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REGULAR ARTICLE

Value chain management for commodities: a case study from the chemical industry

M. Kannegiesser · H.-O. Günther · P. van Beek · M. Grunow · C. Habla

Abstract We present a planning model for chemical commodities related to an industry case. Commodities are standard chemicals characterized by sales and supply volatility in volume and value. Increasing and volatile prices of crude oil-dependent raw materials require coordination of sales and supply decisions by volume and value throughout the value chain to ensure profitability. Contract and spot demand differentiation with volatile and uncertain spot prices, spot sales quantity flexibility, spot sales price–quantity functions and variable raw material consumption rates in production are problem specifics to be considered. Existing chemical industry planning models are limited to production and distribution decisions to minimize costs or makespan. Demand-oriented models focus on uncertainty in demand quantities not in prices. We develop an integrated model to optimize profit by coordinating sales quantity, price

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M. Kannegiesser · H.-O. Günther (✉)
Department of Production Management, Technical University of Berlin,
Wilmersdorfer Str. 148, 10585 Berlin, Germany
e-mail: hans-otto.guenther@tu-berlin.de

P. van Beek
Management Studies Group and Operations Research and Logistics Group,
Wageningen University, Hollandseweg 1, 6706 KN Wageningen, The Netherlands
e-mail: paul.vanbeek@wur.nl

M. Grunow
Department of Manufacturing Engineering and Management, Technical University of Denmark,
Building 425, 2800 Kgs. Lyngby, Denmark
e-mail: grunow@ipl.dtu.dk

C. Habla
Department of Enterprise-Wide Software Systems, The Fern Universität in Hagen,
Universitätsstr. 1, 58097 Hagen, Germany
e-mail: christoph.habla@fernuni-hagen.de

and supply decisions throughout the value chain. A two-phase optimization approach supports robust planning ensuring minimum profitability even in case of worst-case spot sales price scenarios. Model evaluations with industry case data demonstrate the impact of elasticities, variable raw material consumption rates and price uncertainties on planned profit and volumes.

Keywords Value chain management · Sales and supply network planning · Demand uncertainty · Commodities · Chemical industry

1 Introduction

The chemical industry is one of the key global industries with product sales of € 1,776 billion globally in 2004 (CEFIC 2005). In this article, we focus on the segment of chemical commodities. Commodities are mass products produced and sold in high volumes with standardized quality and few variants. Price is the key buying criterion for customers. Examples are standard polymers, certain types of intermediate products or basic chemicals. Sales prices for theses commodities are volatile and can change regularly, e.g., weekly or monthly based on negotiations between the company and its customers.

Prices for raw materials can also change regularly. Specifically, many key raw materials in the chemical industry showed a severe rise in prices due to the increase of the crude oil price over the last years. Raw price volatility and increases have to be considered in sales and supply planning of commodity products to ensure profitability of the business. Therefore, the focus on demand and supply *volume* planning alone is not sufficient since a feasible volume plan might not be profitable for the company due to the volatility of supply costs and sales prices. The monthly planning process needs to support integrated decisions on *volume* and *values*, specifically on sales quantities and prices considering available supply volumes and raw material costs. In this paper, an integrated planning model related to a real-life case from the European chemical industry is presented.

In our investigation, we consider a simplified intra-organizational *value chain network* of a company producing chemical commodities. The industry context of this case is a company operating a complex, multi-stage value chain network producing polymers that also require several intermediate products as raw material. The company is operating at several production sites and is serving different sales locations. The business is a commodity business where raw materials and finished products are characterized by market price and volume volatility. Annual production volumes exceed 1 Mio. tons. In this study we focus on the monthly sales and operations planning process for the entire value chain network for a planning horizon of 6–12 months.

Figure 1 shows a section of the network. The company has grouped multiple customers in regional or industry-specific sales locations. Two production resources are located in one production location, from where sales locations are served. One market-facing multi-purpose resource produces multiple finished commodity products. The second single-purpose resource produces the intermediate product for the multi-purpose resource in continuous production mode. The intermediate product produced

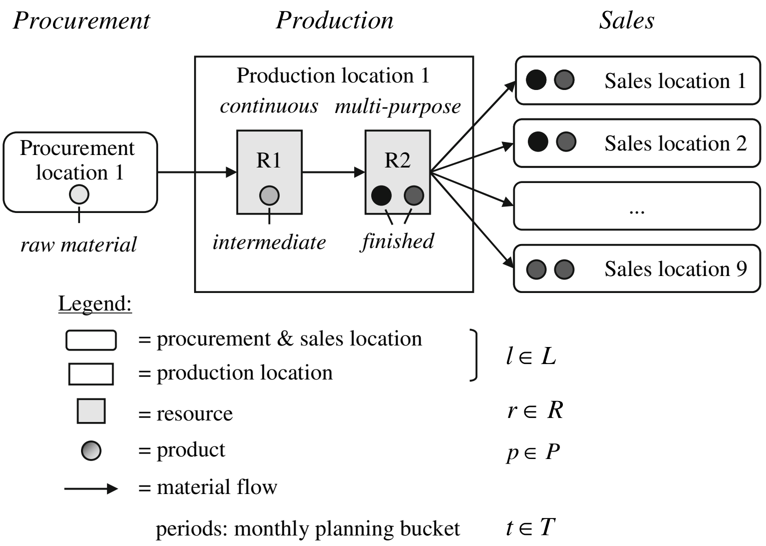


Fig. 1 Section of the considered value chain network

on resource R1 requires a raw material product procured from an external procurement location.

The planning problem at hand shows a number of characteristics that are typical of the chemical industry.

- Spot and contract business differentiation is an important issue in the chemical industry specifically in commodity business.
- Price and volume volatility for chemical commodities in sales and procurement is more significant than in other industries, e.g., in discrete parts manufacturing.
- The entire production system is organized as a multi-stage network with multi-purpose and continuously operated production resources.
- Material flows are predominantly divergent with intermediates used in multiple subsequent products.
- Raw material consumption rates in production are variable depending on the degree of capacity utilization.

These characteristics can be found, for example, in basic chemicals and/or polymer production, while fine chemical and pharmaceutical production can be seen as a specialty type of business relying on smaller quantities and complex batch production mode. The simplified network as shown in Fig. 1 focuses on the interaction between procurement, production and sales. The problem at hand is an excerpt from the global value chain planning problem of a polymer producing company. In our investigation we focus on the interaction between key business functions in the global value chain context. The model developed represents a prototype which is used by the planners to better understand volume and value dynamics from sales to procurement and their impact on profit in a value chain network. In a later stage, the company intends to introduce the Supply Network Planning module of an advanced planning software system for operative planning (cf. Dickersbach 2006). To reduce the complexity of the prototype model, several standard features such as inventory records and transportation are excluded mainly because they do not have a high profit impact compared to sales and procurement issues. Exchange rates and risk hedging inventories are also excluded here though they do represent further important issues in the investigated global value chain network which will be included in the final implementation of the value chain planning model.

Traditionally, supply network planning models focus on the flow of goods in the network while assuming sales and procurement prices as being fixed. Revenue management, however, represents a topic which has recently gained considerable interest both in practice and in academia. For an application in the iron and steel industry and a discussion of dynamic pricing in the US automotive industry, cf. Spengler et al. (2007) and Biller et al. (2005), respectively. Key issues of revenue management are dynamic pricing strategies as well as accept and reject decisions to make more effective use of resources. Booking and pricing systems of airlines, hotels, car rentals, telecommunication systems and cargo transportation are just a few popular examples of revenue management, cf. Gosavi et al. (2007), Bartodziej et al. (2007), Lee et al. (2007), Defregger and Kuhn (2007), Reiner and Natter (2007). These papers focus on revenue maximization based on pricing and decisions to influence the demand for services such as airline seats, rental car capacity or hotel rooms which are in limited supply. Active sales and pricing decisions investigated in revenue management are principally relevant for the industrial planning problem considered in our paper. However, in contrast to service industries we deal with physical products and the complex decision-making process in a global chemical value chain.

This paper aims at integrating ideas of revenue management into supply network planning to optimize profit throughout the entire intra-organizational value chain network. We choose “value chain management” as an overall term for the integration of demand-oriented management concepts such as revenue management as well as supply-oriented logistics management concepts which primarily focus on material flows. Specifically, our modeling approach reflects the following key issues:

- For chemical commodities as well as for many other industrial products (e.g., fertilizers or animal feed products), *contract* and *spot demand* can be distinguished. While sales prices and quantities are fixed for contract demand, spot market sales can be highly variable with regard to both price and quantity. We develop a value chain planning model that, in addition to production and distribution planning, also supports pricing and sales decisions for spot demand.
- Similar to sales commodity markets, raw materials can be procured either based on fixed contracts with suppliers or on the spot market. In the latter case, the company has to decide on the procurement quantity taking the volatility of procurement prices into account. Our modeling approach also reflects these issues which are of increasing importance in many industries specifically confronted with increasing raw material prices.
- Empirical investigations have shown that both spot sales prices for commodities as well as procurement prices for raw materials are characterized by high uncertainty. Modeling these prices as independent random variables, as it is assumed in a

large number of academic contributions, is not always realistic because the drivers behind the market development, e.g., development of crude oil prices, are ignored. Hence, our approach is based on scenario analysis which utilizes human expertise to forecast market developments in combination with subjective probability measures.

