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Solving Planning and Design Problems in the Process Industry Using Mixed Integer and Global Optimization

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Abstract

This contribution gives an overview on the state-of-the-art and recent advances in mixed integer optimization to solve planning and design problems in the process industry. In some case studies specific aspects are stressed and the typical difficulties of real world problems are addressed.

Mixed integer linear optimization is widely used to solve supply chain planning problems. Some of the complicating features such as origin tracing and shelf life constraints are discussed in more detail. If properly done the planning models can also be used to do product and customer portfolio analysis.

We also stress the importance of multi-criteria optimization and correct modeling for optimization under uncertainty. Stochastic programming for continuous LP problems is now part of most optimization packages, and there is encouraging progress in the field of stochastic MILP and robust MILP.

Process and network design problems often lead to nonconvex mixed integer nonlinear programming models. If the time to compute the solution is not bounded, there are already a commercial solvers available which can compute the global optima of such problems within hours. If time is more restricted, then tailored solution techniques are required.

Keywords: Global Optimization, mixed integer programming, portfolio optimization, trilinear terms, concave objective functions, convex underestimators, origin tracing, shelf life time, petro-chemical industry, optimization under uncertainty, stochastic mixed integer optimization, robust mixed integer optimization

1 Introduction

The paper reviews some progress and the current state of planning and design in the process industry as far as mixed integer linear programming (MILP) ([91],[120]), mixed integer quadratic programming (MIQP), mixed integer nonlinear programming (MINLP) and global optimization techniques ([37],[112]) are concerned. We might touch certain aspects of scheduling, as the border line between planning and scheduling is vague [74]. However, scheduling is not the main focus and we refer the reader to Floudas & Lin (2004, [42]), Jia and Ierapetritou (2004,[65]), Janak *et al.* (2004,[64]), and Floudas & Lin (2005,[43]) for up-to-date reviews on scheduling using MIP and, in particular, continuous-time formulations. Readers interested in some excellent reviews on retroperspective and future perspectives of a broader set of optimization techniques are referred to [19] and [50]. In particular, for logic-based modeling and nonlinear discrete/continuous optimization problems we refer the reader to [81].

Planning is part of company-wide logistics and supply chain management. However, to distinguish or separate between planning and design, or even to distinguish between operative planning and strategic planning is often a rather artificial approach leading to unneccessary bottlenecks in operative planning. In reality, the border lines between those areas are diffuse and there are strong overlaps between planning in production, distribution or supply chain management and strategic planning. Kallrath (2003b,[72]) describes a successful case study in which operative and strategic planning aspects are combined in one MILP model. The client reports cost savings of several millions of US$. These cost savings were achieved via a reduction in transportation cost compared to the previous year when the model was not in use. The solution for a one year planning horizon allowed the company to better understand and forecast the flow of products between North America, Europe and Asia. This knowledge was then used to reduce the need and cost of urgent shipments. Moreover, it was beneficial to the client to see that the design solutions (which reactors to be opened or to be closed) were stable against up to 20% changes in the demand forecast.

After a brief discussion of special features and general comments on planning and design in the process industry this paper provides in Section 2 detailed MILP models to add three special features (origin tracing, shelf-life, and customer portfolio optimization) to MILP production and distribution problems. As the authors sees optimization under uncertainties and MINLP/global optimization as the two disciplines which will have a strong impact on planning in the process industry section 3 and 4 focus on these topics. Various case studies are discussed in Section 5. Section 6 provides a generic description of a challenging problem which might involve both optimization under uncertainties and MINLP/global optimization and attract the attention of researchers in those fields.

1.1 Special Features in the Process Industry

The production methods in the process industry but also the production facilities and their connections lead to a number of complications and to mixed integer linear and nonlinear optimization problems. The table summarizes the most frequent features; some of them are described in more detail in this paper):

LP	production planning	simple blending ([76], Section 5.1),
		enterprise-wide annual planning (Section 5.2),
NLP	production planning	blending accessing concentrations explicitly [68]
	multi-component flows	pooling problem ([36], Chap. 11 in [76], or [39])
	process design	reaction kinetics [68]
MILP	production planning	multi-purpose reactors with mode changes [71]
		batch and campaign planning [69], [52], [16] or [86]
		origin tracing (Section 2.1)
	logistics	variable tanks [113], semi-continuous transport [71]
		shelf-life (Section 2.2)
	marketing	customer portfolio analysis (Section 2.3)
	supply chain optimiz.	planning & distribution (Section 5.1)
	process operations	hybrid dynamic optimization problems [31]
MIQP	process operations	hybrid dynamic optimization problems [31]
	predictive control	predictive control of mixed logical dynamic systems [31]
MINLP	process design	process optimization [68], process synthesis and design [14]
		lay-out of reactors (Section 5.5)
		process systems engineering [51]
	network design	topology of production facilities and tanks [68]
		waste water treatment network ([79],[68])
	supply chain optimiz.	short term planning for petrochemical complexes [29]

One of the special features in the process industry is related to the multi-stage *continuous* and *batch production systems* involing multi-purpose equipment subject to sequence-dependent mode changes. Plants producing only a limited number of products each in relatively high volume typically use special purpose equipment allowing a continuous flow of materials in *long campaigns*, *i.e.*, there is a continuous stream of input and output products with no clearly defined start or end time. Alternatively, small quantities of a large number of products are preferably produced using multi-purpose equipment which are operated in *batch mode*, *i.e.*, there is a *well-defined start-up*, *e.g.*, filling in some products, well-defined follow-up steps defined by specific recipes, *e.g.*, heating the product, adding other products and let them react, and a *clearly defined end*, *e.g.*, extracting the finished product. Batch production involves an integer number of batches where a batch is the smallest quantity to be produced. Several batches of the same product following each other immediately establish a *campaign*. Production may be subject to certain constraints, *e.g.*, campaigns are built up by a discrete number of batches, or a minimal campaign length (or production quantity) has to be observed. Within a fixed planning horizon, a certain product demand can be covered by producing that product in several campaigns; this implies that campaigns have to be modeled as individual entities of unknown size. Determining the optimal size of such campaigns is referred to as the *lot sizing* or *campaign planning problem* (*cf.*, [52], [16] or [86]), a challenging problem in (supply chain) planning and design planning leading to MILP or MINLP problems. Kallrath (1999,[69]) shows how these features can be covered within MILP models based on time-discrete formulations. The lot-sizing problem usually occurs in (supply chain) planning problems, but it can also occur in design problems; the design problem posed in Section 6 contains a lot-sizing problem as a subproblem.

Another special feature in the refinery or petrochemical industry or process industry in general is the *pooling* problem (*cf.*, [36], or Chapter 11 in [76]), an almost classical problem in nonlinear optimization resulting from models describing multi-component mass flow problems in which several units of a production network are connected. It is also known as the *fuel mixture problem* in the refinery industry but it also occurs in blending problems in the food industry. The pooling problem refers to the intrinsic nonlinear problem of forcing the same (unknown) fractional composition of multi-component streams emerging from a pool, *e.g.*, a tank or a splitter in a mass flow network. The pooling problem occurs in all multi-component network flow problems in which the conservation of both mass flow and composition is required and both the flow and composition quantities are variable. Structurally, this problem contains bilinear terms (products of variables) appearing in equality constraints, *e.g.*, mass balances. It is therefore a nonconvex nonlinear problem. Nowadays the target is to solve larger pooling problems with global optimization techniques. Especially, the refinery industry due to decreasing margins is strongly interested in computing the global optimum and might benefit from current research activities on solving larger pooling problems (*cf.*, [1], [39], or [80]).

Nonlinear programming (NLP) models have been used by the refining, chemical and other process industries for several decades. State-of-the art NLP solvers use either sequential quadratic programming (`SNOPT` [47] is an example), advanced interior point methods ([118], [18], [50]), or generalized reduced gradient methods implemented in the commercial solver `CONOPT` [30]. In the refinery industry sequential linear programming (SLP) techniques are still in use. SLP solves NLP problems by solving a sequences of LP problems. All the approaches mentioned above suffer from the drawback of yielding only locally optimum solutions. Although many users may identify obviously sub-optimal solutions from experience, there is no validation of those which are not obviously so, as this would require truly globally optimal solutions. However, recent advances in optimization algorithms have yielded experimental academic and commercial codes which compute global optima of such problems and prove their global optimality.

