Planning in the Process Industry

Josef Kallrath¹²

- ¹ BASF-AG, GVC/S (Scientific Computing) B009, D-67056 Ludwigshafen, Germany (e-mail: josef.kallrath@web.de)
- ² University of Florida, Astronomy Dept., Gainesville, 32611 FL, USA (e-mail: kallrath@astro.ufl.edu)

The date of receipt and acceptance will be inserted by the editor

1 Introduction

Since there has been tremendous progress in planning in the process industry during the last 25 years, it might be worthwhile to give an overview of the current state-of-the-art of planning problems in the process industry. This is the purpose of the current contribution which has the following structure: we start with some conceptional thoughts and some comments on special features of planning in the process industry. What is said in this article applies to the chemical but also to the pharmaceutical as well as to the food industry. The reader will find an orientation on production planning, strategic and design planning, planning under uncertainty and multi-objective planning. In Section 2 the focus is on planning features one would expect in a process industry planning model. Section 3 and 4 address planning under uncertainty and multi-criteria planning.

1.1 A Definition of Planning

A definition of the term planning leads to a group of related terms such as strategic planning, design planning, master planning, operative planning, and production planning. Planning needs also be distinguished from scheduling.

A starting point could be Pochet and Wolsey (2006, [21], p. 3) in their definition of production planning: Production planning is defined as the planning of the acquisition of the resources and raw materials, as well as the planning of the production activities, required to transform raw materials into finished products meeting customer demand in the most efficient or economical way. Note that this does not say anything about the length of the time horizon. Their definition of supply chain planning is similar to production planning, but extends its scope by considering and integrating procurement and distribution decisions. They distinguish supply chain design problems which cover a longer time horizon and include additional decisions such as the selection of suppliers, the location of production facilities, and the design of the distribution system.

In this article we use planning for any type of strategic, design or operative planning. We always assume that we are dealing with multi-site production networks. Operative planning includes production planning within multi-site production networks and scheduling of individuals sites. While in production planning the focus is rather on optimizing the trade-off between economic objectives such as cost minimization or maximization of contribution and the less tangible objective of customer satisfaction, in scheduling due dates, makespan, or machine utilization become more relevant. So, instead of the term production planning we use the term operative planning (or just, *planning*) targeting in supporting decision which have an operative impact on a time scale of several months, may be up to a year. Planning involves the determination of operational plans that support different short- or mid-term objectives for the current business and for a given multisite topology. Planning covers a horizon from a few months to 12 months, and can be extended to cover years (when it comes to strategic or design planning) and time-discrete models are used. If the time horizon becomes smaller we are in the realm of scheduling where time-continuous models become more efficient. When we extend the time-horizon we are dealing with strategic planning or design planning covering a year up to 20 years. Design planning includes those parts of the Pochet-Wolsey definition above allows beyond the topology also for the design of production units, or the capacity of warehouses. Strategic planning is more on product and customer portfolio optimization but also on the acquisition of whole production sites. Kallrath (2007, [16]) elaborates more on the concept of operative planning and design planning problem and promotes the idea to combine both in one single model.

1.2 Special Planning Features in the Process Industry

In the process industry *continuous* and *batch production systems* can be distinguished. There exists also semi-batch production which combines features from both. 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 on multi-purpose equipment which are operated in *batch mode*. Batch production is characterized by *well-defined start-ups*, *e.g.*, filling in some products and follow-up steps defined by specific tasks for

Planning in the Process Industry

heating, mixing and reaction, and a *clearly defined end* for extracting the finished product. Batch production involves an integer number of batches where a batch is the smallest quantity to be produced; the batch size may also vary between a lower and upper bound. 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 minimal production quantity) has to be observed. Within a fixed planning horizon, a certain product can be produced in several campaigns; this implies that campaigns have to be modeled as individual entities. One might argue that details of the batch production could be rather found in a scheduling model than in scheduling. However, the model provided in Kallrath & Maindl (2006, [17], Chap. 8) is a clear example where batch and campaign features have been incorporated into a time-discrete planning model enhancing it by some continuous time aspects. This problem has been solved the first time by Kallrath (1999, [10]). An elegant and numerically more efficient formulation to add time continuity to discrete-time models has been developed more recently by Sürie (2005, [24]). However, it seems that this formulation yet needs to be extended to support multi-stage production.