- Finally, it is shown how technological flexibility with respect to consumption rates of raw material and feasible processing modes of the chemical production equipment can be used in order to balance sales market demands and procurement opportunities.

The overall objective of the proposed optimization model is to maximize profit by coordinating sales turnover with quantity and prices as well as supply decisions throughout the value chain. Model evaluations with industry case data demonstrate clearly the applicability of the value chain optimization model. The model has been developed and implemented together with the company proving the industry case and also the problem requirements and assumptions such as contract and spot demand.

The remainder of this article is organized as follows. The next section provides an overview of the relevant literature. In Sect. 3, a mixed-integer linear optimization model for sales and supply planning in intra-organizational value chain networks is developed. Section 4 presents a case study evaluation based on a real application from the European chemical industry.

2 Literature review

In the academic literature a wealth of papers dealing with demand and supply network management has been published. For an overview and classification, see, e.g., Thomas and Griffin (1996), Stadtler (2005) and Tang (2006). Some of these papers focus on demand, others on supply aspects of the problem. Among the demand-focused papers emphasis is given either on demand forecasting, demand uncertainty, or pricing decisions.

The objective of *demand forecasting* is to predict future demand quantities as accurate as possible based on historical data. For an overview of demand forecasting within supply chain management see Kilger and Wagner (2008) and Meyr (2008). The classical approach towards demand forecasting does not apply to the considered chemical commodity business, where contract demand is certain and spot demand does not need to be fulfilled. In addition, the development of demand does not follow historical demand patterns, but is rather influenced by future raw material prices as investigated by Asche et al. (2003) for crude-oil related products.

The paper by Gupta and Maranas (2003) represents one example for dealing with *demand uncertainty* in the chemical industry. The authors propose a demand and supply network planning model to minimize costs. Production decisions are made “here and now” and demand uncertainty is balanced with inventories independently incorporating penalties for safety stock and demand violations. Demand quantity uncertainty is modeled as a normally distributed continuous random variable with known mean and standard deviation and penalty costs are charged for unfilled demand. This approach, however, is not suitable in our commodity case, since spot demand and factors such as demand price uncertainty for chemical commodities or fluctuating raw material and crude oil prices have to be considered. Another example from the chemical engineering literature has been given by Chen and Lee (2004). They develop a multi-company demand and supply network planning model to maximize profit under demand uncertainty and pricing decisions. Demand uncertainty is modeled with quantity scenarios and probabilities. A two-phase optimization strategy is developed to reach robust plans. Pricing decisions are modeled with fuzzy logic considering satisfaction levels of buyer and seller assuming collaboration and preference transparency between both parties. This assumption, however, is not valid in the spot sales commodity business considered in our investigation.

Chakravarty (2005) develops an optimization model for global network design decisions incorporating *sales quantity and price decisions*. Chakravarty uses demand curves, where demand quantity is a function of price, and sales turnover is decided using quadratic optimization. The model scope of profit optimization incorporating variable sales prices and supply quantities as well as costs is similar to the considered problem more on a macro network design level rather than on a monthly planning level for a chemical industry value chain. In addition the assumption of a monopolistic market constellation, where the company is able to influence demand by price setting reflected in the demand curves is not valid in the considered case.

In contrast to demand planning, the supply side of chemical industry value chains has been widely investigated especially with focus on production planning and scheduling. Examples of papers dealing with industrial applications are Blömer and Günther (2000), Neumann et al. (2002), Kallrath (2002a,b) or on multi-site supply network planning with given demand, cf. Timpe and Kallrath (2000), Grunow (2001), Grunow et al. (2003), and Berning et al. (2002). Production scheduling for batch and campaign production and synchronization of production plans across plants considering sequence and production mode constraints are major subjects in this field of research. The specific aspect of variable raw material consumption, which is essential in the industrial application considered in our investigation, has not sufficiently been addressed in the literature so far.

Procurement planning in general and spot and contract procurement planning in the chemical industry particularly have recently been investigated in a number of papers. For instance, Stadtler (2008) discusses general tasks of purchase planning integrated in overall supply chain management at the order level. Recent papers discuss procurement strategies for spot and contract markets. Reiner and Jammernegg (2005) develop a risk-hedging model and compare different procurement strategies including speculation inventories. Marquez and Blanchar (2004) present extended procurement strategies based on real-options to optimize contract portfolios considering in-transit and warehouse inventories. Seifert et al. (2004) underline the importance of spot procurement next to contract procurement and show the advantage, if a fraction of demand is based on spot market procurement.

So far, models presented in the academic literature focus either on demand or on supply aspects. In the academic literature we did not find any realistic value chain planning model that integrates sales and supply decisions by volume and value in a price-volatile chemical commodity business, although this planning problem is of high importance not only in the chemical commodity industry.

3 Sales and supply planning model

To support decision making in the considered intra-organizational *value chain network* a mixed-integer linear programming (MILP) model is proposed. Maximizing profit throughout the entire value chain is seen as the overall objective function. Principally, the value chain profit consists of the following constituents:

Profit = spot sales turnover depending on variable sales prices and quantities
+ fixed contract sales turnover
− spot procurement costs depending on variable procurement prices and quantities
− fixed procurement costs
− variable production costs depending on variable raw material consumption and processing mode

The first two elements of the profit function and related constraints are reflected by the sales model introduced in Sect. 3.1. The supply model presented in Sect. 3.2 considers all other issues related to procurement and production. To solve the model, two different optimization strategies are proposed (see Sect. 3.3).

3.1 Sales model

3.1.1 Demand and sales planning for chemical commodities

In the industrial application considered, the central task is to plan monthly sales volumes and values in the network for 6–12 months. The planning process starts with a monthly demand forecast of quantities and prices submitted by the "Sales and Marketing" department of the company. The forecast aggregates demand of single customers at the sales location level resulting in a cumulated demand quantity and a weighted average price. The planning objective is to maximize profit considering available production and procurement capabilities, sales prices and supply costs. The planning result is a tactical sales and operations plan with sales quantities and prices as well as production and procurement quantities per month. The planning problem shows some specifics as described in the following.

Contract and spot sales quantity management
Contract and *spot* demand can be distinguished in chemical commodities markets. *Contract demand* is based on agreements between the company and customers with sales quantities and prices being fixed for a defined period. Contract demand quantities and prices are fulfilled as forecasted and are deterministic. *Spot demand* is also forecasted by quantity and price. However, spot demand does not need to be fulfilled completely since the company can make active sales decisions on the acceptance or rejection of spot sales requests. The spot price can be bilaterally negotiated, requested by the customer directly or set by the company. In the latter case the customer reacts with a quantity bid. In any case prices are negotiated bilaterally between company and customer. Double auction mechanisms with multiple buyers and sellers submitting offers and bids cleared in one market price are not considered in this context.

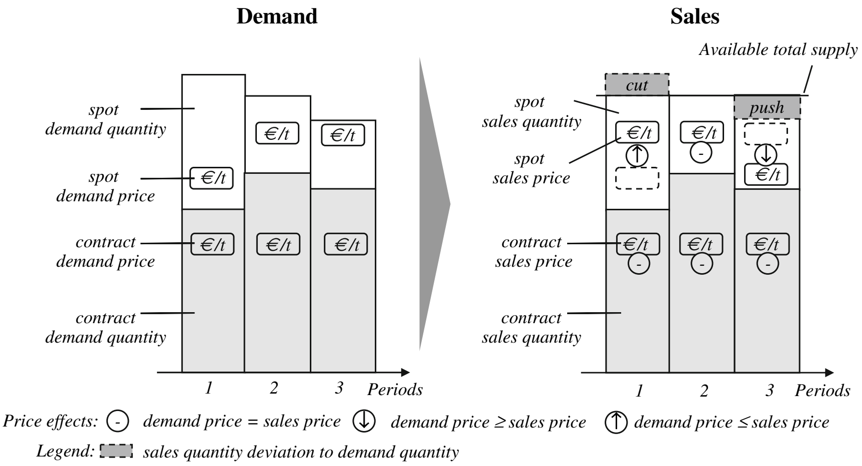


Fig. 2 Principle of contract and spot demand and sales

Spot sales quantities are flexible and can be lower or higher than the forecasted quantities for various reasons as shown in Fig. 2. Firstly spot sales are lower than the demand quantity if the spot demand quantity exceeds the available supply and the company needs to make monthly volume quotation decisions cutting volumes first on an overall sales location level and then also on a detailed, individual customer level. Merely for illustration reasons, the available supply is shown to be constant in Fig. 2. Of course in the real application the available supply can vary, e.g., due to variations in procurement quantities and production capacity. Secondly spot sales are reduced if spot demand prices are too low compared to raw material costs forcing the company to make a loss when supplying the customer. Hence the spot demand forecast has a bid character as in single-sided auctions competing for limited supply. The bid can be successful and is fully supplied or it can be partly or even fully rejected depending on the available supply quantity and the bid price. Like in stock markets and exchanges, bids need not be necessarily executed in the marketplace if the bid volume and price cannot be cleared with a suitable offer.