In the chemical process industry, the proper description of the reaction kinetics leads to exponential terms. If, in addition, plants operate in discrete modes or connections between various units, *e.g.*, reactors, tanks and crackers or vacuum columns have to be chosen selectively [68], then mixed-integer nonlinear optimization problems need to be solved. Process network flow ([79],[80]) or process synthesis problems usually fall into this category, too. Examples are heat exchanger or mass exchange networks. Hybrid models describing process operations involving transitions between operating modes described by their own dynamic models, constraints and specifications lead to MILP or MIQP problems with special structure [31]. Recent reviews on process systems engineering with a focus on optimization applications are Grossmann *et al.* (1999,[51]), Floudas (2000,[38]) and Biegler and Grossmann (2004,[19]). Many design problems in the process industry including process, network, or facility design lead to nonconvex MINLP problems. Thus, they provide a fruitful terrain for global optimization techniques (*cf.*, [48], [19] and [50]). Current challenges in process design optimization are reviewed by Biegler and Grossmann (2004,[18]), and a yet unsolved problem is briefly described in Section 6 to attract researchers' attention.

Nonconvex nonlinear models are, of course not restricted to the oil refining and petrochemical sector, but arise in logistics, network design, energy, environment, and waste management as well as finance and their problems ask for global optimization; see Section 4 and Section 6.

1.2 Comments on Planning and Design in the Process Industry

Typical design problems in the process industry are related to the choice of chemical reactor technology, their size and number, and the production topology, *i.e.*, process design and network design. These design problems often lead to MINLP problems and are ideal to use global optimization techniques. The network design problem may involve the pooling problem described above.

Planning in the process industry is used to create production, distribution, sales and inventory plans based on customer and market information while observing all relevant constraints. In particular, operational plans have to be determined which are aimed to structure future production, distribution and other related activities according to business objectives. It is common practice that, based on these operational plans, detailed schedules are worked out which define the precise timing and sequencing of individual operations as well as the assignment of the required resources over time. Planning tools and software packages from various vendors are designed to incorporate new market and operational information quickly and help business users to keep their operations performing at their optimum. Especially, nowadays it is possible to find the optimal way to meet business objectives and to fulfill all production, logistics, marketing, financial and customer constraints.

Regarding the production facilities the planning (and also the scheduling) problems contain the following structural features:

- multi-purpose (multi-product, multi-mode) reactors,
- sequence-dependent set-up times and cleaning cost,
- combined divergent, convergent and cyclic material flows,
- non-preemptive processes (no-interruption), buffer times,
- multi-stage, batch & campaign production using shared intermediates,
- multi-component flow and nonlinear blending,
- finite intermediate storage, dedicated and variable tanks.

In production or supply chain planning, we usually consider material flow and balance equations connecting sources and sinks of a supply network. Time-indexed models using a relative coarse discretization of time, *e.g.*, a year, quarters, months or weeks are usually accurate enough. LP, MILP and MINLP approaches are often appropriate and successful for problems with a clear quantitative objective function (net profit, contribution margin, cost, total sales neglecting cost, total production for a fixed system of production reactors, energy consumption or the usage of other utilities, deviation of the usage of resources from their average usage), or quantitative multi-criteria objectives usually a subset of those just listed. The supply chain planning problems may contain many special features such as

batch production	order lost cost
buy or sell assets	product swaps
campaign production	production origin tracing
delay cost	shelf-life
nonlinear pricing	transportation and logistics
multi objectives	intermittent deliveries

This list covers many features but may be incomplete. In particular we stress that according to our experience several objectives or criteria need to be considered simultaneously (contribution margin, total production, totals sales, total turnover, costs, stocked products, transported products, etc.). Lexicographic goal programming seems to be a reasonable approach to deal with such situations because it leads to clear interpretations of the solutions.

For design as well as for planning problem one usually assumes that all data of a problem are given, *i.e.*, full knowledge of the future (of course, this is also an approximation since our knowledge of future demand or orders is uncertain), and that they are accurate. However, in reality, the input data are often subject to uncertainties. Those uncertainties can arise for many reasons:

- Physical or technical parameters or process control data, which are only known to a certain degree of accuracy. Usually, for such input parameters safe intervals can be specified.

- In strategic design optimization problems such as described and solved, for instance, by Kallrath (2002, [71]), demand and price forecast are used over a long planning horizon of 10 to 20 years. These predictions are subject to all sorts of uncertainties and can be at best quantified with some probability distribution or scenario approach.

Despite possible uncertainties in some input data, there are optimization problems which can be solved under the assumption of deterministic data without serious problems. Either the data show only small errors or uncertainties, or the problem and its structure is not sensitive with respect to such variations.

However, especially in long term or strategic planning the deterministic assumption is clearly not reasonable, but the results obtained at least provide enough intuition into the problem to justify the model. This reflects the fact that a clear decision on what approach is the best for solving a problem under uncertainty cannot be made *a priori* but rather after the problem is solved. Unfortunately, it may also happen, that assuming deterministic data does not provide accurate enough results to justify the model. Sometimes making that assumption can even be the reason that misleading results are obtained. The goal of optimization under uncertainty is to exploit uncertain data (*w.r.t.* the future) and incomplete information in such a way to improve the final quality of its overall performance, *i.e.*, the quality of decisions over rolling time horizons, or to increase robustness.

2 Special Features in Planning in the Process Industry

The features described in this section are extensions to the models and real world cases described in Kallrath & Wilson (1997,[76]), Timpe & Kallrath (2000,[113]) and Kallrath (2002,[71]). In several projects these features and their corresponding model formulations have been requested by clients. While there are better sources on modeling (*cf.*, [76], or [75]) the following sections are quite detailed stressing the importance of good modeling practice and formulations.

2.1 Keeping Track of the Origin of Products

In some cases customers assign an attribute to their orders. They may wish to get a product from a certain plant only, or that do not want to get it from a particular one, or that shipment should come from one plant only without specifying this plant explicitly. Thus the model incorporates the input data D^{A1}_{dpo} and D^{A2}_{dp}, which have the following meaning: if D^{A1}_{dpo} is specified for a combination of demand point d, product p, and origin o then it is interpreted as follows:

$$D^{A1}_{dpo} = \begin{cases} 1 & : \text{shipment of } p \text{ is allowed to come from origin } o \\ 2 & : \text{shipment of } p \text{ must not come from origin } o \end{cases} \quad .$$

If D^{A2}_{dp} is specified, *i.e.*, it exists, and has one of the following value

$$D^{A2}_{dp} = \begin{cases} 1 & : \text{at least one constraint is specified in } D^{A1}_{dpo} \\ 2 & : \text{shipment of } p \text{ always come from same origin} \end{cases} \quad .$$

If D^{A2}_{dp} is specified the feasible set of origins $\mathcal{O}_{dp}$ (note, it does not depend on time) for demand D_{dpt} is calculated according to the following scheme:

$$\mathcal{O}_{dp} = \cup \left\{ o | D^{A1}_{dpo} = 1 \right\}$$

or, alternatively,

$$\mathcal{O}_{dp} = \mathcal{O} \Big\backslash \cup \left\{ o | D^{A1}_{dpo} = 2 \right\} \quad .$$

Note the in both cases we exploit full complementarity, *i.e.*, the demand attributes for a certain order or demand should, for several origins o, only have $D^{A1}_{dpo} = 1$ or $D^{A1}_{dpo} = 2$ values.

To model the case $D^{A2}_{dp} = 2$ the sales variables s^L_{dpot} are coupled to the binary variables δ^T_{dpo}

$$\delta^T_{dpo} := \begin{cases} 1, \text{ product } p \text{ at demand point } d \text{ can be taken from origin } o \\ 0, \text{ otherwise} \end{cases} \quad ; \quad \forall \{dpo\} \quad ,$$

which control the flow of product p from origin o to demand point d. Note that there must be at least one possible origin for the demand, defined in table D^{A1}_{dpo}, and that these binary variables do not depend on time, *i.e.*, they either enable a connection from an origin o to demand point d for product p, or they forbid it for the whole planning horizon. This is ensured by the equations

$$\sum_{o \in \mathcal{O}_{dp}} \delta^T_{dpo} = 1 \quad ; \quad \forall \{dp\} \quad . \tag{2.1}$$

Let us now couple δ^T_{dpo} and s^L_{dpot}. The inequalities

$$s^L_{dpot} \leq M \delta^T_{dpo} \quad ; \quad \forall \{dpot\} \tag{2.2}$$

ensure that no sale of product p from origin o at demand point d is possible if $\delta^T_{dpo} = 0$. If $\delta^T_{dop} = 1$ then the inequalities (2.2) produce the redundant bounds $s^L_{dpot} \leq M$. Here, M is a sufficiently large upper bound. The best choice [see Kallrath & Wilson (1997,[76]), Section 9.1] is $M = D_{dpt}$. Note that sales variables cannot be created for origin "unknown" ($o =$ "X"), if D^{A2}_{dp} is specified.