Chemical products produced on different production equipment could lead to different performance when further used. Therefore, customers might require that a product always is produced on one particular machine, or at least it is always produced on the same machine. This features is called *origin-tracing* and is treated in Kallrath (2005, [15]). 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. A model formulation is provided in Kallrath (2005, [15]).

Another special feature in the refinery or petrochemical industry or process industry in general is the *pooling* problem (see, for instance, [1], or Chapter 11 in [18]). This is an almost classical problem in nonlinear optimization. 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. Structurally, this problem contains indefinite bilinear terms (products of variables) appearing in equality constraints, *e.g.*, mass balances. 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.

Non-linear programming (NLP) models have been used by the refining, chemical and other process industries for many years. These nonlinear problems are non-convex and either approximated by linear ones which can be solved by linear programming (LP) or approximated by a sequence of linear models. This sequential linear programming (SLP) technique is well established in the refinery industry but suffers from the drawback of yielding only locally optimum solutions. Although many users may identify obviously suboptimal solutions from experience, there is no validation of non-obviously sub-optimal solutions, as this would require truly globally optimal solutions. Recent advances in optimization algorithms have yielded experimental academic codes which do find globally optimal solutions to large scale pooling NLP models (Meyer & Floudas (2006, [20]). Non-convex nonlinear models are 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 solution asks for global optimization.

1.3 Some Comments on Planning and Scheduling in the Process Industry

Planning and scheduling is part of company-wide logistics and supply chain management. Planning and scheduling are often treated as separate approaches to avoid mathematical complexity. Depending on the level of detail required, the border lines between planning and scheduling are diffuse. There could be strong overlaps between scheduling and planning in production, distribution or supply chain management and strategic planning. The main structural elements of planning and scheduling in the process industry are:

- 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.

Structurally, in scheduling these features often lead to allocation and sequencing problems, knapsack structures, or to the pooling problem. Although the horizon of scheduling problems is usually only days to a few weeks, time-discrete models lead to too many binary variables. Thus, timecontinuous formulations are preferable; cf. Janak et al. (2004, [8]) or the reviews by Floudas & Lin (2004, [4]) or Floudas (2007, [2]). The largest scheduling problem using a continuous-time approach has been solved by Janak *et al.* (2006a, b; [6], [7]). It includes over 80 pieces of equipment, considers the processing recipes of hundreds of different products and leads to a MILP problems with up to 463,025 constraints, 55,531 variables among them 8,981 binary variables, and 1,472,365 non-zeroes.

In production or supply chain planning, we usually consider material flow and balance equations connecting sources and sinks of a supply network avoiding some of the complicating details of scheduling. Time-indexed models using a relative coarse discretization of time, *e.g.*, a year, quarters, months or weeks are usually accurate enough. LP, linear mixed integer programming (MILP) and nonlinear mixed integer programming (MINLP) technologies are often appropriate and successful for problems with a clear quantitative objective function as outlined in Section 2, or quantitative multi-criteria objectives. A typical size planning problem with 4 sites, 800 different products, 1,500 different combinations of product and production plant, 10,000 different combinations of customer, product, package and month are involved is reported in Kallrath (2005, [15], Sect. 5.1). This problem leads to over 200,000 variables, 380,000 non-zero elements, 400 integer variables and 900 semi-continuous variables. The number of discrete variables usually can reach a few thousand.

2 Model Features in Planning Problems

In the literature and in available software packages we usually find *discretetime models* supporting multi-period analysis, *i.e.*, nearly all the data may vary over time and allow to evaluate scenarios that involve time dependent aspects such as seasonal demand patterns, new product introductions, shutdown of production facilities for maintenance periods. These models include the following main structural objects which are represented by the corresponding indices of the model:

- Locations can be production or storage sites, hosting plants and tanks, or demand points hosting tanks.
- Facilities typical are production, wrapping or inventory units that are characterized by their functional properties. Especially, in the process industry we find multi-stage production systems involving units with general product-mode relationships. Their functional properties are attributes such as capacity, throughput rates, product recipes, yields, minimum production utilization rates, fixed and variable costs, or storage limitations. Facilities can be existing or potential (for design studies). Production facilities may be subject to batch and campaign constraints across periods.
- Demand Points may represent customers, regional warehouse locations or distributors who specify the quantity of a product they request. A demand point can be also seen as a sink of the planning model, *i.e.*, a point where a product leaves the system and is not further traced. Demand may be subject to certain constraints, *e.g.*, satisfying a minimum quantity of demand, observing origins of production or supplying a customer always from the same origin.
- Inventories may be physically fixed entities such as tanks or warehouses but also moveable entities (*e.g.*, drums, containers, boxes, etc.). They can be defined as dedicated
 - 1. to a single product from one production source,
 - 2. dedicated to a specific product, or

3. free to accept any product from any source or origin.