Note that there are no penalties in spot business as it can be found in supply network planning, where an artificial penalty is applied if demand cannot be met. These often subjective penalties are not related to actual business agreements or actual monetary penalties negotiated between the company and the customer. In our case customers either have a fixed contract or they do flexible spot business on a tactical level. This flexibility, however, does not destabilize the respective value chain operations since it is limited to the tactical planning level and does not impact the operational order level. Customers have a very early information and commitment on a monthly level whether they receive the requested spot quantities or not. If a spot customer has received a confirmation, the supplier delivers the related orders accurately and with high reliability. To summarize, in the considered industrial application demand is not regarded as a given monolithic quantity to be fulfilled in the traditional supply chain management sense but is defined as a mix of fixed contract demand and flexible spot demand.

Spot sales price–quantity functions and elasticities

Spot sales decisions have intuitive price effects as shown in Fig. 2: higher average prices are achieved when cutting spot sales quantities or lower prices are required when pushing additional quantities into the market. However, we do not assume a monopolistic market situation, where the company is able to influence or dominate market prices. In our case, price is a result of the spot sales quantity decision made by the company. Since the price is an average price across several customer forecasts grouped into one sales location, it is intuitive that the average price increases when sales quantities are lower than the demand forecast quantity. It is assumed that customers with lowest prices are cut first. Hence the average price across the remaining customers increases. In this context, competitor behavior has no influence on this price–quantity function. Competitors have influence on the overall market prices and the available supply. However, the model focuses on bilateral negotiations between the company and its customers. This business relationship is confidential, i.e., the competitor does not know about spot quantities ordered by the customers and the corresponding spot sales prices. The competitor does not even know to what extent a customer is supplied on contract or spot basis. Since the business relationships are kept confidential the competitor is not able to take specific reactions.

Spot sales price uncertainty

Spot demand quantity and prices are uncertain in the commodity business for the considered planning horizon. Since price is the main buying criterion, mid-term demand quantity is mainly influenced by the price level. Additionally, commodity suppliers often make supply volume decisions before sales prices are finally fixed due to complex multi-stage production systems, large lead times in production and raw material supply, lack of change-over flexibility in production with production plans fixed for one month, planned shut-downs for maintenance as well as long transportation lead times specifically in global value chain networks. Therefore, supply volumes in commodity business are fixed prior to sales prices in the market. Hence, the spot sales price remains an uncertain parameter. In our investigation, the spot sales price is considered as uncertain leading to different price and sales turnover scenarios for the same sales quantity. Therefore, contract demand quantity and price as well as spot demand quantities are treated deterministic while spot sales prices are considered stochastic.

3.1.2 Derivation of price–quantity functions for spot demand

In the value chain network investigated the following entities have to be considered in the formulation of the sales model:

- *Products* include finished products sold on the market, intermediate products produced and raw materials procured.
- *Locations* represent the nodes of the value chain network such as sales, production or procurement locations.
- The planning horizon is divided into discrete time buckets (*periods*), months by default.

Demand and sales are planned for all valid product–sales location combinations $\{p, l\} \in PL^S$ and a medium-term planning horizon covering periods $t \in T$.

Given the simplifying assumption that transit times between production and sales locations and thus inventory balances can be neglected, the model can be separated by time periods and periods could even be neglected. The same is true for locations. However, from an industry-practice perspective, it is important to show the monthly development and interrelationships of sales and operation figures thus making the dynamics in the value chain across business functions and the volatility in profits, prices and volumes more transparent. Thus, instead of performing single period experiments a model formulation is suggested that integrates all activities within the entire planning horizon. Locations are essential as reference points for the aggregation of demand and the determination of the price–quantity functions. In the real application, transit times as well as intermediate inventories, safety stocks, etc. can easily be embedded into the model formulation.

Demand input data comprise the demand forecast provided by the “Sales and Marketing” organization of the company. Demand forecasts are aggregated from a single customer level to an aggregated sales location level. The contract demand forecast indicates the total demand quantities of all relevant products for each period and product–location combination. In addition, the corresponding average sales price can be derived from the customer contracts. Owing to the usual contract terms, total sales turnover achieved from contract sales is fixed.

In contrast, total sales turnover achieved from spot sales depends on the decisions of the company on spot prices and sales quantities for each period and product-location combination. As explained in the previous subsection, the company receives quantity and price bids from its spot market customers. In addition, the local “Sales and Marketing” units forecast expected bids for future periods. It is important that *all* spot sales opportunities are forecasted as total demand bids regardless of whether production capacity needed to fulfill this demand is available or not. It should be noted that the resulting average spot sales price increases if the spot demand exceeds the production capacity and the company selects the spot demand bids with the best spot sales prices. This relationship is expressed by the elasticity ε defined as $-\varepsilon = (\Delta p/p) : (\Delta x/x)$. Here, the elasticity can be interpreted as the change of the average spot price p with respect to the change of the spot sales quantity x. Forecasting individual customer spot demand for 6–12 months is more difficult than forecasting the overall spot market demand. The latter is essential in order to evaluate if spot demand exceeds own supply. To model the relationship between spot price and quantities, we show how adequate *price–quantity functions* can be derived from the forecasted customer bids.

The derivation of price–quantity functions is based on the following major assumptions:

- The relationship between spot sales price and spot sales quantity can be modeled as a linear function within the feasible minimum and maximum quantities defined by the management of the company. Of course, the price–quantity relationship could also be modeled using a non-linear function depending on the actual price–quantity bids the company receives. In our case we found that the linear function showed a sufficient statistical fit based on the real data provided by the company.

- External factors affecting the spot demand quantity, e.g., competitor actions, are not considered, i.e., spot sales demand only depends on spot sales price for each period and product–location combination.

The detailed steps of the algorithm for determining the price–quantity function for spot sales demand and a numerical example are provided in Table 1. To keep the presentation simple, we assume one single period and one individual product–location combination, i.e., the corresponding indices are omitted. Given are spot demand quantity q_c and price forecast p_c for individual customers $c \in C$ (step 1). The spot demand forecast by price and quantity represent future sales opportunities defined by the "Sales and Marketing" unit of the company. Historical sales can provide some guidance. However, anticipating future price trends in the market also depends on future demand and the raw material price development. Note that the forecast does not have to be necessarily discussed with the customer but can and should be based on the market knowledge of the "Sales and Marketing" organization also reflecting targets and new sales opportunities which "Sales and Marketing" wants to actively pursue in the market. Next, all price forecasts are sorted in non-increasing order giving ranks $r = 1, \ldots, R$ (step 2). In step 3, demand forecast quantities q_c are summed up to a cumulated spot demand quantity Q_r for each rank $r = 1, \ldots, R$ with Q_R being the total demand quantity across all forecasts In step 4, the corresponding average spot demand price forecast P_r for each rank $r = 1, \ldots, R$ is determined with P_R being the average price across all forecasts. In the following steps 5 and 6, the quantity share Q_r/Q_R and the average price ratio P_r/P_R of each rank $r = 1, \ldots, R$ are determined.

Table 1 Algorithm to determine the price–quantity function of spot demand and numerical example

Algorithmic steps	Customer			
	A	B	C	D
1. List individual customers $c \in C$ with spot demand quantity q_c and price forecast p_c				
Quantity (t)	100	200	100	200
Price (€/t)	100	90	80	70
2. Sort forecasts in non-increasing order of price using ranks $r = 1, \ldots, R$				
Rank	1	2	3	4
3. Determine cumulated spot demand quantity Q_r for rank $r = 1, \ldots, R$				
Σ Quantity (t)	100	300	400	600
4. Determine average spot demand price P_r for rank $r = 1, \ldots, R$				
Ø Price (€/t)	100	93.3	90	83.3
5. Determine quantity share Q_r/Q_R of rank $r = 1, \ldots, R$				
Δ Quantity (%)	17	50	67	100
6. Determine average price ratio P_r/P_R of rank $r = 1, \ldots, R$				
Δ Price (%)	120	112	108	100
7. Perform linear regression for price ratios and quantity shares				
Regression	$y = -0.2407 \cdot x + 1.2408$; $R^2=1.00$			
8. Determine price elasticity				
Elasticity	$\varepsilon = 0.2407$			

In step 7 a linear regression for price ratios with respect to quantity shares is carried out giving the price–quantity function. Finally, the spot demand elasticity is obtained as the negative slope of the regression function (step 8). Note that the elasticity is determined based on linear regression considering the quantity shares and average price shares and not the absolute quantity and average prices in the price–quantity function.

