2}_{j,s,t} = y^d_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.8}$$

where $y^{d_1}_{j,s,t},\; y^{d_2}_{j,s,t} \in \{0, 1\}$, and $U^d_{j,s,t}$ is a number large enough (e.g., process capacity).

AppendixA.2. Bulk Discount Contract

Contract type $c = b$ and two price schemes, b_1 and b_2.

$$\text{COST}^b_{j,s,t} = \varphi^{b_1}_{j,s,t} P^{b_1}_{j,s,t} + \varphi^{b_2}_{j,s,t} P^{b_2}_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.9}$$

$$P^b_{j,s,t} = P^{b_1}_{j,s,t} + P^{b_2}_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.10}$$

$$0 \le P^{b_1}_{j,s,t} \le y^{b_1}_{j,s,t} \sigma^b_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.11}$$

$$y^{b_2}_{j,s,t} \sigma^b_{j,s,t} \le P^{b_2}_{j,s,t} \le y^{b_2}_{j,s,t} U^b_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.12}$$

$$y^{b_1}_{j,s,t} + y^{b_2}_{j,s,t} = y^b_{j,s,t} \qquad \forall\, j \in \text{JR},\; s \in ST,\; t \in T \tag{A.13}$$

where $y^{b_1}_{j,s,t},\; y^{b_2}_{j,s,t} \in \{0, 1\}$, and $U^b_{j,s,t}$ is a number large enough (e.g., process capacity).

AppendixA.3. Fixed Duration Contract

Contract type $c = l$ and three price-quantity schemes, l_p for $p \in \mathrm{LC} = T_{1:3}$, where the notation $T_{m:n}$ means a subset of the ordered set T containing all its elements in between and including the m-th and n-th elements. For example, if $T = \{1,2,3,4,5,6\} \subset \mathbb{Z}$, then $\mathrm{LC} = T_{1:3} = \{1,2,3\}$.

$$\mathrm{COST}^{l}_{j,s,t} = \varphi^{l_1}_{j,s,t} P^{l_1}_{j,s,t,t} + \sum_{p \in \mathrm{LC}_{2:|\mathrm{LC}|}} \sum_{\substack{t' \in T \\ t' \leq t \\ t' \geq t - l_p + 1}} \varphi^{l_p}_{j,s,t'} P^{l_p}_{j,s,t,t'} \quad \forall\, j \in \mathrm{JR},\ s \in ST,\ t \in T \tag{A.14}$$

$$P^{l}_{j,s,t} = P^{l_1}_{j,s,t,t} + \sum_{p \in \mathrm{LC}_{2:|\mathrm{LC}|}} \sum_{\substack{t' \in T \\ t' \leq t \\ t' \geq t - l_p + 1}} P^{l_p}_{j,s,t,t'} \quad \forall\, j \in \mathrm{JR},\ s \in ST,\ t \in T \tag{A.15}$$

$$y^{l_p}_{j,s,t} \sigma^{l_p}_{j,s,t} \leq P^{l_p}_{j,s,t,t'} \leq y^{l_p}_{j,s,t} U^{l}_{j,s,t} \quad \forall\, j \in \mathrm{JR},\ s \in ST,\ p \in \mathrm{LC},\ (t,t') \in T,\ t' \leq t,\ t' \geq t - l_p + 1 \tag{A.16}$$

$$\sum_{p \in \mathrm{LC}} y^{l_p}_{j,s,t} = y^{l}_{j,s,t} \quad \forall\, j \in \mathrm{JR},\ s \in ST,\ t \in T \tag{A.17}$$

$$y^{l_p}_{j,s,t} \leq 1 - y^{l_{p'}}_{j,s,t'} \quad \forall\, j \in \mathrm{JR},\ s \in ST,\ (p,p') \in \mathrm{LC},\ (t,t') \in T,\ t' < t,\ t' \geq t - l_p + 1 \tag{A.18}$$

where $y^{l_p}_{j,s,t} \in \{0,1\}$, for $p \in \mathrm{LC}$, and $U^{l}_{j,s,t}$ is a number large enough (e.g., process capacity).