We may encounter tank farms, and especially *multi-purpose storage entities, i.e.*, variable and multi-product tanks.

- Products may be classified as raw materials, intermediates, finished and salable products. A product may have several of these attributes, and it can be purchased from suppliers, produced or sold. Products are produced according to the capabilities at the facilities and the recipes assigned; they may establish a product group, *e.g.*, additives. Product requirements are based on market demand which is characterized by volume, selling price, package type, time, origin and location or by other products in which they are used as intermediate products.
- Suppliers or vendors may provide products for purchase under different offering schemes. This includes the ability to link the product supply to locations and describe contractual pricing mechanisms or availability. The solver may choose the optimal supplier.

Regarding the overall business and strategic objectives the model needs to incorporate data describing the

- costs, *i.e.*, certain fixed costs, variable costs (production, transportation, inventory, external product purchase, energy, resources and utilities), and further
- commercial aspects: financial aspects such as depreciation plans, discount rates, investment plans, foreign currency exchange rates, duties and tariffs, as well as site dependent taxes.

Maximize operating cash flow and maximize net present value (NPV) objective functions are used to determine the financial and operating impacts of mergers, acquisitions, consolidation initiatives, and capital spending programs effecting business. In detail this may include:

- 1. maximize the net profit (free design reactors; open and close facilities),
- 2. maximize the contribution margin for a fixed system of production units,
- 3. maximize the contribution margin while satisfying a minimum percentage of demand,
- 4. minimize the cost while satisfying full demand (allow external purchase of products),
- 5. maximize total sales neglecting cost,
- 6. maximize total production for a fixed system of production reactors,
- 7. maximize total production of products for which demand exists,
- 8. minimize energy consumption or the usage of other utilities,
- 9. minimize the deviation of the usage of resources from their average usage,
- 10. multi-criteria objectives, *e.g.*, maximize contribution margin and minimize total volume of transport.

The objective function 2 to 10 support different short- or mid-term objectives for the current business. By using different objective functions it is possible to create operational plans that support strategies such as market penetration, top-line growth, or maximization of cash flow to support other business initiatives.

If, besides this broad structure, the focus is on a more detailed representation of physical entities, we find that planning models and their constraints may involve the following features (in alphabetic order):

- Batch production [cf. Kallrath (1999, [10])]: The quantity of a specific product being produced in a campaign possibly over several periods must be an integer multiple of some pre-defined batch size.
- Buy, build, close or sell specific production assets [cf. Kallrath (2002, [12])]: This feature is used for closing, or selling acquisition, consolidation and capacity planning to determine the NPV and operational impacts of adding or removing specific assets or groups of assets to the network.
- Campaign production [cf. Kallrath (1999, [10])]: This allows to impose a lower and/or an upper bound on a contiguous production run (campaign) possibly across periods; this feature is also known under the name minimal runs.
- Delay cost: Penalty cost apply if customer orders are delivered after the requested delivery date.
- Minimum production requirements: Minimum utilization rates modelled as semi-continuous variables have to be observed for specific production units and/or entire production locations for each production time period.
- Multi-locations: This can be production sites, storage sites, and demand points.
- Multi-purpose production units [cf. Kallrath & Wilson (1997, [18]), or Kallrath & Maindl (2006, [17]), Chap. 8]: If a unit is fixed to a certain mode, several products are produced (with different mode-dependent daily production rates), and vice-versa, a product can be produced in different modes. Daily production can be less than the capacity rates. A detailed mode-changing production scheme may be used to describe the cost and time required for sequence-dependent mode-changes.
- Multi-stage production [cf. Kallrath & Maindl (2006, [17]), Chap. 8]: Free and fixed recipe structures can be used for the production of multiple intermediate products before the production of the final product with convergent and divergent product flows. The recipes may depend on the mode of the multi-purpose production unit.
- Multi-time periods [cf. Timpe & Kallrath (2000, [25])]: Non-equidistant time period scales are possible for commercial and production needs. For instance, demand may be forecast weekly for the first quarter of the year and then quarterly for the remainder of the year.
- Nonlinear pricing for the purchase of products [cf. Kallrath (2002, [12])] or utilities (energy, water, etc.) or nonlinear cost for inventory or transportation may lead to convex and concave structures in order to model volume and price discount schemes for the products or services

purchased, while in addition, contract start-up and cancellation fees may lead to additional binary variables.