This proposed algorithm requires a sufficient number of individual customer bids or forecasts within one sales location and thus relies on effective support by the local “Sales and Marketing” units. If the number of price–quantity bids is not sufficient and the regression is not accurate enough, elasticities cannot be directly used for decision making. In this case, elasticity is assumed to be 0 meaning no price effects are included in the model and calculated profits are lower and more cautious than in reality. If all customers have the same spot prices, the average price is equal to the individual prices and the elasticity is equal to 0 meaning that no average price effects occur in case of volume reductions. In the investigated example from the chemical industry, we observed that price elasticities were volatile and ranked mainly between 0.1 and 0.5 different by month, product and locations analyzed for 12 months. The number of customers for one product and one location varied each month between 10 and 36. The R-squared value for the linear regression varied monthly between 0.4 and 0.99. Without having conducted a full elasticity analysis across the entire portfolio, the analysis helps to prove market perceptions such as a higher elasticity exists in one market compared to another market or comparing elasticity between products being perceived to have a different elasticity. The statistical quality of the linear regression analysis in selected months was considered as good in terms of the number of customers involved and the R-squared value proving the applicability of the approach. Alternatively, a quadratic regression of the sales turnover curve could be applied. This concept, however, does not create the same basis for understanding in the “Sales and Marketing” organization of the company since elasticity is the parameter known in “Sales and Marketing” to discuss and understand price–quantity dynamics in the market rather than discussing quadratic regression parameters that cannot be well understood and translated into direct price-quantity-relations.

Another issue of considerable practical importance in commodity markets is the uncertainty of market prices arising from a great number of external factors. In our case study investigation, price uncertainty is reflected by alternative price scenarios $s \in S$. In the real application, scenarios have to be defined for each product–location combination. To keep the presentation simple, we again consider only one single product–location combination.

To model the volatility of market prices, a price factor δ_s for spot demand price, e.g., 0.8, 1.0 and 1.2, and a corresponding subjective scenario probability ω_s valid for the entire planning horizon have to be defined by management. Typically three scenarios *“worst”*, *“best”* and *“average”* are used in order to limit the complexity and keep the scenario planning pragmatic. The price scenario philosophy of the company is to have only one single sales plan with quantity x_0 that is executed in the market at different price levels p_s. In addition we assume identical price–quantity functions, i.e., identical spot demand elasticity for all price scenarios meaning that the price factor δ_s is impacting all customers homogenously not changing their spot demand volume.

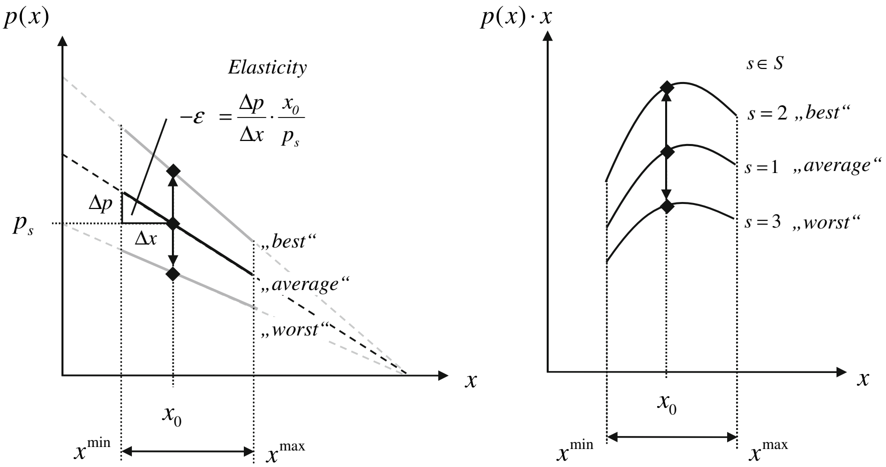


Fig. 3 Price–quantity function and sales turnover curve for individual price scenarios

Figure 3 illustrates the concept of scenario-based price–quantity functions, which basically describe the dependency of sales price p on quantity x. With price–quantity function $p(x)$ the resulting sales turnover is given as $p(x) \cdot x$. The scenario-based price–quantity functions have different slopes but the elasticity considering relative average price shares and relative quantity shares is identical in each scenario. In addition to given input data, *sales control data* are defined by the planner executing sales and marketing business rules to set the boundaries for spot sales quantities. Control parameters $x^{\min}$ and $x^{\max}$ indicate the minimum and maximum spot demand that needs to be fulfilled as shown in Fig. 3.

The concept of scenario-dependent sales turnover functions represents a significant advantage of demand *price* scenarios compared to demand *quantity* scenarios, since the company does not have to manage different volume scenarios creating high complexity in all areas of planning from sales to procurement. Moreover, the scenario price factors can be directly applied to model the sales turnover in the objective function of the optimization model without affecting quantity constraints of the model. This advantage might change the perspective on demand uncertainty from quantity scenarios towards price scenarios related to a defined sales quantity. This is even more practicable, since prices can be changed faster in practice compared to production volumes and material flows. In particular in the production of chemical commodities, considerable changeover times of the processing equipment have to be considered. Moreover, transportation lead times and limitations on transit stock often reduce the flexibility to adjust production quantities and redirect material flows on short notice.

3.1.3 Linear approximation of spot sales turnover

Since spot price and quantity depend on each other according to the linear price–quantity function, the profit function is quadratic. In the following, we show how a piecewise linear approximation of the sales turnover function can be achieved. This

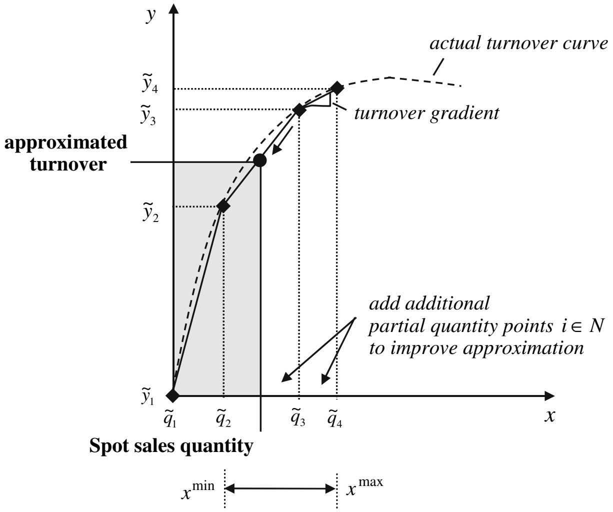


Fig. 4 Linear sales turnover approximation approach

approach is based on the concavity property of the sales turnover function and the limited region of sales quantity flexibility to be considered. For a review of linear approximation techniques for non-linear functions see Kallrath (2002b). For the optimization problem investigated in this paper, some application-specific features have to be considered which are described in the following. As in the previous subsection, we skip the indices for periods and product–location combinations in order to improve the understandability of the presentation.

The sales turnover approximation approach illustrated in Fig. 4 is based on partial quantity points subdividing the sales turnover curve into multiple sections, for which sales turnover is linearly approximated. As explained in the previous subsection, $x^{\min}$ and $x^{\max}$ are given as management-defined control parameters, which indicate the minimum and maximum spot demand that needs to be fulfilled, respectively. The set of partial quantity points $i \in N$ has four elements by default: 0, $x^{\min}$, Q_R and $x^{\max}$, where Q_R indicates the total quantity of all forecasted customer quantities (see the algorithm for determining the price–quantity function in the previous subsection). Note that $x^{\max} > Q_R$ expresses the possibility of gaining additional spot market qauantity at lower sales prices. In the case of $x^{\max} = Q_R$ only forecasted orders are considered. The three non-zero points are fixed and indexed by $i^{\min}$ for $x^{\min}$, i^{mid} for Q_R and $i^{\max}$ for $x^{\max}$. The approximation can be improved by adding additional partial quantity points i^+ between $i^{\min}$, i^{mid} and i^{mid}, $i^{\max}$, respectively. Partial spot sales quantities $\tilde{q}_i$ are determined at each partial quantity point $i \in N$. Corresponding partial spot sales turnover $\tilde{y}_i$ values are calculated for each partial spot sales quantity $\tilde{q}_i$ using the exact sales turnover function. Partial spot sales turnover between two partial quantity points is approximated based on the spot sales turnover gradient of the linear connection for the partial quantity section $j = 1, \ldots, N - 1$ between two partial quantity points.

Since the sales turnover curve is concave and the linear sales turnover gradients decrease monotonically, no integer variables are required to decide which partial quantity section is filled first. The objective function to maximize sales turnover will ensure to fill the partial quantity sections from left to right. It should be noted that the linear sales turnover approximation does not depend on the individual sales price scenario.

3.1.4 Constraints of the sales model

Before the constraints that make up the sales model are presented, the respective notation has to be defined. Note that some variables, e.g., for modeling aggregate sales figures, are introduced to improve the readability of the model formulation. These variables could be replaced by the corresponding expressions.

