Noname manuscript No.
(will be inserted by the editor)

Combined Strategic and Operational Planning - An MILP Success Story in Chemical Industry

Josef Kallrath[1,2]

[1] BASF-AG, GVC/S (Scientific Computing) - C13, D-67056 Ludwigshafen, Germany (e-mail: `josef.kallrath@basf-ag.de`)
[2] University of Florida, Astronomy Dept., Gainesville, 32661 FL, USA (e-mail: `kallrath@astro.ufl.edu`)

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

Abstract We describe and solve a real world problem in chemical industry which combines operational planning with strategic aspects. In our simultaneous strategic & operational planning (SSDOP) approach we develop a model based on mixed-integer linear (MILP) optimization and apply it to a real-world problem; the approach seems to be applicable in many other situations provided that people in production planning, process development, strategic and financial planning departments cooperate.

The problem is related to the supply chain management of a multi-site production network in which production units are subject to purchase, opening or shut-down decisions leading to an MILP model based on a time-indexed formulation. Besides the framework of the SSDOP approach and consistent net present value calculations, this model includes two additional special and original features: a detailed nonlinear price structure for the raw material purchase model, and a detailed discussion of transport times with respect to the time discretization scheme involving a probability concept. In a maximizing net profit scenario the client reports cost saving of several millions US$.

The strategic feature present in the model is analyzed in a consistent framework based on the operational planning model, and vice versa. The demand driven operational planning part links consistently to and influences the strategic. Since the results (strategic desicions or designs) have consequences for many years, and depend on demand forecast, raw material availability, and expected costs or sales prices, resp., a careful sensitivity analysis is necessary showing how stable the decisions might be with respect to these input data.

Key words MILP modelling – Strategic and operational planning – Supply chain – Chemical industry – Transportation

1 Introduction

This contribution evolved from a project in chemical industry in which we developed and successfully applied a mixed-integer model to a real world problem which combines strategic and operational planning aspects in one model (a second example which encourages this approach is described in [9, Section 8.2]); operational planning aspects involve decisions on short or mid-term time-scale which are transformed into operational activities, *e.g.*, producing, shipping or selling something. Let us first give some motivation why this simultaneous strategic & operational planning (SSDOP) approach based on mixed-integer optimization may greatly improve a company's situation and let us focus on some problems we might expect.

1.1 Solving design and operational planning problems simultaneously

It is a frequent experience that clients ask for support on a production planning or scheduling problem for a plant or reactor which just went into operation. Often, especially in scheduling problems, it turns out that there exist certain bottlenecks. It would greatly improve the situation if the design of a plant or reactor would be analyzed simultaneously with the planning or scheduling problem. Certainly, this problem is mathematically demanding because scheduling problems alone are already very difficult to solve [10], *e.g.*, because of resources (raw material, machine availability, or personnel) too strongly limited. Thus, if the design and planning/scheduling problem are part of one embracing model this bottleneck situation might be avoided. This simultaneous approach requires the availability of realistic and detailed demand forecast, and expected cost or sales prices, resp., and that the departments being responsible for the design and the planning/scheduling cooperate. The latter problem is by far the more difficult one, especially in large companies. A concrete example of this type, a process design network problem, is discussed in [9, Section 9.2].

1.2 Solving strategic and operational planning problems simultaneously

A company running a complex production network consisting of several plants, (see, for instance, [11, Section 10.4]) wishes to buy additional plants, open new reactors based on improved technology, or to shut down some older reactors. In their multi-stage production system there might exist logical implications between the status of certain reactors. The data governing the investment or deinvestment decisions are the costs to buy a plant, or the costs to open or shut down a reactor. The investments or deinvestments should be sound over a time horizon of, say, up to 15 years. The best approach to analyze such situations is to develop a quantitative planning model and to enhance it by additional plants or reactors (leading to so-called design variables and constraints) and let the model provide suggestions on optimal design decisions. Regarding the database, it is necessary to provide the full data set (recipes, production rates and capacity, etc.) for all design plants or design reactors. All cost data should be discounted over the time horizon in order to support a net present value analysis. Such a case for a real production division of a chemical company is discussed in Section 2. To model this problem we partly use the model formulation published in [7], [11, Section 10.4], or [13]; the current project required major extensions related to design reactors, transport arriving over several time slices, non-linear pricing structures to purchase raw materials and additional objective functions such as *maximize net profit*, *multi-criteria objectives* (*i.e.*, maximize profit & minimize the quantity of transport in tons), *maximize sales volume* or *maximize turnover*.