- Order lost cost: Penalty cost are incurred if products are not delivered as requested and promised.
- Packaging machines are optimized to increase machine throughput and assure that priority is given to the most profitable products.
- Product swaps: With the objective of saving transportation and other cost companies often arrange joint supply agreements called *swaps*. For example: Company 1 based in Europe as well in the US has a production shortage of product A in the US and thus purchases a defined quantity of product A in the US from company 2. Company 2 (also located in the US and Europe) has a customer in Europe requesting product A and thus purchases a defined quantity product A from company 1 in Europe. Both companies get product A where they need it and avoid the cost of shipping the product. Without this type of supply agreement company 1 would have to ship product A from its US manufacturing plant to Europe.
- Production origin tracing [cf. Kallrath (2005, [15])]: It is possible to define fixed, free or unique origins for specific demands. For example, a customer may require that his demand is satisfied only from a specific plant in the network, or it may not be supplied from a set of plants, or the customer only requests that he is supplied from one unique plant during the whole planning horizon.
- Shelf-life time [cf. Kallrath (2005, [15])]: Product aging time can be traced. This allows for the application of constraints such as: maximum shelf-life time, disposal costs for time expired products, and the setting of selling prices as a function of product life.
- Transportation and logistics [cf. Kallrath (2002, [13])]: Transportation quantities are appropriately modeled by the use of semi-continuous variables. This allows minimum and maximum shipment quantities to be defined for each source location, destination location, product, and transport mean combination. The logistics involves the costs, lead times and constraints (minimum shipment quantities) associated with moving intermediate and finished products between facilities and demand points. The mean of transport may be chosen by the optimizer and nonlinear cost functions have to be considered as well.

This list covers many features but may be enhanced depending on the planning problem at hand. A model supporting this features caters to the overall business and strategic objectives. The model incorporates data describing the variable costs for production, transportation, inventory, external product purchase, energy, resources and utilities, and further commercial aspects: financial aspects such as depreciation plans, discount rates, investment plans, foreign currency exchange rates, duties and tariffs, as well as site dependent taxes. Maximize operating cash flow and maximize net present value (NPV) objective functions can also be used to determine the financial and operating impacts of mergers, acquisitions, consolidation initiatives, and capital spending programs effecting business. One would expect that a planning model supports various objective functions among them net profit (free design reactors; open and close facilities), contribution margin, cost, sales, total production, or multi-criteria objectives, e.g., maximize contribution margin and minimize total transportation volume.

A possible extension which could relatively easy connected to such a model are customer or product portfolio features as described in Kallrath (2005, [15]).

3 Planning Under Uncertainty

In many instances, the data are not in a deterministic form and this naturally leads to optimization under uncertainty, that is, 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 from 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, processing times.
- Demand and price uncertainties occur in many situations: supply chain planning, investment planning, or strategic design optimization problems involving uncertain demand and price over a long planning horizon of 10 to 20 years.

For planning, the third point is most relevant. It is difficult to predict demand and prices, especially in strategic or design planning problems where the time horizon covers several years. Scenario based optimization in the sense of stochastic optimization leads to large number of variables. A decision taker might be more inclined to hedge against certain risks than to find the most probable scenario. Therefore, the robust optimization framework developed by Floudas and co-workers seems to be more appropriate; cf. Lin *et al.* (2004, [19]) and Janak *et al.* (2007, [9]). It provides a) an explicit trade-off between the effect of uncertainties on the objective function of choice, (b) the unified treatment of uncertainties in product demands, processing times, processing rates, prices of products, and prices of raw materials, (c) the alternative deterministic equivalent models for a variety of types of representations of uncertainties through bounded, symmetric, normal, difference of normal, binomial, discrete, and Poisson probability distributions.