Indices, index sets

$p \in P$	products
$l \in L$	locations
$l \in L^S$	sales locations
$i \in N$	partial quantity points
$j = 1, \ldots, N-1$	partial quantity sections
$t \in T$	periods
$\{p, l\} \in PL^{\text{Sal}}$	valid product–sales location combinations for sales products

Parameters

q^{Sc}_{plt}	contract demand quantity forecast for product–sales location combination $\{p, l\}$ and period t
$\underline{X}^{Ss}_{plt}, \overline{X}^{Ss}_{plt}$	minimum and maximum spot sales quantity for product–sales location combination $\{p, l\}$ and period t, respectively
τ^{Ss}_{jplt}	spot sales turnover gradient of the linear sales turnover approximation for partial quantity section j, product–sales location combination $\{p, l\}$ and period t
$\tilde{q}^{Ss}_{iplt}$	partial spot sales quantity at partial quantity point i for product-sales location combination $\{p, l\}$ and period t
p^{Sc}_{plt}	contract sales price for product–sales location combination $\{p, l\}$ and period t

Decision variables

x^{S}_{plt}	total sales quantity for product–sales location combination $\{p, l\}$ and period t
x^{Ss}_{plt}	spot sales quantity for product–sales location combination $\{p, l\}$ and period t
$\tilde{x}^{Ss}_{jplt}$	partial spot sales quantity for partial quantity section j for product–sales location combination $\{p, l\}$ and period t
y^{Ss}_{plt}	spot sales turnover for product–sales location combination $\{p, l\}$ and period t

$\tilde{y}^{Ss}_{jplt}$	partial spot sales turnover for the partial quantity section j for product–sales location combination $\{p, l\}$ and period t

In the following, only the constraints of the sales model are presented. Additional constraints of the supply model are presented in Sect. 3.2.3. Finally, the objective function for maximizing the profit for the entire value chain network is defined in Sect. 3.3. It should be noted that constraints of the sales model do not depend on the individual spot sales scenario.

The total sales quantity is obtained as the sum of contract sales and spot sales quantity:

$$x^{S}_{plt} = x^{Ss}_{plt} + q^{Sc}_{plt} \quad \forall \{p, l\} \in PL^{\mathrm{Sal}}, t \in T \tag{1}$$

The spot sales quantity is limited between minimum and maximum boundaries:

$$\underline{X}^{Ss}_{plt} \leq x^{Ss}_{plt} \leq \overline{X}^{Ss}_{plt} \quad \forall \{p, l\} \in PL^{\mathrm{Sal}}, t \in T \tag{2}$$

The total spot sales quantity equals the sum of the partial spot sales quantities:

$$x^{Ss}_{plt} = \sum_{j=1}^{N-1} \tilde{x}^{Ss}_{jplt} \quad \forall \{p, l\} \in PL^{\mathrm{Sal}}, t \in T \tag{3}$$

Partial spot sales quantities need to fit in the respective section between consecutive partial spot sales quantities:

$$\tilde{x}^{Ss}_{jplt} \leq \tilde{q}^{Ss}_{iplt} - \tilde{q}^{Ss}_{i-1,plt} \quad \forall \{p, l\} \in PL^{\mathrm{Sal}}, i \in N, i > 1, j = 1, \ldots, N-1, t \in T \tag{4}$$

Partial spot sales turnover is given as the product of partial quantity and partial sales turnover gradient:

$$\tilde{y}^{Ss}_{jplt} = \tau^{Ss}_{jplt} \cdot \tilde{x}^{Ss}_{jplt} \quad \forall \{p, l\} \in PL^{\mathrm{Sal}}, j = 1, \ldots, N-1, t \in T \tag{5}$$

The spot sales turnover equals the sum of the partial spot sales turnovers:

$$y^{Ss}_{plt} = \sum_{j=1}^{N-1} \tilde{y}^{Ss}_{jplt} \quad \forall \{p, l\} \in PL^{\mathrm{Sal}}, t \in T \tag{6}$$

Further constraints, for example, on sales contract quantity rules and flexibility are possible but excluded here.

3.2 Supply model

3.2.1 Procurement and consumption of raw materials for chemical commodities

Variable raw material consumption rates in production
Raw material consumption in production is traditionally treated as constant based on given recipe factors. Recipe in the chemical industry is a synonym for the bill-of-material in discrete parts manufacturing and includes all input products with their respective input fraction required to produce one unit of one or several output products in a production process. However, in chemical production the degree of raw material consumption rates and hence the recipe factors often depend on the processing mode of the equipment, which can be employed at different utilization or throughput levels. In this case the recipe is not composed of static input factors but of recipe functions, which express the relationship between the input consumption and the output quantity produced. Hence the problem of how to decide on raw material consumption and how to balance volatile raw material costs with sales quantities and prices needs to be solved.

Spot and contract procurement
Raw materials are procured either based on fixed contracts or on the spot market. Differences in spot and contract prices have been observed in many business sectors, cf., Reiner and Jammernegg (2005). In analogy to the demand side, procurement contracts are fixed by quantity and price with the objective to ensure a basic supply of raw materials. Spot procurement supports the requirements of the company for flexibility in supply and sales planning facing uncertain market prices. By utilizing spot procurement the company can decide the actual procurement quantity with certain flexibility around the offered quantity. Price levels for contracts and spot business differ and are volatile.

3.2.2 Modeling flexible recipes

Key issues of the supply model are to decide on the variable raw material consumption rates in production and on spot procurement quantities. Both issues are highly interrelated, i.e., high production rates determine the amount of raw material that has to be supplied. Moreover, raw material costs per output ton produced can grow with higher production utilization and throughput rates. In the overall context of value chain optimization, production rates have to comply with decisions reflected by the sales model, e.g., on spot sales quantities and prices.

In the following, the basic principle of flexible recipes is presented. To keep the explanations simple, we consider only one single type of finished product that is produced from one single raw material on one resource at a specific location during a given period, i.e., indices for input and output products, resources, locations, and periods are omitted. In the real application, however, there are multiple input products. Typically, one input product represents the main feed into the production process while the others are auxiliary substances which can be procured on short notice.

Let C denote the production capacity of the resource measured in tons of output per period and let x^{in} and x^{out} indicate the input of raw material and output of finished products, respectively. Capacity utilization is defined as $U = x^{\text{out}}/C$. Minimum utilization rates and the capacity as maximum utilization rate have to be maintained. Even in periods with extremely low demand, production processes must run at a minimum utilization rate to ensure process stability and product quality. A complete shut-down of an asset is technically feasible, for example, in the case of planned maintenance or in emergency cases but not considered as a planning option in regular operations. In many types of chemical mass production, raw material consumption depends on the utilization rate of the equipment employed. Hence, linear recipe functions can be derived, which indicate the input of raw material required to produce the desired amount of output.

In Table 2 the derivation of linear recipe functions is explained using a numerical example. Utilization rates are given in steps of 20% assuming that all rates are used with equal probability. Capacity is given at 1,440 tons per day. The next two rows indicate pairs of input and output quantities for each utilization rate. These figures can be derived from the technological parameters of the production equipment. The recipe factor is defined as the ratio of input to output quantities. Note that recipe factors only refer to the main raw material and do not include other input materials. This explains the value of the recipe factor of less than 1.0 for $U = 20\%$. Finally, linear regression is applied with respect to the recipe factors. As a result, a variable consumption factor of $a = 1.3$ and a constant factor of $b = -144$ are obtained based on the given utilization rates and the underlying technological parameters.

The special case of a static recipe is given for $b = 0$. In this case, the raw material consumption does not change with capacity utilization. Otherwise the recipe factor grows with increasing resource utilization. The linear recipe function for the example of Table 2 is illustrated in Fig. 5. As a reference case, the static recipe is shown. Linear recipe functions are one type of recipe found in chemical industry. Of course other forms of recipe functions are possible depending on the consumption pattern analyzed for a specific resource.

In the supply model production input and output quantities depend on each other according to the recipe functions. Output and utilization decisions determine the raw material quantities to be supplied at each location. As mentioned before, raw materials are procured in both spot and contract mode. While contract procurement needs to be executed as agreed, spot procurement is flexible with minimum and maximum quantities for each type of raw material and each product–location combination. The company decides on spot procurement quantities within these intervals.

Table 2 Linear recipe function example

Utilization rate U	20%	40%	60%	80%	100%
Capacity C	1,440	1,440	1,440	1,440	1,440
Raw material input quantity x^{in}	230	605	979	1,354	1,728
Production output quantity x^{out}	288	576	864	1,152	1,440
Recipe factor ($x^{\text{in}}/x^{\text{out}}$)	0.80	1.05	1.13	1.18	1.20
Linear regression w.r.t. recipe factors	$x^{\text{in}} = 1.3 \cdot x^{\text{out}} - 144$; $a = 1.3,\ b = -144$ $R^2 = 0.99$				

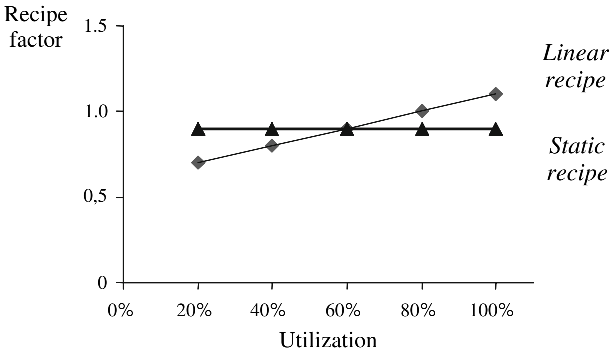


Fig. 5 Static recipe and linear recipe function

3.2.3 Constraints of the supply model

Before the constraints which make up the supply model are presented, the respective notation has to be defined. Note again that some aggregate (redundant) variables are introduced to improve the readability of the model formulation.