2.2 Shelf Life Time - Keeping Track of Time Stamps

Certain performance chemicals or goods in the food industry have a limited shelf-life and are subject to an expiration date, or can only be used after a certain aging time. To trace those time stamps requires that individual storage means are considered, *e.g.*, containers or drums, which carry the time stamp or the remaining shelf-life.

Therefore, most of the data associated with inventories have to be duplicated for problems involving shelf-life w.r.t. to an additional shelf-life index. Other data are required in addition, *e.g.*, besides the amount given for the initial inventory we need to know when the product has been produced.

If the shelf-life of products expires, we assume that they have to be disposed. That might require them to be shipped to a certain disposal site. However, it is not necessary to model this process in details if we just restrict ourselves to some variable disposal cost (\$/ton) associated with each tons left over in an inventory and therefore identified as an amount to be disposed.

When product moves from a location to another location, a portion of the shelf-life is used for transport. When it arrives at the demand point its effective shelf-life is the total life minus the transport time.

The practical use of such the shelf-time feature would be if a customer (*e.g.*, food or a pharmaceutical company) ordered a batch of 200 kg of product that had a shelf-life of 6 months. If the product were not consumed by the customer in the 6 month window, then the product would be disposed at a cost of x \$/kg. Depending on the remaining shelf-life time h, a price of E^p_{dpth} can be achieved.

As an example we discuss the vitamin example in which vitamin tablets are made. The produce would mix pure vitamins A, B_{12}, C, etc. per a defined recipe in a blender to create 200 kg of a blend. The blend would then be packaged and a time stamp applied. The shelf-life in this case is one year and the manufacturer must sell the product within this window or dispose of the product at a cost of C^D_{lph} \$/kg. The vitamin producer would be able to sell the blends per a nonlinear schedule that is a function of the age of the product or the remaining shelf-life time, resp., *e.g.*, he receives 100% of the selling price if the product is sold from 1-6 months of its production, 80% within 7-10 months and 50% within 11-12 months. If the product is stocked longer than 12 months then the disposal costs of C^D_{lph} \$/kg need to be paid.

Let us add the shelf-life aspect to some dedicated product tanks. If for each product p there is an own tank available attached to each production site s then we talk about a dedicated product tank i with no restriction on origin o (note that the index o can take the value "free" or any value i). Such inventory entities are called *fixed-product variable-origin tanks* and are described by the balance equation for time period k

$$\begin{array}{c} s^S_{sipok} = s^P_{sipok} + \sum\limits_{v\in\mathcal{V}} p^E_{spvk} + t^{IS}_{spk} - t^{OS}_{spk} \\ - \sum\limits_{r|I^{Pipi}_{sr}=1} u^s_{srpk} + \sum\limits_{r\in\mathcal{R}\left|\left(I^{SRP}_{srp}=1\wedge I^{Pipi}_{sr}=1\right)\right.} p^T_{srpok} \end{array} \quad , \quad \forall\{sipok|o=\text{"free"}\} \tag{2.3}$$

with the source, s^P_{sipok}, entering from initial stock or stock from the previous time slice, $k-1$

$$s^P_{sipok} := \begin{cases} S^0_{sipo} & , k=1 \\ s^S_{sipok-1} & , 2\le k\le N^K_s \end{cases} \tag{2.4}$$

with the initial product stock, S^0_{sipo}, and stock, $s^S_{sipok-1}$, from the previous time slice. External purchase from vendor v is denoted by p^E_{spvk}, while u^s_{srpk} and p^T_{srpik} are used to describe the consumption and generation of products in the production process. The most complicated terms are t^{IS}_{spk} (t^{OS}_{spk}) denoting all incoming (outgoing) transport at site s. The incoming transport, t^{IS}_{spk}, at site s includes all incoming transport from other locations as well as shipment in transit from previous periods prior to the beginning of the planning horizon.

This is a generic description of shelf-life used to outline the concept. Products subject to shelf-life constraints are indicated by the table I^{SLP}_p; if $I^{SLP}_p=1$ then p is a shelf-life product, otherwise it is not. It is assumed that within the whole production network a product p is either a shelf-life product or it is not.

Let p^{PM}_{srpmk} be the production variable. A part (or all) of this amount of product p may be charged to tank i at site s. This amount is denoted by $p^{TS}_{srpikS^{LT}_{srpm}}$ where S^{LT}_{srpm} is the shelf-life of product p if it is produced on reactor r in mode m at site s. Note that the shelf-life depends on mode m, and the that the charge-to-tank variable p^{TS} also to depends on $h=S^{LT}_{srpm}$ to have a clear assignment to the appropriate tank (may be this is not really necessary). Therefore, the inventory balance equations which distributes products to tanks needs to be modified in order to account for the additional index shelf-life.

Now let us consider the tank balance equations at site s for a shelf-life product for a dedicated product tank (no restriction on origin). The original inventory balance equation (2.3) is modified and looks like

$$\begin{array}{c} s^{SH}_{sipokh} = s^{PH}_{sipok} + \sum\limits_{v\in\mathcal{V}} p^{EH}_{spvkh} \\ - \sum\limits_{r|I^{Pipi}_{sr}=1} u^{SH}_{srpkh} + \sum\limits_{r\in\mathcal{R}\left|\left(I^{SRP}_{srp}=1\wedge I^{Pipi}_{sr}=1\right)\right.} p^{TS}_{srpikh} \\ +t^{ISH}_{lspykh} - t^{OSH}_{lspykh} \end{array} \quad , \quad \begin{array}{c} \forall\{sipok|o=\text{"free"}\} \\ \forall\{1\le h\le S^{LT}_p\} \end{array}$$

with

$$s^{PH}_{sipok} := \begin{cases} S^0_{sipo} & , k=1 \\ s^S_{sipok-1} & , 2\le k\le N^K_s \end{cases} \quad , \tag{2.5}$$

and appropriately modified expressions for incoming and outgoing transport.

The sales variable s_{srpt}^L can extract product from all tanks with appropriate shelf-life

$$s_{srpt}^L = \sum_{u=1|}^{L_{srpm}} s_{srptu}^L \quad ,$$

where s_{srptu}^L denotes the amount of product taken from storage tank s_{srptu} with remaining shelf-life u. The balance equations for these tanks read

$$s_{siptu-1} = s_{sipt-1u} + f_{spt}^+ - s_{srptu}^L - f_{spt}^- \quad , \quad u = 2, \ldots, L$$

For $u = 1$ this balance equation involves a disposal variable s_{srpt}^W and the balance equation reads

$$s_{srpt}^W = s_{srpt-1u} + f_{spt}^+ - s_{srptu}^L - f_{spt}^- \quad , \quad u = 1 \quad .$$

Note that f_{spt}^+ and f_{spt}^- denote the material flow entering the inventory (production, incoming transport from the production sites or other sales points, external purchase, etc.) and leaving the inventory (sales, outgoing transport to other sales points, etc.), respectively. The model might associate disposal or penalty costs with the variable s_{srpt}^{DISP}.

Example 1: Consider a fixed site s, reactor r, product p with shelf-life time $u = 6$ weeks, 20 tons produced in mode $m = 3$ in week $\tau = 2$ (this means it still can be sold in week 8) put into inventory s_{sp26}, 10 tons produced in mode $m = 2$ in week $\tau = 4$ put into inventory s_{sp46}; no more of product p is produced. Now consider sales in week $t = 5$. So the total amount of sales s_{srpt}^L can be covered by what can be extracted from appropriate tanks, in this case $s_{sp53} = 20$ and $s_{sp55} = 10$.