4 Multi-Criteria Planning Problems

In planning we may encounter the situation that there are conflicting objectives. Maximizing contribution margin and minimizing the amount of stocked material might conflict. The novice might think if the storage costs are appropriately included in the objective function both objectives would go along with each other very well. However, some promising sales could be lost because not enough material had been stocked. Thus, the goal to minimize the amount of stock is different from maximizing contribution margin. At least in this example it might be possible to measure both goals in the same unit of measure, in this case a monetary unit. The more general situation is that we are facing conflicting goals which cannot even be measured on a common scale.

Multi-objective optimization, also called multi-criteria optimization or vector minimization problems, allows to involve several objective functions. A simple approach to solve such problems is to express all objectives in terms of a common measure of goodness leading to the problem how to compare different objectives on a common scale. Basically, one can distinguish two cases. Either the search is for *Pareto optimal* solutions, or the problem has to be *solved for every objective function separately*.

When minimizing several objective functions simultaneously the concept of *Pareto optimal solutions* turns out to be useful. A solution is said to be *Pareto optimal* iff no other solution exists that is at least as good according to every objective, and is strictly better according to at least one objective. When searching for Pareto optimal solutions, the task might be to *find one*, *find all*, or *cover the extremal set*.

A special solution approach to multiple objective problems is to require that all the objectives should come close to some targets, measured each in its own scale. The targets we set for the objectives are called *goals*. Our overall objective can then be regarded as to minimize the overall deviation of our goals from their target levels. The solutions derived are Pareto optimal.

Goal programming can be considered as an extension of standard optimization problems in which targets are specified for a set of constraints. There are two basic approaches for goal programming: the preemptive *(lexicographic)* approach and the *Archimedian* approach. In the Archimedian approach weights or penalties are applied for not achieving targets. A linear combination of the violated targets weighted by some penalty factor is added, or establishes the objective function. We consider only the first approach.

In preemptive goal programming, goals are ordered according to importance and priorities. Especially, if there is a ranking between incommensurate objectives available, this method might be useful. The goal at priority level i is considered to be infinitely more important than the goal at the next lower level, i + 1. But they are relaxed by a certain absolute or relative amount when optimizing for the level i + 1. In a reactor design problem we might have the following ranking: reactor size (i = 1), safety issues (i = 2), and eventually production output rate (i = 3).

Here we provide an illustrative example for *pre-emptive (lexicographic)* goal programming with two variables x and y subject to the constraint $42x + 13y \le 100$ as well as the trivial bounds $x \ge 0$ and $y \ge 0$. We are given

name	criterion	type	A/P	Δ
goal 1 (OBJ1):	5x + 2y - 20	\max	Р	10
goal 2 $(OBJ3)$:	-3x + 15y - 48	\min	А	4
goal 3 (OBJ2):	1.5x + 21y - 3.8	max	Р	20

where the attribute A or P indicates whether we have to interpret Δ as an absolute value, or percentage-wise. The multi-criteria LP or MILP problem is converted to a sequence of LP or MILP problems. The basic idea is to work down the list of goals according to the priority list given. Thus we start by maximizing the LP w.r.t. the first goal. This gives us the objective function value z_1^* . Using this value z_1^* enables us to convert goal 1 into the constraint

$$5x + 2y - 20 \ge Z_1 = z_1^* - \frac{10}{100} z_1^* \quad . \tag{1}$$

Note how we have constructed the target Z_1 for this goal (P indicates that we work percentage wise). In the example we have three goals with the optimization sense {max, min, max}. Two times we apply a percentage wise relaxation, one time absolute. Solving the original problem with the additional inequality (1) we get:

$$z_1^* = -4.615385 \quad \Rightarrow \quad 5x + 2y - 20 \ge -4.615385 - 0.1 \cdot (-4.615385)$$
(2)

Now we minimize w.r.t. to goal 2 adding (2) as an additional constraint. We obtain:

$$z_2^* = 51.133603 \quad \Rightarrow \quad -3x + 15y - 48 \ge 51.133603 + 4 \tag{3}$$

Similar as the first goal, we now have to convert the second goal into a constraint (3) (here we allow a deviation of 4) and maximize according to goal 3. Finally, we get $z_3^* = 141.943995$ and the solution x = 0.238062 and y = 6.923186. To be complete, we could also convert the third goal into a constraint giving

$$1.5x + 21y - 3.8 \ge 141.943995 - 0.2 \cdot 141.943995 = 113.555196$$

Note that lexicographic goal programming based on objective functions provides a useful techniques to tackle multi-criteria optimization problems. The great advantage is that the absolute or percentage-wise deviations used in lexicographic goal programming based on objectives are easy to interpret. However, we have to keep in mind that the sequence of the goals influences the solution strongly. Therefore, the absolute or percentage deviations have to be chosen with care. It is very important that the optimization problem can be solved to exact optimality or at least closely to optimality because otherwise the interpretation of the permissible deviation from targets becomes difficult if not impossible.