Indices, index sets

$p \in P$	products
$l \in L$	locations
$r \in R$	resources
$t \in T$	periods
$l \in L^P$	production locations
$l \in L^O$	procurement locations
$l \in L^S$	sales locations
$\{p, r\} \in PR^{\text{in}}, PR^{\text{out}}$	valid input/output product–resource combinations
$\{p, l\} \in PL^{\text{in}}, PL^{\text{out}}$	valid input/output product–production location combinations
$\{p, l\} \in PL^{\text{Proc}}$	valid product–procurement location combinations for procured products
$\{p, l\} \in PL^{\text{Sal}}$	valid product–sales location combinations for sales products

Parameters

C_{rt}^P	capacity of production resource r in period t
$U_r^{P\,\text{min}}$	minimum utilization rate of production resource r
a_{pr}, b_{pr}	parameters of the linear recipe function for product–resource combination $\{p, r\}$
d_t	number of production days in period t
$c_{pr}^{P\text{var}}$	variable production cost per unit for product–resource combination $\{p, r\}$
$c_{plt}^{P\text{spot}}$	average cost rate per unit for spot procurement for product–procurement location combination $\{p, l\}$ in period t

$c_{plt}^{P\text{con}}$	average cost rate per unit for contract procurement of product–procurement location combination $\{p, l\}$ in period t
$q_{plt}^{P\text{con}}$	contract procurement quantity for product–procurement location combination $\{p, l\}$ in period t
$\underline{X}_{plt}^{P\text{spot}}, \overline{X}_{plt}^{P\text{spot}}$	minimum and maximum spot procurement quantity for product–procurement location combination $\{p, l\}$ in period t, respectively

Decision variables

$x_{prt}^{P\text{out}}$	production output quantity for product–resource combination $\{p, r\}$ in period t
$x_{prt}^{P\text{in}}$	production input quantity for product–resource combination $\{p, r\}$ in period t
$x_{plt}^{P\text{out}}$	production quantity for product–production location combination $\{p, l\}$ in period t
$x_{plt}^{P\text{in}}$	secondary demand in product–production location combination $\{p, l\}$ in period t
$x_{plt}^{P\text{spot}}$	procurement spot quantity for product–procurement location combination $\{p, l\}$ in period t
x_{plt}^{Proc}	procurement quantity for product–procurement location combination $\{p, l\}$ in period t
x_{plt}^{S}	total sales quantity for product–sales location combination $\{p, l\}$ and period t
$v_{prt}^{P\text{var}}$	variable production costs for product–production location combination $\{p, l\}$ in period t
v_{plt}^{Proc}	procurement costs for product–production location combination $\{p, l\}$ in period t

In the following, the constraints of the supply model are presented.

Capacity and minimum utilization rate limit the total production quantities of all products produced on the resource in a specific period:

$$U_r^{P\min} \cdot C_{rt}^P \le \sum_{\{p,r'\} \in PR^{\text{out}}: r'=r} x_{pr't}^{P\text{out}} \le C_{rt}^P \quad \forall r \in R, t \in T \tag{7}$$

The input quantity of intermediate or raw material products required depends on the production rate of the resource and the linear recipe function which is determined on a tons per day basis. Hence the number of production days needs to be considered in constraint (8).

$$x_{prt}^{P\text{in}} = \left(a_{pr} \cdot \sum_{\{p',r'\} \in PR^{\text{out}}} x_{p'r't}^{P\text{out}} \right) + \left(b_{pr} \cdot d_t \right) \quad \forall \{p, r\} \in PR^{\text{in}}, t \in T \tag{8}$$

Production output and input quantities are aggregated at the location level.

$$x_{plt}^{P\text{out}} = \sum_{\{p',r\} \in PR^{\text{out}}:p'=p} x_{p'rt}^{P\text{out}} \quad \forall \{p,l\} \in PL^{\text{out}}, t \in T \tag{9}$$

$$x_{plt}^{P\text{in}} = \sum_{\{p',r\} \in PR^{\text{in}}:p'=p} x_{p'rt}^{P\text{in}} \quad \forall \{p,l\} \in PL^{\text{in}}, t \in T \tag{10}$$

Given the simplified network with two dedicated resources at a single production location these constraints are not required. However, for practical reasons it is important to keep locations and resources separated, since key effects such as flexible recipes are related to specific resources and their technology rather than to an entire production location.

The total variable production costs are obtained as product of production quantity and variable production cost rate:

$$v_{prt}^{P\text{var}} = c_{pr}^{P\text{var}} \cdot x_{prt}^{P\text{out}} \quad \forall \{p,r\} \in PR^{\text{out}}, t \in T \tag{11}$$

Total procurement costs are calculated based on variable spot procurement quantities and fixed contract procurement quantities:

$$v_{plt}^{P\text{var}} = (x_{plt}^{P\text{spot}} \cdot c_{plt}^{P\text{spot}}) + (q_{plt}^{P\text{con}} \cdot c_{plt}^{P\text{con}}) \quad \forall \{p,l\} \in PL^{\text{Proc}}, t \in T \tag{12}$$

Total procurement quantities are obtained by summing up spot and contract procurement quantities:

$$x_{plt}^{\text{Proc}} = x_{plt}^{P\text{spot}} + q_{plt}^{P\text{con}} \quad \forall \{p,l\} \in PL^{\text{Proc}}, t \in T \tag{13}$$

Total spot procurement quantity is limited between the minimum and maximum boundaries:

$$\underline{X}_{plt}^{P\text{spot}} \leq x_{plt}^{P\text{spot}} \leq \overline{X}_{plt}^{P\text{spot}} \quad \forall \{p,l\} \in PL^{\text{Proc}}, t \in T \tag{14}$$

The following equation balances total supply quantities consisting of production and procurement quantities with total demand consisting of total sales quantity and secondary demand of production based on the assumption of single sourcing. In practice, material balances also include inventories and transportation quantities which are important in global networks with several weeks lead times and considerable transit inventories. Since we focus on the integration of business functions in value chains, these issues are beyond the scope of this paper.

$$\begin{aligned} &\sum_{l' \in L^P:l'=l} x_{pl't}^{P\text{out}} + \sum_{l' \in L^O:l'=l} x_{pl't}^{\text{Proc}} \\ &\quad = \sum_{l' \in L^P:l'=l} x_{pl't}^{P\text{in}} + \sum_{l' \in L^S:l'=l} x_{pl't}^{S} \quad \begin{array}{l} \forall \{p,l\} \in PL^{\text{out}},\ PL^{\text{in}}, \\ PL^{\text{Proc}},\ PL^{\text{Sal}},\ t \in T \end{array} \end{aligned} \tag{15}$$

3.3 Optimization strategies

The objective of the proposed modeling approach is to maximize profit for the entire value chain network. It is assumed that the company behaves risk-averse in face of the price uncertainty and seeks to ensure minimum profits. Two optimization strategies can be applied incorporating spot sales price scenarios to reflect price uncertainty (cf. Chen and Lee 2004):

- *One-phase optimization*: maximize expected profit across one or multiple price scenarios. This approach corresponds to the classical "expected value" maximization known from decision theory.
- *Two-phase optimization*: maximize expected profit across multiple price scenarios taking into account the constraint that a given minimum profit value is reached. From a practical point of view, this approach seems to be more appropriate in situations where a high variability of profit can be expected and the risk of low profit outcomes shall be minimized.

The one-phase optimization strategy considers one or multiple spot price scenarios. Each scenario (see Sect. 3.1.2) is characterized by the spot price factor δ_{plst}, which expresses possible spot price levels, e.g., 0.8, 1.0, and 1.2, for each relevant product–location combination $\{p, l\}$, period t and scenario $s \in S$. Each scenario is assigned a subjective probability ω_s. While supply decisions remain unchanged, the various spot price scenarios lead to multiple sales turnover scenarios that are realized with the same spot sales quantity. Since price scenarios are represented by specific price factors, they can be directly applied to model spot sales turnover in the objective function.