Now consider the case that a product with remaining shelf-life is shipped to another inventory; the transport duration is finite. Therefore the balance equation reads

$$s_{dptu-1}^D = s_{dpt-1u}^D - s_{dptu}^L - \sum_{d_d \in \mathcal{D}_d} t_{dd_dptu}^{LL} + \sum_{\mu=1|u=\mu-T_{ldp}^D}^{L_{sp}} t_{ldpt-T_{ldp}^D\mu-T_{ldp}^D}^{LL} \quad , \quad u = 2, \ldots, L$$

with transport variables $t_{dd_dptu}^{LL}$ for shelf-life products and

$$L_{sp} := \max_{\{(r,m)|I_{sr}^{SR}=1 \wedge I_{srpm}^{SRPM}=1\}} \{L_{srpm}\} \quad .$$

For $h = 1$ we get again the equation involving the disposal variable

$$s_{dipt}^W = s_{dipt-1h}^D - s_{dipth}^L - \sum_{d_d \in \mathcal{D}_d} t_{dd_dpth}^{LL} + \sum_{\mu=1|u=\mu-T_{ldp}^D}^{L_{sp}} t_{ldpt-T_{ldp}^D\mu-T_{ldp}^D}^{LL} \quad , \quad h = 2, \ldots, L$$

The sales variables s_{dptu}^L associates with shelf-life products also allow to apply nonlinear specific revenue which might depend on remaining shelf-life:

$$\sum_{d \in \mathcal{D}} \sum_{p \in \mathcal{P}} \sum_{o \in \mathcal{O}} \sum_{t=1}^{N^T} \sum_{u=1}^{L_p} S_{dptu}^P s_{dpotu}^L \quad .$$

The disposal variable s^W_{dpt} can be associated with disposal cost.

$$\sum_{d\in\mathcal{D}}\sum_{p\in\mathcal{P}}\sum_{o\in\mathcal{O}}\sum_{t=1}^{N^T}\sum_{u=1}^{L_p} C^W_{dptu} s^W_{dpotu} \quad .$$

This model description is minimal with respect to the number of variables. The number of variables increases with the shelf-life.

2.3 Customer Portfolio Optimization

A more special feature in demand satisfaction is related to semi-continuous requirements on demand. There is a chance that some customers could be lost completely if they are not satisfied. This approach is a first step towards *customer portfolio optimization*.

In a more general framework solution a user might want to enter the percentage, D^{AF}_{dp}, of demand (aggregated over the whole planning horizon) that at a minimum must be satisfied for a customer. The alternative is not to satisfy any of the demand, *i.e.*, we are facing a semi-continuous constraint. If the percentage to which a certain demand needs to be specified is not specified, then the model can chose how much and when to supply as is currently practiced. If the general solution is implemented and the user specifies a percent value less than 100, then we also need a flag that indicates if the minimum percent of demand should be applied to all commercial periods equally or if the solver can chose when to supply the minimum total quantity. For example, if the user selects 50% as the minimum demand that must be satisfied, the commercial time horizon is 1 year with 12 periods, and the demand is 100 tons/period. Then the model may return the solution where the constraint of 600 tons is supplied during periods 7 - 12. This may not be practical as the user/customer wants to take 50 tons per period for periods 1-12.

Another likely scenario is to ask for solution which pick out 2 of 3 customers, *i.e.*, sell all of customer A and B's demand but not C. Or all of B and C's demand but not A. This is a realistic business scenario that is actually quite common.

We could deal with this type of situation if we classified customers (demand points) with a flag that indicates the condition that if any demand is satisfied then all demand must be satisfied. This flag would be active when you have a account that must either always have its demand satisfied or you make the choice not to sell to the account and therefore do not satisfy any of the demand.

Of course, this constraint is different from the one that requires a certain percentage of demand to be satisfied. The new constraint is not time dependant and it lets the solver choose to supply or not to supply. If supply is chosen then it must be fulfilled to 100% (or any other pre-fixed percentage, D^{AF}_{dp}).

To support customer portfolio optimization, we use at first the real variables, s^A, which express the aggregated sales for a given customer specified by the index combination $\{dp\}$. These variables are generated if the entry D^A_{dp} exist, where D^A_{dp} is generated if $\sum_{o\in\mathcal{O}_{dp}}\sum_{t=1} s^L_{dpot} > 0$. The aggregated sales is just

$$s^A_{dp} = \sum_{o\in\mathcal{O}_{dp}}\sum_{t=1}^{N^T} s^L_{dpot} \quad , \quad \forall \left\{ dp \,\middle|\, \exists D^A_{dp} \right\} \quad .$$

A simple customer portfolio analysis is performed by exploiting the input table D_{dp}^{AF}, $0 \leq D_{dp}^{AF} \leq 1$. D_{dp}^{AF} puts a semi-continuous minimum requirement on the total sales s_{dp}^{A} for the total demand D_{dp}^{T}, *i.e.*,

$$s_{dp}^{A} = 0 \vee D_{dp}^{AF} D_{dp}^{T} \leq s_{dp}^{A} \leq D_{dp}^{T} \quad .$$

Here, D_{dp}^{T} is the total demand of product p specified by customer $\{dp\}$ over the whole planning horizon, *i.e.*,

$$D_{dp}^{T} = \sum_{t=1}^{N^T} D_{dpt} \quad .$$

The additional parameter M^C is used to limit the number of total demands to be delivered. To model this feature, the binary variables δ_{dp}^{sA} are introduced which indicate whether demand d for product p should be considered or not. These variables are subject to the inequalities

$$D_{dp}^{AF} D_{dp}^{T} \delta_{dp}^{sA} \leq s_{dp}^{A} \leq D_{dp}^{T} \delta_{dp}^{sA} \quad , \tag{2.6}$$

and

$$\sum_{d \in \mathcal{D}} \sum_{p \in \mathcal{P}} \delta_{dp}^{sA} \leq M^C \quad . \tag{2.7}$$

3 Optimization Under Uncertainty

So far, in this article we focussed only on deterministic models. If the assumption that all data have to be treated as deterministic data is given up, we are lead to optimization under uncertainty, *i.e.*, optimization problems in which at least some of the input data are subject to errors or uncertainties, or in which even some constraints hold only with some probability or are just soft. Those uncertainties can arise for many reasons:

- Physical or technical parameters which are only known to a certain degree of accuracy. Usually, for such input parameters safe intervals can be specified.
- Process uncertainties, *e.g.*, stochastic fluctuations in a feed stream to a reactor, or processing times subject to uncertainties.
- Demand uncertainties occur in many situations: supply chain planning [53], investment planning [24], or strategic design optimization problems [71] involving uncertain demand and price over a long planning horizon of 10 to 20 years.

Regarding the conceptual problems involved in optimization under uncertainty it is not a surprise that it took until now that the number of applications using, for instance, stochastic programming is strongly increasing. The first step to model real world problem involving uncertain input data is to analyze carefully the nature of the uncertainty. Zimmermann (2000,[123]) gives a good overview what one has to take into consideration. It is very crucial that the assumptions are checked which are the basis of the various solution approaches. Below we list and comment on some techniques which have been used in real world projects or which one might think of to use.

- *Sensitivity analysis* is conceptually a difficult problem in the context of MIP, and is, from a mathematical point of view, not a serious approach to solve optimization problems under uncertainty [119]. Nevertheless, it is frequently used by engineers or logistic people to study the role of certain parameters or scenarios.

- *Stochastic Programming*, in particular *multi-stage stochastic models,* also called *recourse models*, have been used since long [see, for instance, Dantzig (1955,[28]), Kall (1976,[66]), Kall & Wallace (1994,[67]), Schultz (1995, [107]), Birge (1997,[20]), Birge and Louveaux (1997,[21]), or Carøe and Schultz (1999, [23])]. In stochastic programming, the models contain the information on the probability information of the stochastic uncertainty and the distribution does not depend on the decision in most cases. By now, most of the modeling languages used in mathematical optimization [*cf.* Kallrath (2004,[75])] use scenario-based stochastic programming for LP problems. While stochastic MILP (S-MILP) is an active field of research [detailed discussions on various algorithms for stochastic integer optimization can be found in the survey of Klein-Haneveld & van der Vlerk (1999,[78]) or Sen & Higle (1999,[111]), and, more recently, in the *Handbook of Stochastic Programming* [100], Schultz (2003,[108]), or Andrade *et al.* (2005,[9])] industrial strength software is still to enter the stage. We refer the reader also to a review of stochastic integer programming by S. Sen (2004,[110]). In another recent review Mitra *et al.* (2004,[89]) describe a classification of stochastic integer programs and they also describe case studies of solving very large scale SIPs applying Lagrangean relaxation technologies using serial and parallel machines ([88], [85]). In this context the work of Alonso-Ayuso *et al.* ([8], [7]) and Ahmed *et al.* [6] are also to be noted. To keep up-to-date, the reader might visit van der Vlerk's *Stochastic Programming Bibliography* [114] from time to time. Finally, a list of stochastic programming applications, especially for design and optimization of chemical processes, is given in [103].