Goal programming offers an alternative approach but should not be regarded as without defects. The specific goal levels selected greatly determine the answer. Therefore, care is need when selecting the targets. It is also important in which units the targets are measured. Detailed treatment of goal programming appears in such books as Ignizio (1976, [5]) and Romero (1991, [22]) who introduce many variations on the basic idea, as well as in Schniederjans (1995, [23]).

5 Solution Approaches

Most of the planning problems in the process industry lead to MILP or MINLP models and contain the following building blocks: tracing the states of plants, modeling production, balance equations for material flows, transportation terms, consumption of utilities, cost terms, and special model features. Mode-changes, start-up and cancellation features, and nonlinear cost structures require many binary variables. Minimum utilization rates and transportation often require semi-continuous variables. Special features such as batch and campaign constraints across periods require special constraints to implement the concept of contiguity; cf. Kallrath (1999, [10]) and Sürie (2005, [24]). The model, however, remains linear in all variables. Only if the pooling problem occurs, *e.g.*, in the refinery industry or the food industry, we are really facing a MINLP problem. For a review on algorithms used in LP, MILP, NLP, and MINLP the reader is referred to [11]. State-of-the art global solution techniques to non-convex nonlinear problems are reviewed by Floudas *et al.* (2004, [3]).

It is very convenient and saves a lot of maintenance work if the planning model is implemented in an algebraic modeling language. In modeling languages one stores the *knowledge* about a model. A model coded in a modeling language *defines the problem*; it usually does not specify how to solve it. Unlike procedural languages such as Fortran or C, modeling languages are *declarative languages* containing the problem in a declarative form by specifying the properties of the problem. *Algebraic modeling languages* – *cf.* Kallrath (2004, [14]) – are a special subclass of declarative languages, and most of them are designed for specifying *optimization problems*, *i.e.*, the model can be written in a form which is close to the mathematical notation. Usually they are capable of describing problems of the form

$$\min f(x) \tag{4}$$

$$s.t. \ q(x) = 0 \tag{5}$$

$$h(x) \ge 0 \quad , \tag{6}$$

where **x** denotes a subset of $X = \mathbb{R}^m \times \mathbb{Z}^n$.

Planning in the Process Industry

The problem is flattened, *i.e.*, all variables and constraints become essentially one-dimensional, and the model is written in an *index-based* formulation, using *algebraic expressions* in a way which is close to the mathematical notation. Typically, the problem is declared using *sets*, *indices*, *parameters*, and *variables*.

In a modeling language, model and model data are kept separately. There is a clear cut between the model structure and the data. Thus, many different instances of the same model class with varying data can be solved. Many systems provide an ODBC (open database connectivity) interface for automatic database access and an interface to the most widely used spreadsheet systems. This relieves the user from the laborious duty of searching for the relevant data every time the model is used. A second advantage of this concept is that during the development phase of the model (in the cycle) the approach can be tested on *toy problems* with small artificial data sets, and later the model can be applied without change for large scale industry-relevant instances with real data.

In an algebraic modeling language, the formulation of the model is *inde*pendent of solver formats. Different solvers can be connected to the modeling language, and the translation of models and data to the solver format is done automatically. This has several advantages. The formerly tedious and error prone translation steps are done by the computer, and after thorough testing of the interface errors are very unlikely. There is a clean cut between the problem definition and the solution approach, *i.e.*, between the modeling and the numerical, algorithmic part. In addition, for hard problems different solvers can be tried, making it more likely that a solution algorithm is found which produces a useful result. Algebraic modeling languages such as AIMMS, GAMS, LINGO, MPL, Mosel or OPL studio are well suitable to implement such models; cf. Kallrath (2004, [14]).