AppendixB. Concavity of Sales Term when using Logit Demand-Response Model

In this appendix, we show the following result: the function

$$f(d) = \frac{1}{\beta_5}\left[\ln\left(\frac{\beta_3 - d}{d}\right) - \beta_4\right] d \tag{B.1}$$

is concave if $\beta_3 \cdot \beta_5 > 0$ and $\beta_4 \in \mathbb{R}$. This function arises in the sales term (selling price $\times$ sales) when using the logit demand-response model (see Table 2). This is a univariate function, and its concavity can be verified by analyzing the sign of its second derivative with respect to d evaluated at critical points. Symbolic calculations were performed with Maple 18.01 (Maplesoft, 2014).

Setting the first derivative of $f(d)$ with respect to d to zero yields

$$f'(d) = \frac{1}{\beta_5}\left[\ln\left(\frac{\beta_3 - d}{d}\right) - \beta_4\right] - \frac{\beta_3}{\beta_5(\beta_3 - d)} = 0$$

Solving the equation for d gives the single stationary point

$$d^* = \beta_3 \frac{W\left(e^{-1-\beta_4}\right)}{1 + W\left(e^{-1-\beta_4}\right)}$$

where $W(\cdot)$ is the Lambert W function (Corless et al., 1996) that satisfies the following equation

$$W(x)e^{W(x)} = x \tag{B.2}$$

The second derivative of $f(d)$ with respect to d is given by

$$f''(d) = -\frac{\beta_3^2}{\beta_5(\beta_3 - d)^2 d}$$

which evaluated at d^* yields

$$f''(d^*) = -\frac{\left[1 + W\left(e^{-1-\beta_4}\right)\right]^3}{\beta_3\beta_5 W\left(e^{-1-\beta_4}\right)} \leq 0 \tag{B.3}$$

If the relation in equation (B.3) is true, then the stationary point d^* is a maximizer of $f(d)$, i.e., $f(d)$ is concave. Let $u = e^{-1-\beta_4}$ denote the argument of the Lambert W function in equation (B.3). Note that u is non-negative for $\beta_4 \in \mathbb{R}$. From the definition of $W(\cdot)$ in equation (B.2), since the right-hand side (u) and the exponential term in the left-hand side ($e^{W(u)}$) are non-negative, the first-term in the left-hand side ($W(u)$) must also be non-negative. Consequently, the numerator $[1 + W(u)]^3$ is non-negative. Finally, the second derivative in equation (B.3) is negative if $\beta_3 \cdot \beta_5 > 0$.

AppendixC. Data for Example 1

The parameters for the stochastic production planning model (see Subsection 4.4) are given in the following tables. Example 1 considers only a single site; therefore, in all tables below, $s =$ S1.

Table C.7: Deterministic spot market price ($\alpha_{j,s,t}^{\text{spot}}$) [\$/t].

Raw Material	**Time Period**					
	1	2	3	4	5	6
A	2.91	2.90	4.44	2.83	4.38	5.45

Table C.8: Operating cost ($\delta_{i,s,t}$) [\$/t].

Process	**Time Period**					
	1	2	3	4	5	6
P1	0.26	0.26	0.26	0.14	0.14	0.14
P2	0.16	0.16	0.16	0.13	0.13	0.13
P3	0.32	0.32	0.32	0.32	0.32	0.32

Table C.9: Inventory cost ($\xi_{j,s,t}$) [$/t].

Product	**Time Period** 1 – 6
D	0.03

Table C.10: Mass factor ($\mu_{i,j,s}$) [-].

Process	**Material**			
	A	B	C	D
P1	0.83	−1.00		
P2		0.95	−1.00	
P3		1.11		−1.00

Table C.11: Production capacity ($Q_{i,s,t}$) [t].