- *Chance constrained programming* has also a long history and dates back to Charnes and Cooper (1959,[25]). A more recent overview on general chance-constrained methods is given by Prékopa (1995,[98]). While usually it is seen as a special approach within stochastic programming, it is here listed separately because it differs significantly from the multi-stage recourse approach. Chance constrained programming deals with probabilistically constrained programming problems, *i.e.*, a constraint holds with a certain probability, and is quite useful to model, for instance, service level features in supply chain optimization problems [*cf.*, Gupta *et al.* (2000,[54]), or Gupta and Maranas (2003,[53])]. Orçun *et al.* (1996,[94]) considered uncertain processing times in batch processes and used chance constraints to model the risk of violating temporal constraints. Arellano-Garcia *et al.* (2003,[10]) proposed a systematic approach to solving approach to solving nonlinear chance constrained optimization problems. In a follow up paper [11] they present a novel chance constrained optimization approach for solving optimal process design problem under uncertainty, in which optimal operational aspects and robust analysis are simultaneously considered. As stochastic programming, chance constrained programming also requires probability distributions to be specified. Unfortunately, chance constrained programming is not yet found in commercial software packages.

- *Fuzzy set modeling* supporting uncertainties which fall into the class of vague information and which are expressible as linguistic expressions [fuzzy set theory in the context of LP problems has been used, for instance, by Zimmermann (1987,[122]; 1991,[121] and Rommelfanger (1993,[99])]. This methodology is much younger than SP and is used when, from the SP point of view, the information is incomplete. Balasubramanian and Grossmann (2003,[13]) applied a fuzzy based approach to batch scheduling with uncertain times. A detailed list of applications of fuzzy programming has been compiled in the review article by Sahinides (2004,[103]).

- *Robust optimization* [see, for instance, Ben-Tal *et al.* (2000, [15])] is a relatively new approach to deal with optimization under uncertainty in case that the uncertainty does not have a stochastic background and/or that information on the underlying distribution is not or hardly available (which is, unfortunately, often the case in real world optimization problems). The approach replaces linear models by nonlinear ones. Direct extensions of Ben-Tal's approach for MILP problems have been developed for batch scheduling under uncertainty by Lin *et al.* (2004,[84]). A different approach to robust optimization has been developed by Bertsimas (2003,[17]). This approach claims to have the advantage that the type and the complexity of the problem does not change, and it is applicable to MILP problems. While in stochastic programming the number of variables increases drastically, in this robust optimization approach the number of variables approximately only doubles.

- Stochastic decision processes based on *Markov processes* [87] and/or the control of *time-discrete stochastic processes* allow for decision-dependent probability distributions but typically require stronger assumptions on the stochasticity. The paper by Cheng *et al.* (2003,[26]) gives an excellent illustration of such techniques applied to design and planning under uncertainty.

- *Global optimization* and the techniques, such as interval arithmetic, used in this field (*cf.*, [37], [60], [77] and [59]) may, to SP people, not appear as a particular tool to deal with uncertainties. Indeed, it has nothing to do with uncertainties as such (although uncertainties can be part of the deterministic equivalent model). However, global optimization, in particular when based on interval analysis, can provide safe results, for instance, in safety analysis. The author was once involved in a project modeling a chemical reactor, in which, under no circumstances, the pressure was allowed to increase a certain value. Thus, the problem was to establish, for a range of temperatures and other physical parameters subject to deviations from the nominal value, that the maximum pressure could never exceed the critical value. The problem briefly outlined in Section 6 may establish some further research in which optimization under uncertainty and global optimization will meet each other.

The variety of approaches (the list above is not complete, *e.g.*, Ryu *et al.* (2004,[101]) treat enterprise-wide supply chain networks under uncertainty by bilevel and parametric programming) supports the argument that the difficulties in modeling optimization problems under uncertainty are by far larger than those in deterministic optimization.

Despite the conceptual difficulties, it is strongly recommended that if some data, *e.g.*, demand forecast in planning models, or production data in scheduling are subject to uncertainties, one should consider whether the assumption that planning and modeling is exclusively based on deterministic data can be given up and uncertainty can be modeled. If probability distributions for the uncertain input data can be provided, stochastic programming is the mean of choice. Nowadays, there exist powerful solution techniques to solve stochastic mixed integer programming problems [100]. Successful applications of this techniques to scheduling problems in the chemical process industry are reported, for instance, by Sand *et al.* [105], Engell *et al.* [33], Sand and Engell (2004,[104]) and Lin *et al.* (2004,[84]); see Section 5.4 for details.

Process design optimization under uncertainty has also a long history in the process industry (*cf.*, [55], [97], [26]). Even global optimization techniques have been applied to design under uncertainty (*cf.*, [56] or [41]). This is another indication that optimization under uncertainty will play an important role in the near future because the available algorithms become better and better to address such problems.

Finally, it is worthwhile to mention that in the chemical process industry optimization under uncertainty has not been applied only to planning and scheduling but even to the detailed modeling of the underlying chemical processes. Henrion *et al.* (2001,[58]) have developed a detailed nonlinear physical, differential-equation based model to describe a distillation column with a feed tank. Process and feed stream uncertainties are modeled by scenario-based stochastic optimization. Probabilistic constraints are used to control stochastic storage tank levels. This work serves as a good example illustrating the importance to discuss carefully the kind of uncertainties occurring in the problem.

4 Mixed Integer Nonlinear and Global Optimization

Mixed integer nonlinear optimization is a field which benefitted strongly from the chemical engineering community and its process design and process engineering problems. Especially, Ignacio Grossmann (Carnegie Mellon University), Chris A. Floudas (Princeton University) and Nick V. Sahinidis (University of Illinois) have provided many fruitful ideas and algorithms to the community. The tremendous effort in this field has been reviewed recently by Floudas (2000,[37]), Tawarmalani and Sahinidis (2002,[112]), Grossmann (2002,[49]), and Floudas *et al.* (2004,[40]). The contributions in the book *Frontiers in Global Optimization* edited by Floudas and Pardalos (2004,[44]) give a good overview about trends and activities in the field. Below we focus on nonconvex NLP and MINLP problems. Here we mention only briefly that there exist already many algorithms and software packages to solve convex MINLP problems: `DICOPT` [32], `MINOPT` [109], or `LOGMIP` ([115], [116]) to mention a few which are properly published. Information on other packages, such as `AIMMS-OA` by Bisshop & Roelofs, `Alpha-ECB` by Westerlund & Lundquist, `MINLPBB` by Fletcher and Leyffer, or `SBB` by Bussieck & Drud can be found on the authors' webpages.

Process design and process engineering problems as well as other nonlinear problems in the process industry, unfortunately in most cases, are nonconvex problems and thus have many local optima. The problem of the existence of multiple local optima in nonlinear optimization is treated in a mathematical discipline of its own: global optimization, a field including theory, methods and applications of optimization techniques aimed at detecting a global optimum of nonlinear problems. Global optimization applies to both, NLP and MINLP. Problems analyzed in the context of global optimization are seen to be attacked by stochastic and deterministic solution approaches.

Stochastic methods are based on random sampling the search space providing upper bounds on nonconvex minimization problems. The metaheuristics genetic algorithms, evolution strategies, tabu search and simulated annealing are refinement of such random sampling methods. In the strict sense one might consider such techniques not as optimization methods at all because, due to the lack of lower bounds, they do guarantee neither optimality nor a certain quality of feasible points they may find.

In contrast, *deterministic methods* are based on progressive and rigorous reduction of the solution space until the global solution has been determined with a pre-given accuracy closing the gap between the upper and lower bound. Deterministic methods to solve nonconvex NLP or MINLP problems may be classified as primal-dual methods, interval methods, and B&B methods; they have in common that they derive upper and lower bounds including the objective function value of the global optimum. These methods are quite different from the classical concepts of gradients and Hessians used by local NLP solvers. Typical B&B methods, for instance, exploit convex underestimators of the objective function and convexify the feasible region; they divide the feasible region in subregions, solve the NLP problem on that reduced set, derive bounds and branch if necessary. While the B&B method in MILP problem is known to terminate unconditionally after a finite number of steps, B&B methods in global optimization are subject to convergence proofs. However, if we want to find the global optimum only up to a small number $\varepsilon > 0$ between the upper and lower bound, then the B&B will also terminate after a finite number of steps. Not only B&B methods, but all deterministic algorithms in global optimization have more in common with what is used in discrete optimization rather than in nonlinear continuous optimization. The *Journal of Global Optimization* or the books ([59], [61], [60], [77], [37] or [112]) are good and recommended starting points. Nowadays, there exist reliable and advanced solution algorithms and software package to solve nonconvex NLP and MINLP problems (*cf.*, Arnold Neumaier webpage mentioned below).