Modern algebraic modeling languages such as AIMMS, GAMS, LINGO, MPL, Mosel or OPL studio are well suitable to implement such models - cf. Kallrath (2004, [14]) to get a flavour of all of them – use state-of-the art commercial solvers, e.g., XPressMP [by Dash Optimization, http://www.dashoptimization.com] or CPLEX [by ILOG, http://www.ilog.com], and allow to solve even huge MILP problems with several hundred thousand variables and constraints quite efficiently. In the case of MINLP, the solution efficiency depends strongly on the individual problem and the model formulation. However, as stressed in [11] for both problem types, MILP and MINLP, it is recommended that the full mathematical structure of a problem is exploited, that appropriate reformulations of models are made and that problem specific valid inequalities or cuts are used. Software packages may also differ with respect to the ability of pre-solving techniques, default-strategies for the Branch&Bound algorithm, cut generation within the Branch&Cut algorithm, and last but not least diagnosing and tracing infeasibilities which is an important issue in practice.

There is great progress on solving planning problems more efficiently by constructing efficient valid inequalities for certain substructures of planning problems. The well written book by Wolsey (1998, [26]) and Pochet & Wolsey (2006, [21]) contain many examples. These inequalities may a priori be added to a model, and in the extreme case they would describe the complete convex hull. As an example we consider the mixed-integer inequality

$$x \le C\lambda$$
 , $0 \le x \le X$; $x \in \mathbb{R}_0^+$, $\lambda \in \mathbb{N}$ (7)

which has the valid inequality

$$x \le X - G(K - \lambda)$$
 where $K := \left\lceil \frac{X}{C} \right\rceil$ and $G := X - C(K - 1)$ (8)

This valid inequality (8) is the more useful, the more K and X/C deviate. A special case arising often is the situation $\lambda \in \{0, 1\}$. Another example, taken from ([26], p. 129) is

$$A_1\alpha_1 + A_2\alpha_2 \le B + x \quad ; \quad x \in \mathbb{R}^+_0 \quad , \quad \alpha_1, \alpha_2 \in \mathbb{N}$$

$$\tag{9}$$

which for $B \notin \mathbb{N}$ leads to the valid inequality

$$\lfloor A_1 \rfloor \alpha_1 + \left(\lfloor A_2 \rfloor \alpha_2 + \frac{f_2 - f}{1 - f} \right) \le \lfloor B \rfloor + \frac{x}{1 - f}$$
(10)

where the following abbreviations are used:

$$f := B - \lfloor B \rfloor \quad , \quad f_1 := A_1 - \lfloor A_1 \rfloor \quad , \quad f_2 := A_2 - \lfloor A_2 \rfloor \tag{11}$$

The dynamic counterpart of valid inequalities added a priori to a model leads to cutting plane algorithms which avoid adding a large number of inequalities a priori to the model (note, this can be equivalent to finding the complete convex hull). Instead, only those useful in the vicinity of the optimal solution are added dynamically.

Using these techniques, for some BASF planning problems including up to 100,000 constraints and up to 150,000 variables with several thousand binary variables, good solution with integrality gaps below 2% have been achieved within 30 minutes on standard Pentium machines [11].

6 Conclusions

Planning is strongly based on mathematical optimization exploiting large MILP problems. Strategic, design and operative planning models including several hundred thousand variables and constraints can be solved efficiently using commercial algebraic modeling languages and attached MILP solvers. These models are connected to company wide databases.