Another problem of this type ([8] and [9, Section 9.1]), linking strategic and operational aspects is the optimization of a network of processing units at a large production site connected by a system of pipes. The purpose of this model was to design an integrated production network minimizing the costs for raw material, investment and variable costs for re-processing units, and a cost penalty term for low product quality. The investment decisions are considered on a 10-year linear depreciation rate.

1.3 Mathematical problems of combined models: complexity

Although company wide supply chain production models exist, see, for instance, [1] in most cases, because of their high complexity, even pure production planning or supply chain optimization problems are often seen as academic and not suitable for practical application. Instead, either simplifications (like linear relaxations) or simulation approaches are used, especially if there are several plants, tank storages, and the production planning problem is just a part of the comprehensive problem of optimizing the whole supply chain with regard to a detailed description of the commercial environment, such as demands with different prices for different customers, availability of raw material or quality commitments.

Therefore, if one suggests a simultaneous strategic/design & operational planning (SSDOP) approach it is not a surprise that the sceptics might argue *embedding a complex mixed-integer programming model in an even bigger problem including design features "is by far too difficult"*. Indeed, the problem might be large and complex, but as the case discussed in Section 2 shows, it is worthwhile to try and it can be done.

1.4 Mathematical problems of combined models: structure of the objective function

It is important that the problem is – within the limits and the assumptions of the model – approached as an exact optimization problem with a well-defined objective function representing the economic structure of the business process. We need to be able either to prove optimality, or to derive safe bounds enabling us to compare different scenarios reliably and to perform sensitivity analyses. A simulation approach is no substitute because it does not strictly (in the mathematical sense) support these items as it could happen that the scenarios A and B have the optimal solutions 110 and 105 but a simulation based approach produces best evaluations 103 and 104 which would indicate that B is better. In the SSDOP approach there are a few complicating factors related to the structure of the objective function.

Since the objective function may contain terms related to operational planning (variable costs for production and processing, transport, raw material, utilities, inventories, mode-changes, etc.) and the design decision (event costs to close or open reactors, to purchase plants, etc.) the scaling in the objective function terms might be poor. This problem might be overcome by appropriate branching strategies and prioritizing the branching variables. Since the planning horizon considered may cover up to 15 years, nonlinear (usually concave) terms describing a price structure might enter in addition. If these terms are not too complicated they can be described sufficiently accurate as shown in Section 4.2, for instance.

1.5 Mathematical problems of combined models: reliability of data

A point of practical concern is the availability of demand forecast data, costs or sales prices over a long period. People not favoring the SSDOP approach might use this as a strong argument against it. There are two arguments to meet these concerns: a) on what grounds would they base their investment decisions otherwise? (the problem related to accurate data concerns both mathematical planning and non-mathematical planning) and b) the mathematical planning approach supports sensitivity analyses and allows to estimate the stability of the decisions with respect to variability of the forecast data. In addition, when building the model and collecting the data, it is necessary to try to balance the degree of details entering the model. Finally, depending on the specific purpose, the overall model might be adapted to its use on different application levels (pure strategic, pure operational planning with fixed design decisions, etc.) requiring different accurateness of the data.