The family of products (α`BB` [4], [2], or [5]; `SMIN-`α`BB` and `GMIN-`α`BB`B [3]) developed in Chris A. Floudas's group at Princeton University is very advanced. Recent efforts at Princeton University and the Imperial College in London (England) allow it to apply this techniques also to optimization problems involving ordinary or partial differential equations [95], parameter estimation problems of differential-algebraic system [34], and optimal control problems (*cf.*, [35] or [90]).

Another center of activity in global optimization is Arnold Neumaier's working group at the University of Vienna. His group developed the global optimization program `GLOBT` [27] and his webpage http://www.univie.ac.at/˜neum is best and most informative one on global optimization and optimization in general – a visit is strongly recommended.

A Branch&Cut&Price algorithms has been developed by Nowak (2004a,[93]) to solve general nonconvex MINLP. This algorithms has been implemented in his C++ library `LaGO` [92] and provides promising results for smaller problems.

Finally, Nick Sahinidis's effort and progress he achieved with `BARON` (*cf.* [102], [46]), a general Branch&Bound solver based on polyhedral relaxation and box reduction, is remarkable and found its way into the GAMS modeling system [22]. Although nowadays the size of problems which can be solved is limited to a few hundred variables the presence of BARON in GAMS makes global optimization techniques more accessible to a wider audience of user, which in turn produces much more feedback leading to improvements in the development of algorithms.

The field of global optimization is growing. A few commerical solvers are already available: BARON and LGO by Janos Pintér [96] based on interval arithmetic. The number of applications is increasing (*cf.*, the case study in Section 5.5) and it is worthwhile at this stage to get in contact with the field; it may knock at your door tomorrow anyway.

5 Real World Case Studies and Success Stories

This section provides case studies and success studies which give more detail on some of the features listed in the table in Section 1. They cover problems from three continents, which have been solved by LP, MILP, global optimization techniques or stochastic programming and give a good snap shot about real world problem solving in the process industry. It is remarkable that MILP models in production planning can nowadays be solved so efficiently and fast that it is possible to integrate them into Web-based optimization tools giving access to a wide range of end-users. An example related to BASF Corp. is described in Section 5.3. Another Web interface system has been implemented at DOW Chemicals solving a nonlinear model for a polymer plant [63].

5.1 BASELL Supply Chain Optimization for Polypropylene Business - A Large MILP Problem

In the late 1990's the author was involved in the development of a MILP model for one of BASF's large production units which later became part of BASELL, the world's largest producer of polypropylene, a leading supplier of polyethylene and advanced polyolefin products, and a global leader in the development and licensing of polypropylene and polyethylene processes and catalysts. Some preliminary technical background on this optimization project has already been described by Kallrath (2000,[70], Sect. 4.2). During the years plants had been added and the model size increased. The mathematical formulation of the model was improved and tightened by efficient cuts derived by Laurence Wolsey (CORE, Louvain-la-Neuve, Belgium). Many of the ideas which made its way into the model can be found in his book [120]. The case study described below is taken in its present form with kind permission from Dash Optimization's home page www.dashoptimization.com/casestudy_7.html.

5.1.1 Problem

The Polypropylene-Business currently has over 10 supply points located in different European countries such as Benelux, Germany, France, Italy, Spain, United Kingdom. BASELL sells about 1500 different finished products belonging to a number of different product families like homopolymer products, impact and random copolymer products, metocene, adstif, and clyrell products.

About 3000 different customers for these products are located in Europe and Overseas. Customers are in the film, packaging, car supplier, furniture, house ware, paint and other industries.

Every month, a 3 month sales forecast is provided by the BASELL sales department. This forecast gives expected sales quantities per customer, product, package, and month. Sales quantities are qualified by customer categories that distinguish between customers that must be served from sales opportunities where optimization might or might not decide to serve depending on profits that can be achieved.

The problem is to find a sales plan and a production plan that takes into account:

- Given minimum and maximum sales quantities
- Production and stock capacities
- Opening stock quantities
- Production constraints such as minimum lot sizes, fixed lot sizes ("batches"), raw material availability and more
- All relevant costs such as raw material prices, production costs, inventory costs, transport prices
- Sales prices per customer, product, and package

The objective function maximizes the profit: sales income minus costs.

5.1.2 Implementation

The user interface is implemented in MS Access and has interfaces on one hand to the company's SAP systems, on the other hand to the MILP solver `Xpress-MP` [57].

A typical planning session comprises the following steps:

- Load current data from SAP: material and customer master data, production data (recipes, raw material costs), sales data (forecast and sales prices)
- Verify correctness and completeness of the data: Do all expected sales have a potential source? Are the raw materials needed during different production steps available? Are there any contradictions in the constraints? and others.
- Run the optimization and look for "flaws" in the results. Such "flaws" could be: stock quantities becoming higher or lower than desirable; unbalanced plant utilization rates; erroneous input data leading to "strange" results; and others.
- Define additional constraints in order to avoid "flaws" described above. Repeat optimization until a satisfactory result is found.
- The final result is documented in reports and sent back to SAP as basis for (1) production scheduling executed at the different production plants and (2) reservation of sales quantities for the specified customers.

The system is built in a way that different versions of the current data can easily be generated and administered, allowing to create "what-if" analyses and to go back to historical data.

5.1.3 Details

- In every planning session, about 800 different products, 1,500 different combinations of product and production plant, 10,000 different combinations of customer, product, package and month are involved.
- These numbers lead to over 200,000 variables, 380,000 non-zero elements, 400 integer variables and 900 semi-continuous variables.
- Solution time for the linear solution is about 1 minute; for a "good" integer solution, that takes into account semi-continuous and integer variables like minimum lot sizes and fixed lot sizes and that is guaranteed to be within 5% of the best possible solution, solution time is about 15 minutes.

5.1.4 Summary

The optimization system described above was first implemented in 1996 with the author being involved, where it had to deal with four production plants and about 100 different final products only. Through various acquisitions and mergers of the company, the system grew to the size it has today.

The BASELL planning department says: "It is of major importance for us to have an instrument that gives us the ability to integrate the complex planning and logistics process. Our optimization systems for Polypropylene Standard Products has become a key element in production and logistics planning. During the last big merger in 2001, optimization had a most prominent role: merge two polypropylene suppliers by first merging their planning activities!"

5.2 A LP-Based Planning System for the Petro-Chemical Industry

This case study focuses on the IT problems of an optimization project lead by Ikenouye Susumu (Ike Ltd., Tokyo). It has not so much to say about the mathematics but rather on the acceptance of optimization, and the importance of graphical user interfaces (GUIs) and data management.

5.2.1 Current Issues of Enterprise-wide Planning and Scheduling System

There have been many applications of pure LP for practical planning work in the process industry, such as oil, petrochemistry and chemistry. Even pure LP has a great power to generate production plans including many trade-off constraints in the production of joint products through continuous production plants. Current applications of LP in petrochemistry are almost completely for the selection of crude naphtha for ethylene cracking.

Now in Japan, the chemical industry is facing very hard problems caused by the competition of Far East Countries producing at much cheaper cost. Therefore, there are many enhancement projects to improve planning and scheduling procedures in various way. One of them is to renew planning and scheduling system by utilizing mathematical optimization.

The oil industry has already sufficient experience in exploiting LP for its planning work. But most Japanese companies in chemical industry do not have qualified personnel to do so. For the past 30 years, some companies have installed LP for production planning. But many of these implementations covered only partial aspects.

From 2001 to 2003, Ike Ltd. and a client in the petrochemical industry have been closely cooperated. This case study reviews briefly the project in which an LP model has been developed for enterprise-wide production planning, including both business planning including budget planning.

A first analysis yielded the following results:

1. There is no full model application to cover an enterprise-wide model for the petrochemical industry.

2. There is no strong relationship between production control and budget control in the practical work process and in planning methods.

3. There is no good software for LP modeling and LP data handling for the petrochemical industry.

4. A lot of days are required to generate production plans and annual budget plans.

5. Consideration for work process of planning work is not sufficient from the point of collaboration.

5.2.2 Approach of Enhancement in Enterprise-wide Planning and Scheduling Work

To enhance planning and scheduling functions, we considered two approaches, *re-organizing the business process* and *improving the information system including LP*.