References

- M. Fieldhouse. The Pooling Problem. In T. Ciriani and R. C. Leachman, editors, *Optimization in Industry: Mathematical Programming and Modeling Techniques in Practice*, pages 223–230. John Wiley and Sons, Chichester, UK, 1993.
- C. A. Floudas. Short-term and Medium-term Scheduling. In L. G. Papageorgiou and M. C. Georgiadis, editors, *Supply Chain Optimization*. Wiley-VCH, Wiesbaden, Germany, 2007, in print.
- C. A. Floudas, I. G. Akrotiriankis, S. Caratzoulas, C. A. Meyer, and J. Kallrath. Global Optimization in the 21st Century: Advances and Challenges for Problems with Nonlinear Dynamics. In A. Barbossa-Povoa and A. Motos, editors, *European Symposium on Computer-Aided Process Engineering* (*ESCAPE*) 14, pages 23–51. Elsevier, Dordrecht, North-Holland, 2004.
- C. A. Floudas and X. Lin. Continuous-Time versus Discrete-Time Approaches for Scheduling of Chemical Processes: A Review. *Computers and Chemical Engineering*, 28(11):2109–2129, 2004.
- J. P. Ignizio. Goal Programming and Extensions. Heath, Lexington, Massachusetts, USA, 1976.
- S. L. Janak, C. A. Floudas, J. Kallrath, and N. Vormbrock. Production Scheduling of a Large-Scale Industrial Batch Plant: I. Short-Term and Medium-Term Scheduling. *Industrial and Engineering Chemistry Research*, 45:8234–8252, 2006a.
- S. L. Janak, C. A. Floudas, J. Kallrath, and N. Vormbrock. Production Scheduling of a Large-Scale Industrial Batch Plant: II. Reactive Scheduling. *Industrial and Engineering Chemistry Research*, 45:8253–8269, 2006b.
- S. L. Janak, X. Lin, and C. A. Floudas. Enhanced Continuous-Time Unit-Specific Event-Based Formulation for Short-Term Scheduling of Multipurpose Batch Processes: Resource Constraints and Mixed Storage Policies. *Ind. Chem. Eng. Res.*, 43:2516–2533, 2004.
- S. L. Janak, X. Lin, and C. A. Floudas. A New Robust Optimization Approach for Scheduling under Uncertainty - II. Uncertainty with Known Probability Distribution. *Computers and Chemical Engineering*, 31:171–195, 2007.
- J. Kallrath. The Concept of Contiguity in Models Based on Time-Indexed Formulations. In F. Keil, W. Mackens, H. Voss, and J. Werther, editors, *Scientific Computing in Chemical Engineering II*, pages 330–337. Springer, Berlin, 1999.
- J. Kallrath. Mixed Integer Optimization in the Chemical Process Industry: Experience, Potential and Future Perspectives. *Chemical Engineering Research and Design*, 78(6):809–822, 2000.
- J. Kallrath. Combined Strategic and Operational Planning An MILP Success Story in Chemical Industry. OR Spectrum, 24(3):315–341, 2002.
- 13. J. Kallrath. Planning and Scheduling in the Process Industry. OR Spectrum, 24(3):219–250, 2002.
- J. Kallrath. Modeling Languages in Mathematical Optimization. Kluwer Academic Publishers, Norwell, MA, USA, 2004.
- J. Kallrath. Solving Planning and Design Problems in the Process Industry Using Mixed Integer and Global Optimization. Annals of Operations Research, 140:339–373, 2005.

- J. Kallrath. Multi-Site Design and Planning Problems in the Process Industry. In L. G. Papageorgiou and M. C. Georgiadis, editors, *Supply Chain Optimization*. Wiley-VCH, Wiesbaden, Germany, 2007, in print.
- 17. J. Kallrath and T. I. Maindl. *Real Optimization with SAP-APO*. Springer, Heidelberg, Germany, 2006.
- J. Kallrath and J. M. Wilson. Business Optimisation Using Mathematical Programming. Macmillan, Houndmills, Basingstoke, UK, 1997.
- X. Lin, S. L. Janak, and C. A. Floudas. A New Robust Optimization Approach for Scheduling under Uncertainty - I. Bounded Uncertainty. *Computers and Chemical Engineering*, 28:1069–1085, 2004.
- C. Meyer and C. A. Floudas. Global Optimization of a Combinatorially Complex Generalized Pooling Problem. *AIChe*, 52:1027–1037, 2006.
- Y. Pochet and L. A. Wolsey. Production Planning by Mixed Integer Programming. Springer, New York, 2006.
- 22. C. Romero. Handbook of Critical Issues in Goal Programming. Pergamon Press, Oxford, 1991.
- M. J. Schniederjans. Goal Programming: Methodology and Applications. Kluwer Academic Publishers, Boston, MA, 1995.
- C. Suerie. Time Continuity in Discrete Time Models New Approaches for Production Planning in Process Industries, volume 552 of Lecture Notes in Economics and Mathematical Systems. Springer, Heidelberg, Germany, 2005.
- C. Timpe and J. Kallrath. Optimal Planning in Large Multi-Site Production Networks. European Journal of Operational Research, 126(2):422–435, 2000.
- 26. L. A. Wolsey. Integer Programming. Wiley, New York, US, 1998.