The expected profit determines the average profit across all price scenarios weighted with their scenario probability ω_s. With the notation defined in Sects. 3.1.4 and 3.2.3 the expected profit function can be defined as follows:

Contract sales turnover ↓ *Contract and spot procurement costs* ↓

Maximize

$$z^{\exp} = \sum_{t\in T}\left[\sum_{\{p,l\}\in PL^S}\sum_{s\in S} y_{plt}^{Ss}\cdot\delta_{plst}\cdot\varpi_s + \sum_{\{p,l\}\in PL^S} p_{plt}^{Sc}\cdot q_{plt}^{Sc} - \sum_{\{p,r\}\in PR^{out}} v_{prt}^{Pvar} - \sum_{\{p,l\}\in PL^{Proc}} v_{plt}^{Proc}\right] \tag{16}$$

Expected spot sales turnover ↑ *Variable production costs* ↑

The expected profit across multiple scenarios provides a more realistic picture of the future profit situation compared to one single scenario. However scenarios are consolidated and expressed as a single value based on their probability weights. The planner would have no information about potential worst case profits and might like to sacrifice expected profit opportunities for safety in exchange. This is addressed by the two-phase optimization approach.

The two-phase optimization strategy (see Figure 6) first maximizes the minimum scenario profit $z^{\min}$, which is lower or equal to all single scenario profits z_s, where z_s

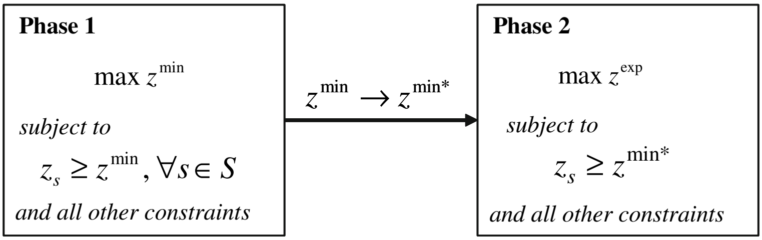


Fig. 6 Two-phase optimization strategy

is defined as follows:

$$z_s = \sum_{t \in T} \left[\sum_{\{p,l\} \in PL^S} y_{plt}^{Ss} \cdot \delta_{plst} + \sum_{\{p,l\} \in PL^S} p_{plt}^{Sc} \cdot q_{plt}^{Sc} - \sum_{\{p,r\} \in PR^{\text{out}}} v_{prt}^{P\text{var}} - \sum_{\{p,l\} \in PL^{\text{Proc}}} v_{plt}^{\text{Proc}} \right] \tag{17}$$

This first phase determines the best minimum profit $z^{\min}$ from all scenarios. $z^{\min}$ is then fixed as baseline profit $z^{\min *}$ for the second phase of the optimization, where the expected profit $z^{\exp}$ is maximized across all scenarios given the condition that each scenario profit reaches the minimum scenario $z^{\min *}$. This concept aims to obtain more robust solutions considering probabilistic demand quantity scenarios.

4 Case study evaluation

The optimization model presented in the previous section was implemented in ILOG OPL Studio 3.71 using CPLEX 9.1 as solver and was tested with industry case data on an Intel Pentium 4 PC with 1598 MHz and 256 MB RAM. Table 3 indicates the number of entities included in the case study evaluation.

For confidentiality reasons data from the company are sanitized in a way that data used for the case study evaluation are generated reflecting realistic dimensions of the investigated business application. However, data used in the simulation show the same scale. Several numerical experiments were carried out in order to analyze the impact of integrating sales and supply decisions by volumes and values based on the developed value chain planning model. Numerical results are presented in the following subsections.

4.1 Price scenario experiments

In the first experiment we compare the optimization strategies introduced in subsection 3.3 for different spot price scenarios. Two alternative demand spot price scenarios "best case" and "worst case" with equal probability of 0.25 are defined in addition to

Table 3 Number of entities in the case study evaluation

Basic elements	Number of entities
Products	50
- Finished	48
- Intermehdiate	1
- Raw material	1
Locations	11
- Sales	9
- Production	1
- Procurement	1
Resources	2
- Continuous	1
- Multi-purpose	1
Periods	6

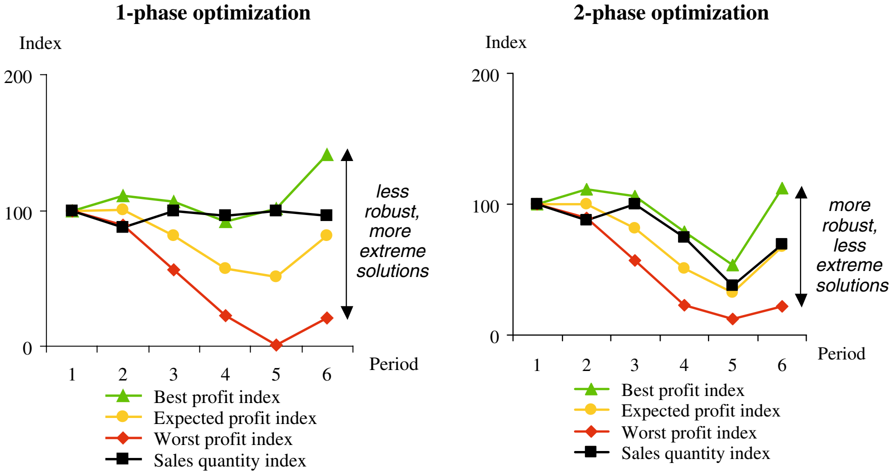
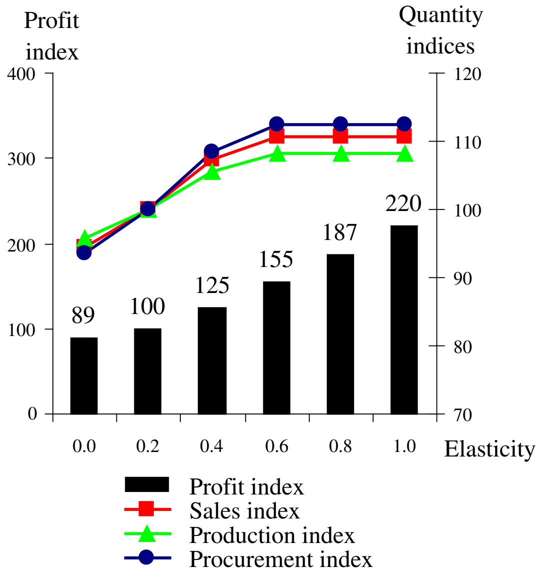


Fig. 7 Comparison of the 1-phase and 2-phase optimization strategies

the standard scenario with probability 0.5. The best case assumes a continuous price increase while the worst case assumes a continuous price decrease. Consequently the expected profit is the average of the best and worst case scenario results and equivalent to the standard scenario result in this special case. Numerical results are shown in Figure 7 for a planning horizon of six periods. Results of the one-phase optimization strategy show relatively constant sales quantities and expected profits slightly below the index value of 100. The results of the first period are indexed at 100 in order to compare the results of the subsequent periods with the first period.

Executing this sales plan can lead to very positive best-case scenario profits but also to very poor profits, if the worst-case price scenario occurs. Less extreme plans can be reached with the two-phase optimization strategy: scenario profits are less variable and the worst case scenario results are comparatively better than in the

Fig. 8 Elasticity model reaction test results



one-phase-optimization strategy. The overall value chain plan in sales, production and procurement is more cautious with lower sales quantities and lower expected profits as the pay-off for better minimum profits.

To conclude, the two-phase optimization results in lower average profits. In the real application, planners might also vary the subjective weights for the different scenarios or set alternative minimum profit levels. This way additional information on the robustness of the obtained solution and a better understanding of the complex relationships between volumes and values in a price-volatile commodity business could be gained.

4.2 Spot price elasticity test

The price elasticity of spot demand for all finished products is varied in multiple scenarios from 0 to 1. The base plan has the elasticity 0.2 and results for the elasticity value of 0.2 are indexed at 100. Elasticity of 0.2 means that the average sales price increases by 2%, if sales volumes are decreased by 10% and vice versa. Experiments are conducted applying the sales turnover approximation method with 24 partial quantity points to reach a high accuracy of the approximation as it will be evaluated in subsection 4.4. Experimental results shown in Figure 8 reveal that different elasticities lead to different optimal profits and quantities in sales, production and procurement, since sales volume-dependent average price effects are considered in the model.

In the specific case the base plan with an elasticity of 0.2 leads to a situation of under-utilization of production capacity, since high raw material costs can not always be compensated by sales prices. Higher elasticities lead to higher sales volumes, capacity utilization and profit increase since the relative sales volume increase can be realized with a lower relative average sales price decrease. In this situation it is profit-optimal to increase production and push additional sales volume into the market with lower sales prices. Full utilization is reached for elasticities of 0.6. Consequently an elasticity of 0.0 leads to lower profits, lower sales volumes and production utilization, since the insufficient sales price level does not change with sales quantity decisions.

Note that higher elasticity leads to higher sales and production volumes in this specific case of under-utilization due to the specific raw material prices and recipe functions. In case of full-utilization and different raw material prices and recipe functions, higher elasticities can also lead to a reduction of sales and production volumes if reduction of sales volumes and the respective increase of the average price is profit-optimal compared to supply costs. To conclude, the test demonstrates the influence elasticity can have on commodity sales and supply decisions and resulting profits.