Re-organization of the business process in practice means to establish a cross functional team. Members of this team are selected from departments that have strong responsible to generating plans from each function of the enterprise, such as crude purchasing, marketing, production management (head quarter and chemical farm) and budget control. These members are working in a collaborative atmosphere supported by information systems and planning tools as a task force team.

Improvements of the information systems are planned including the following items:

1. establish a enterprise-wide LP model,

2. install a GUI to make the LP model easier to use for person unfamiliar with the LP technology

3. set up a database to manage all data related to the LP case study, and

4. combine these LP functions and the estimation function of enterprise profit.

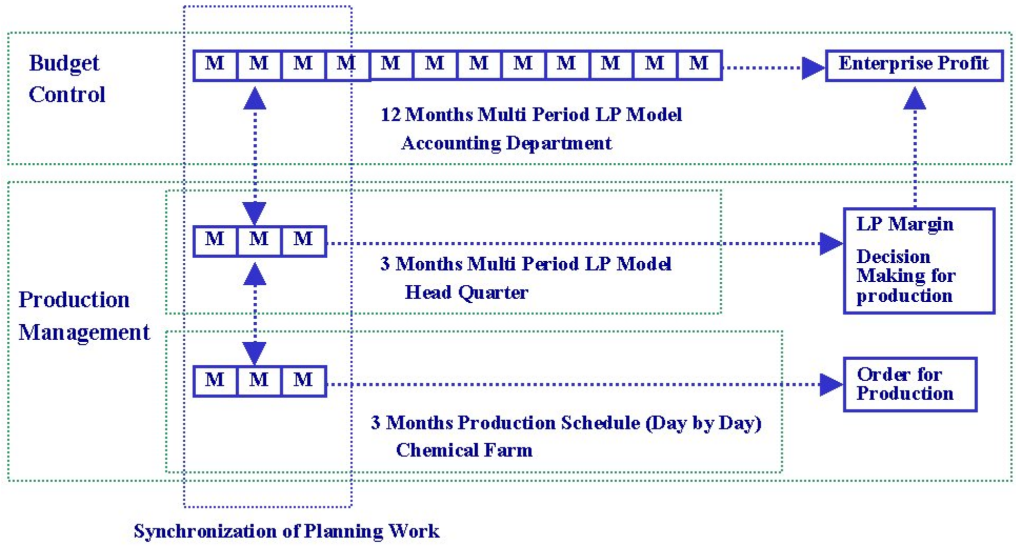

Figure 1: The Three Levels of the Planning and Scheduling System

We structured the planning and scheduling work process according to the three levels shown in Fig. 1: annual production plan (budget plan and profit estimation), monthly production plan and monthly production schedule.
Annual production plans for budget planning are computed based on a 12-months multi-period LP model. The result of this LP yields the profit estimation function. Monthly production planning is presented by a three-months multi-period LP model for each monthly planning work. Monthly (day-by-day) production schedules are prepared for chemical farm production management.

These LP models contain several ten thousands of variables and constraints. There should be some data management function to keep integrity and accuracy of huge data for LP model and results of many case studies. In real world, unexpected changes happen so often and the LP models must be adjusted to those changes as soon as possible. We feel a strong need to produce an easy-to-use a GUI to develop and adjust the LP model for planners without mathematical modeling knowledge.

In big companies, the collaboration between production management work and budget control is in general not too smooth. From the need of real-time performance (profit) management, there should be practical combined functions for both management works. We are preparing a system of planning LP and Profit/Loss calculation in one box.

5.2.3 Technical Enhancement in Planning Systems

(Graphical LP Model Generator) In this case study it is very complicated to develop and to solve the LP problem, but is not difficult mathematically. The most important point is how to design a GUI which allows to develop the LP model for persons unfamiliar with LP. This GUI should allow and support that the process flow is drawn on PC's panel by mouse, selecting box and drawing line. A box represents specific parts of the matrix set by the operator to define the process units including yields of material balance. Upper and lower bounds, costs and prices are set in this box to convert to the LP mathematical model. Process flow and matrix (data table) are very clear and acceptable for the operator who has enough knowledge of production planning. We are developing a *Graphical LP Model Generator* for this function.

(Data Base System for planning work) The LP models developed for chemical production planning in this case study contain several ten thousands of variables and constraints. We have to prepare some data management functions to keep integrity and accuracy of huge data for LP model and results of case studies. Advanced data handling functions, such as data inputting format editing, free reporting editor and coping model data are developed with a database management software [Fig. 2].

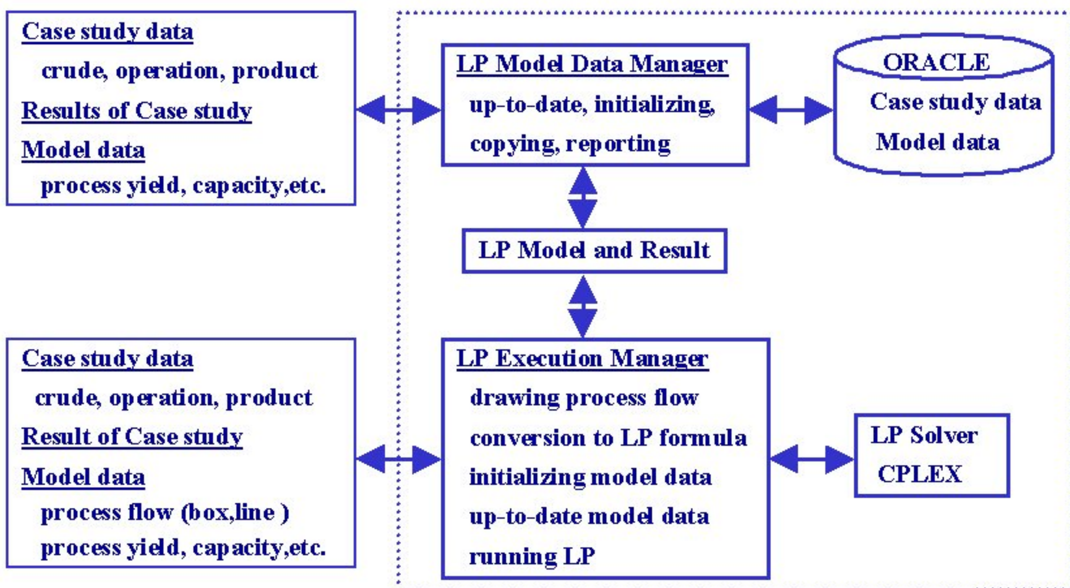

Figure 2: The Architecture of the Planning System

5.2.4 Improvement of the Planning Work

(Planning Work Process) Cross Functional Term uses this system to combine with business sense and engineering sense, at the same time, with accounting and production management. Now in Japan, every open company is forced to disclose it's business performance to stock market four times a year. From this reason, budgeting work is so busy to complete. Production planning work should be done more frequently than budgeting work. To make planning time short is necessarily needed besides improvement of integrity and accuracy of plan. At the same time, optimization of plan should be done as possible. We estimate that planning work time will be 1/3 comparing than current procedure.

This system we presented is qualified to become a very good supporting tool for the decision makers. In our feasibility study, the optimization tool produced schedules reducing the cost by 1% compared to hand-made plans.

(Improvement of the quality of the plan) In our feasibility study, we were able to compute schedules reducing the cost by 1% compared to hand-made plans. This system can brash up accuracy, integrity and optimality in practical planning work of petrochemical enterprise.

5.3 BASF's Web-based Production Optimization Tool

Lee & Cheng (2002,[82]) developed a computational framework for optimization based practical production planning tools on the internal BASF Intranet. This framework enables users equipped with standard web browsers to access complex optimization tools to interactively compute production plans on any computer platform. Lee & Cheng provided a MILP model for a production planning problem for one of BASF's multi-purpose chemical manufacturing plants with multiple production lines. During mode changes the quality of the products allows to sell the product only at a reduced price. Thus there is an inclination to avoid or at least to minimize mode changes. Each production line has a minimum length for production campaigns during which product change overs are not allowed. The goal of the production planning is to compute a production plan that minimizes the inventory holding costs and mode changing cost while satisfying all demand for finished goods and the other production constraints. The implemented model contains only 1,452 variables (308 of them are binary variables) and 1,113 constraints. While, without this optimization based approach, it took several days to generate a production schedule it is now possible to compute it within seconds. The short response time of the integrated model has allowed the production plant to adjust its production schedule to accommodate quickly to sudden market changes. The quality of production planning and the use of production and inventory capacity improved; especially, the storage levels have been decreased.