Process	**Time Period** 1 – 6
P1	85
P2	35
P3	65

Table C.12: Lower (Upper) raw material availability ($a^{\mathrm{L}}_{j,s,t}$ and $a^{\mathrm{U}}_{j,s,t}$) [t].

Raw Material	**Time Period** 1 – 6
A	0 (60)

Table C.13: Upper bound on inventory ($V^{\mathrm{U}}_{j,s,t}$) [t].

Product	**Time Period** 1 – 6
D	6

Table C.14: Purchase price under discount (‘d’) contract type ($\psi^{d,cs}_{j,s,t}$ for $j = \mathrm{A}$) [$/t].

Time Period	**Scheme (cs)**	**Price**
1 – 6	1	3.15
1 – 6	2	2.47

Table C.15: Purchase threshold under discount (‘d’) contract type ($\sigma^{d}_{j,s,t}$ for $j = \mathrm{A}$) [t].

Time Period	**Threshold**
1 – 6	20

Table C.16: Purchase price under bulk discount ('b') contract type ($\psi^{b,cs}_{j,s,t}$ for j = A) [\$/t].

Time Period	**Scheme (cs)**	**Price**
1 – 6	1	3.06
1 – 6	2	2.38

Table C.17: Purchase threshold under bulk discount ('b') contract type ($\sigma^{b}_{j,s,t}$ for j = A) [t].

Time Period	**Threshold**
1 – 6	40

Table C.18: Purchase price under fixed duration ('l') contract type ($\psi^{l_p}_{j,s,t}$ for j = A) [\$/t].

Length (p)	**Time Period**
	1 – 6
1	3.40
2	2.04
3	1.70

Table C.19: Purchase threshold under fixed duration ('l') contract type ($\sigma^{l_p}_{j,s,t}$ for j = A) [t].

Length (p)	**Time Period**	**Threshold**
1	1 – 6	5
2	1 – 6	25
3	1 – 6	30

Table C.20: Purchase spot price for the deterministic base case ($\alpha^{\text{spot}}_{j,s,t}$ for j = A) [\$/t].

Time Period					
1	2	3	4	5	6
2.90	2.91	4.44	2.83	4.38	5.45

Table C.21: Sales spot price for the deterministic base case ($\psi^{\text{spot}}_{j,t}$) [\$/t].

Product	**Time Period**					
	1	2	3	4	5	6
C	2.65	2.87	2.93	2.72	3.35	2.83
D	2.46	2.58	2.94	2.54	2.74	2.99

Table C.22: Stochastic spot market price ($\alpha^{\text{spot}}_{j,s,t,k}$ for j = A) [$/t]. Simulated values from an ARIMA(0,1,1)(0,1,0)$_{12}$ time series model.

Time Period	**Scenario** 1	2	3	4	5	6	7	8	9	10
1	1.37	2.47	4.98	2.57	3.36	1.44	1.96	2.56	6.12	2.27
2	4.02	2.96	4.50	3.20	2.62	0.04	3.28	0.93	3.76	3.83
3	5.97	2.60	4.25	4.93	5.99	0.68	2.41	2.49	7.78	7.26
4	1.01	3.00	3.49	3.43	4.12	1.91	2.11	1.49	4.20	3.51
5	5.55	3.02	4.29	2.96	4.63	2.61	2.52	2.21	7.76	8.23
6	5.49	2.46	8.84	5.16	4.19	5.13	1.29	2.68	10.83	8.47

Table C.23: Stochastic part of demand-response models (ϵ_k) [$/t].

Product	**Scenario** 1	2	3	4	5	6	7	8	9	10
C	−0.18	−0.17	−1.37	−0.17	0.85	0.70	0.55	−0.40	−0.20	−1.19
D	−0.11	0.51	3.41	2.00	−0.99	0.71	−2.27	1.76	1.95	4.24

Inter-site transfer limits and costs ($F^{\text{U}}_{j,s,s',t}$ and $\eta_{j,s,s',t}$) are zero. All scenarios are assumed to have the same probability, i.e., $\pi_k = 0.1$, $k = 1, \ldots, 10$.

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