Our numerical results reveal that considering average price effects reflected by elasticities can have significant influence on the overall volume plan. Hence, a profit-optimal supply and production plan does not necessarily maximize capacity utilization. Therefore, firms should not try to change or reduce elasticities but consider them in their sales and production planning taking the profit impact of price effects into account. Focusing on volumes alone and not considering existing price elasticity will lead to suboptimal plans and reduced profits.

4.3 Raw material price experiments

The influence of raw material prices on profit and utilization is investigated in the third experiment. Production capacity appears to be a bottleneck not sufficient to serve demand with full spot sales flexibility and elasticity of 0.2. Prices for the raw material required in the intermediate production process are varied around a basis index of 100 from 80 to 140. Two raw material recipe scenarios are considered: a static recipe factor of 1.2 and a linear recipe function, where raw material consumption rates increase from 0.8 at 50% utilization to 1.2 at 100% utilization. Figure 9 shows the results of the raw material price scenario experiments.

It is obvious from Fig. 9 that profit decreases in all cases, the more procurement prices increase. However the static recipe leads to comparatively higher sales and production volumes and lower profits compared to the case with the linear recipe function. The reason is that the static recipe represents the maximum factor of the recipe function that does not change. In comparison raw material consumption rates and costs can be decreased in the case of linear recipe functions by reducing the production utilization. Therefore, all volume indices are reduced in the case of linear raw material consumption, since raw material costs due to higher prices can be saved lowering production and raw material consumption. The opposite effect occurs if the maximum value of the recipe function values is higher than the static recipe factor. In both cases raw material unit costs cannot be directly allocated to production output as basis for product profitability and contribution margin analysis since raw material quantities and costs depend on overall value chain planning decisions. Our numerical results reveal that a recipe function with different raw material consumption rates depending on production utilization has a major impact on the optimal profit and on capacity

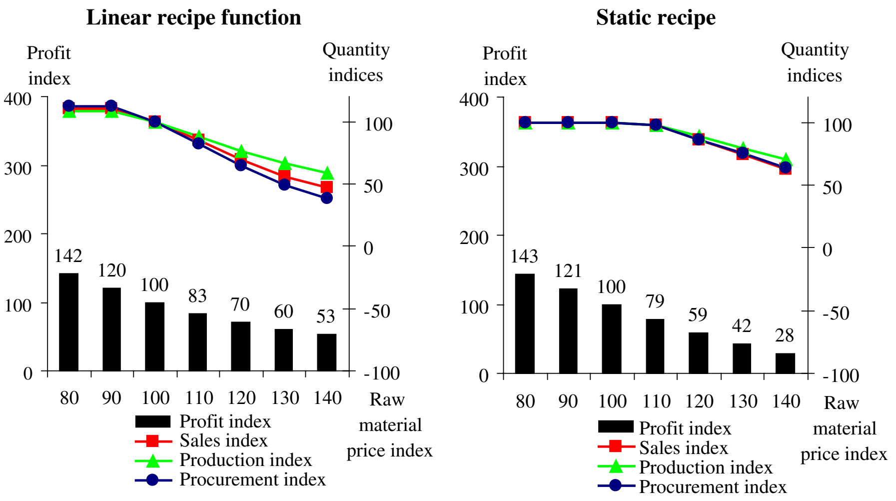


Fig. 9 Raw material price model reaction test results

Table 4 Sales turnover approximation model performance test

Partial quantity points	4	6	8	14	24	44	64
Constraints (thou.)	27	37	48	79	131	234	338
Variables (thou.)	24	35	45	76	128	232	335
Solution time (s)	1	2	2	5	28	118	276
Profit gap (%)	10.79	2.35	1.05	0.25	0.07	0.01	Basis

utilization. Not considering these dynamics would endanger a company's profitability when focusing only on maximizing production utilization.

4.4 Accuracy of the sales turnover approximation

Finally, the accuracy of the piecewise linear sales turnover approximation method is tested using the industry test data set and elasticities of 0.2. The number of partial quantity points is varied from 4 to 64 as shown in Table 4. Numerical results reveal that already 24 partial quantity points are sufficient to reach 99.93% of the objective function value obtained for the very accurate approximation based on 64 partial quantity points. The approximation is even more accurate if sales quantity flexibility is close to the forecast point. The approximation is less accurate, if spot sales quantities can be cut entirely as in the test data, since the sales turnover curve has highest gradients near the point of origin, where the gap between actual and approximated sales turnover is highest.

Considering the tactical planning purpose, run times of 1 min or less are acceptable in practice. These short run times even enable a planner to evaluate different scenarios, i.e., running the model with different parameter settings. To utilize the scenario mode of the optimization model, a small number of partial quantity points would suffice thus permitting solutions within only a few seconds.

4.5 Industrial application

As mentioned before, the presented optimization model has been developed as a prototype model to support the introduction of the Supply Network Planning module of an advanced planning system. In particular, our model helps to determine the required scope of the Supply Network Planning module implementation, to reveal the necessity of customizing the standard advanced planning software, and to evaluate the possible benefits for the company. Hence, the focus of our model formulation was to reflect the company's key optimization problem, namely balancing the consumption of a basic price-volatile raw material which is processed in continuous production mode with output volumes of more than 1 Mio. tons per year and coordinating the respective sales, production and procurement activities.

Prior to the implementation of an enhanced optimization model, the industrial company started a major business reorganization project in order to improve the coordination of business functions from procurement to sales for their global production sites and sales representations. In the course of this project several of the key instruments included in our model formulation were put into practice, in particular, the concept of spot and contract demand management and the instruments of demand elasticities and turnover functions as well as linear raw material recipe functions. Major effects of their application are the following.

- Changing the planning philosophy from pure demand fulfilment, which can be seen as the traditional supply chain management orientation, towards focussing on the global value chain profit by introducing demand management concepts based on the differentiation between spot and contract demand with active spot sales decisions helped the company to turn around the loss-making business unit into a highly profitable one.
- Recognizing the effects of spot demand elasticity and applying them in an integrated value chain planning effort provided the company additional insights into the dynamics of the global markets they are operating in. In fact, several markets show very high elasticities with significant price differences for the same product while demand on other markets is fairly insensitive to sales prices. These insights helped the company to make better sales decisions. Specifically, in the case of supply shortages decisions on cutting spot sales volumes could directly be derived from the model calculations.
- Incorporating linear raw material consumption functions and variable prices into the value chain planning model directly identified potential cost savings of several Mio. $ per year. Formerly, the company used to fully utilize production capacity. After gaining insights from the model application into the interdependencies between procurement and sales volume and prices and the use of different production modes, the company recognized that this is not necessarily the profit-optimal production strategy. Now managers seek to determine differentiated profit-optimal utilization levels for their key production assets at three global sites. As a result,

production volumes are shifted from less resource-efficient assets to the more efficient ones in the global network.
- The basic model is used by three global value chain planners for monthly planning of a global business unit. The model helped them to better understand the profitability levers in the value chain network from procurement to sales.

Further benefits are expected from introducing the Supply Network Planning module of an advanced planning software system to be used jointly with the Demand Planning and ATP/CTP modules which have already been implemented.

5 Summary and outlook

In this paper a model is presented to coordinate sales and supply decisions for commodities in a chemical industry value chain. Price–quantity functions, volatile and uncertain prices, flexible quantities in sales, procurement and production as well as utilization-dependent recipes create complex interdependencies which make it extremely difficult for the human planner to determine profit-optimal network-wide sales and supply plans even for small-sized value chain networks. Price–quantity function elasticities support decisions toward sales volume reductions or increases considering the effect of increasing or decreasing average prices. We evaluated the piecewise linear approximation approach to decide on sales turnover with sales price and volumes as variables. The approximation delivered very accurate results within short solution times and thus can be seen as an efficient approach to solve the underlying quadratic optimization problem. Variable raw material recipes have a direct impact on volumes and values, if raw material prices cannot be compensated by sales prices. Applying two-phase optimization strategies for sales price scenarios leads to more robust plans ensuring target profitability even in case of worst-case prices with the pay-off of more cautious and lower expected profits.

The model presented in this paper has been implemented by the company as basis for numerical investigations. The company has extended the basic model with further features such as inventory balances and transportation activities as well as exchange rates and further specifics of chemical commodity production such as throughput smoothing. Contract and spot sales planning has been implemented in their APS-based demand planning system and procurement planning for key raw materials have been established by their global purchasing department. Implementing these integrated sales and supply planning tools has shown major effects on the overall profitability of the business unit. Specifically the spot price mechanism used to better coordinate sales and supply decisions showed a major impact for the company.

Integrating sales and supply decisions throughout the value chain poses new interdisciplinary research questions as an outlook. Neither supply network planning minimizing costs to fulfill given demand nor revenue management maximizing revenue based on a given supply adequately addresses the problem of managing an industrial value chain end-to-end by volumes and value. Business rules for selling production output profit-optimal in contract or spot business as well as alternative methods to model price–quantity functions considering the impact on supply and profit are potential further areas of research. The overall research focus may shift from supply flexibility and cost minimization towards end-to-end supply, sales and pricing decisions to utilize the value chain in the most profitable way.

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