5.4 Scheduling Under Uncertainty - Industrial CaseStudies

Besides several publications on several approaches to solve scheduling problems in the process industry (*cf.*, [62], [106], [117], [12]), there are also industrial success stories. Successful applications of stochastic optimization to production scheduling problems in the chemical process industry are reported, for instance, by Sand *et al.* [105] and Engell *et al.* [33]. They describe the production of an expandable polystyrene in a plant which consists of a preparation stage operated in a batch mode, a polymerization stage with four batch reactors and two continuously operating finishing lines. This recipe-driven multi-product batch process is subject to limited capacity of equipment items, shared and non-shared intermediates, different types of storage policies, and the following uncertainties: unknown or varying demands, customer orders are uncertain, the chemical reactions are not completely reproducible, stochastic changes of the plant capacity, and varying process times as well as breakdown or reactors or storage tanks. As usually in production planning and scheduling one wants to know the starting times of certain acting, batch sizes and in this case choices of recipes. There is a list of objectives to be reached. Highest priority is on fulfilling demand without any or with minimal delay. Next comes cost efficiency and shut down of the finishing lines should be avoided. A monolithic model of the decision problem for a horizon of several weeks, parameterized by the data available online about the demands and the process state as well as by probability distributions of the uncertain parameters would lead to a large-scale mixed-integer and nonlinear real-time optimization problem. Instead the authors propose a telescopic decomposition with a number of layered sub-models of different degrees of temporal aggregation.

Lin *et al.* (2004,[84]) present a robust optimization approach applicable to MILP problems with bounded uncertainty. Their industrial case study considers three of the most common sources of bounded uncertainties in scheduling: the processing times of tasks, market demands for products, and prices of products and raw materials.

5.5 Global Minima in a Nonconvex Portfolio Optimization Problem

The goal of this problem presented by Kallrath (2003,[73]) was to compute minimal cost solutions satisfying the demand of pre-given product portfolios and to investigate the dependence of the fix costs and investment costs on the product portfolio. The most important parameters characterizing the production facilities are the number and the size of the reactors. The production is subject to shelf-life constraints, *i.e.*, products cannot be stored longer than one week.

Even if analyzed under the simple assumption of constant batch sizes and considering only one time period covering one week, the computation of minimum cost scenarios requires the determination of global minima of a nonconvex MINLP problem. An objective function built up by the sum of concave functions and trilinear products terms involving the variables describing the number of batches, the utilization rates and the volume of the reactor are the nonlinear features in the model.

A complex portfolio with 40 products leads to more costly scenarios requiring more reactors. A 20 products scenario requires only two reactors. The 40 product scenario, which requires the same total production amount cannot be produced on two reactors, but it is possible to find feasible solutions for three reactors with no surplus production satisfying the utilization rates.

This result has been obtained by computing the global minimum of the sum of investment and fixed costs with respect to the number and volume of the reactors. We have successfully applied four different solution techniques to solve this problem. (1) An exact transformation allows us to represent the nonlinear constraints by MILP constraints. Using piecewise linear approximations for the objective function the problem is solved with `Xpress-MP` [57], a commercial MILP solver. (2) The local MINLP Branch-and-Bound solver `SBB` [45] which is part of the modeling system `GAMS` [22]. (3) The Branch&Reduce Optimization Navigator (`BARON`; *cf.* [102] or [46]) also called from `GAMS`. (4) A tailored Branch&Bound approach based on the construction of a lower bounding problem by underestimating the concave objective function with piecewise linear approximations described in Lin *et al.* (2004,[83]).

For the scenarios tested the solution process suffers from weak lower bounds which improve only very slowly. The equivalent linear representation approach provides the global solution for Scenario 2 within a few minutes while Scenario 2 requires almost 6 hours to prove optimality. The commercial solvers, SBB and BARON, produce solutions for the small, 20-product scenario; BARON needs about 12 CPU hours on a Pentium III processor running at 750 MHz to prove global optimality. For the 40-product scenario no solutions have been produced with either SBB and BARON, in 40 hours. Only the tailored Branch&Bound coupled with convex underestimators shows reasonable scaling properties and generates the globally optimal solution of the 40-product scenario with reactors of size 20, 100 and 250 m^3 and the objective function value 37.1758 in about 13 minutes.

Thus, the overall conclusion is that the problem, for some cases, can be solved with current standard solvers but it requires a lot of CPU time. Therefore, in order not to cover only special cases and also to cope with the scaling properties, it is recommended to use tailored approaches in addition.

6 A Challenge: Global Optimization Under Uncertainty

The purpose of this section is to encourage further research on a problem which may benefit from both global optimization and optimization under uncertainty. The following decision problem is kept somewhat generic in order to allow really different solutions approaches. What are the optimal sizes of tanks (and, possibly in addition: what are the optimal safety stocks) if for a set of products (case A) continuous demands (mass/time) or (Case B) discrete demands (mass) in a set of given time slices need to be fulfilled. Demands may be constant for every day, may show seasonal dependencies and are in any case subject to scenario-based uncertainties. The demands should be satisfied by extracting the products from dedicated tanks which are subject to lower bounds (safety stock) and their capacity (a design variable). The tanks are filled during the production and are charged by a multi-stage production network (in the simplest case only one stage) of several multi-purpose reactors. The reactors (in the simplest case: only one) either have a variable continuous output rate (mass/time) and may be operated in campaign (subject to minimal campaign size) or batch mode. In case A the time horizon might be determined by a (hard or soft) periodic constraint on the initial and terminating tank level. The objective function should contain the sum of the investment costs to built tanks of a certain size, the variable storage costs and sequence-dependent setup- or cleaning costs after a campaign. It might be normalized by the time horizon. The tank investments costs are given by concave functions of the tank size. In case A the variable costs are given by a sum of bilinear terms.

Even for the deterministic case (no uncertainties in the demands) this leads to a non-convex MINLP problem (binary variables are needed to assign products to campaigns or batches, nonlinear product terms occur which involve the variable production rates, the length of the campaign and possibly the binary assignment variables). Due to the embedded lot-sizing problem (unknown number, lengths and sequence of the campaigns) this problem has many local minima.

7 Summary

We have provided an overview on mixed integer optimization in the process industry with a special focus on planning, design, global optimization techniques and optimization under uncertainty. The state-of-the-art technology based on mathematical, especially mixed-integer optimization for planning is quite advanced, is able to map many detailed features such as tracing mode-changes, product origins and shelf life, and is thus appropriate for solving real world planning problems. Mixed integer optimization can provide a quantitative basis for decisions and allow to cope most successfully with complex problems and it has proven itself as a useful technique to reduce costs and to support other objectives. MILP models in production planning can sometimes be solved so efficiently and fast that it is possible to integrate them into Web-based optimization tools giving access to a wide range of end-users. While for scheduling problems, there is not yet a commonly accepted state-of-the-art technology and the majority of software packages is still based on pure heuristics there is light at the end of the tunnel: A promising approach, continuous-time formulation has been developed [42], and batch scheduling problems leading to MILP problems can be extended to multi-stage stochastic optimization solved by special decomposition techniques. Solution techniques for computing robust solutions not requiring probability distributions functions are now available for MILP problems.

What will the future hold for us in planning and scheduling? There is a growing number of software packages available which support - at least to some extent - the application of exact methods for a variety of (deterministic) planning problems. That way, planning based on mathematical, especially mixed-integer optimization becomes more and more the state-of-the art in the chemical, food and pharmaceutical industry and as well in refineries. The same problems will more and more be solved considering input date subject to uncertainties.

Network and process design have been solved using MINLP approaches for a long time in the process industry. While MILP has already well established itself not only in the process industry, further quantum leaps in practical optimization of design problems are to be expected. Global optimization of nonlinear mixed integer nonlinear problems knocks at our doors and might, say, within 5 to 10 years, play a similar role as does MILP nowadays. It is remarkable that a substantial part of the progress in the development of exact algorithms in global optimization comes from the chemical engineering community and the first commercial packages are available now.

On top of all that, or in addition, not only deterministic planning and design models, but rather models involving uncertain data will play an increasing role asking for industrial strength solution approaches for optimization under uncertainty, and, in particular, stochastic and/or robust mixed integer programming.

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