2 Strategic decisions in a worldwide production-network

The core production planning problem covers large parts of the supply chain including several plants, multi-stage production using multi-purpose reactors with some logical rules in the production scheme, tank storages, transport with a detailed representation of the commercial environment, such as demands with different prices for different customers and availability of raw material. Products are subject to aggregate demand requirements at certain demand points. Variable costs for production, inventory, transport are given. The raw material purchase follows a nonlinear price structure. The client asked to consider the production planning problem as a part of larger problem. This larger problem comprises a production network in which gaseous raw materials along a line of up to six intermediate products are converted into finished products, and in which a production unit from a given set of design units is subject to shutdown or opening, or in which even some whole plants can be purchased. To avoid duplication of material most details of production and other features are specified in Subsection 4.1. The most important objective is to maximize the total net profit (contribution margin minus fixed costs minus investment costs) of the entire production network. In addition the following objective functions are maximized: contribution margin, total sales neglecting cost, turnover and total production. Costs can be minimized and multi-criteria objectives, for instance, maximize profit & minimize transport, are supported. The most relevant decision variables indicate how much time per time-slice a reactor spends in a certain mode, how much of a product is produced, stored or shipped to another location. Binary variables trace the status and mode changes of a reactor. Structurally, most of the constraints are balance equations tracing inventories, connecting production and production recipes over several production levels and tracing mode changes. Other constraints relate production quantities, production rates and available time to each other, or guarantee that capacity limits are observed.

3 The mathematical model: preliminaries

3.1 The structure of the model and its basic objects

The problem sketched above has some common features with modeling *multi-purpose plants* which are frequently used in the food or chemical process industry. In each mode such a reactor can produce several products according to free or fixed recipes (joint production, coproduction) leading to a general mode-product relation described by a set of yield coefficients: in a certain mode several products are produced (with different maximum daily production rates), and vice-versa, a product can be produced in different (but not all) modes. *Mode changes* correspond physically, for instance, to a change of the temperature or pressure of a reactor, put the reactor in a new feasible mode and result in a considerable loss of production time, which in our case is sequence-dependent, and are modeled as a proportional lotsizing and scheduling problem (PLSP, [5, p.150]), *i.e.*, based on time-indexed formulations with at most one setup- or mode-change per period; see also [12] for a survey on lot sizing problems.

We thus transform the problem into a model describing a multi-site production network including multi-stage production in plants (a plant hosting sets of reactors) depending on the mode chosen for the reactors. Parts of the model have already been published in [7], [11, Section 10.4], or [13]; the current project required major extensions related to design reactors, transport arriving over several time slices, nonlinear pricing structures to purchase raw materials and additional objective functions such as *maximize net profit*, *multi-criteria objectives* (*i.e.*, maximize profit & minimize the quantity of transport in tons), *maximize sales volume* or *maximize turnover*. We thus extend and develop an elaborated version of the model [11, Section 10.4]. In our model we use the following set of objects and indices:

$b \in \mathcal{B}$	$:= \{1, \ldots, N^B\}$	: break points (nonlinear price function)
$c \in \mathcal{C}$	$:= \{1, \ldots, N^C\}$	: sales categories
$d \in \mathcal{D}$	$:= \{1, \ldots, N^D\}$	: demand points
$k \in \mathcal{K}_s$	$:= \{1, \ldots, N_s^K\}$	: production periods at site s
$m \in \mathcal{M}_{sr}$	$:= \{1, \ldots, N_{sr}^M\}$	: modes at site s for reactor r
$p \in \mathcal{P}$	$:= \{1, \ldots, N^P\}$	: products
$r \in \mathcal{R}$	$:= \{1, \ldots, N^R\}$	: reactors
$s \in \mathcal{S}$	$:= \{1, \ldots, N^S\}$	: production sites / plants
$t \in \mathcal{T}$	$:= \{1, \ldots, N^T\}$	: commercial periods

Break points are points at which the unit price as a function of volume changes. *Sales categories* allow, for instance, to model that the first 80% of an order can be purchased at a price of 100 US$, the next 20% at 90US$. *Demand Points* may represent customers, regional warehouse locations or distributors who specify the quantity of a product they request, and are sinks in the supply network, *i.e.*, points 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 from the same origin.

3.2 Discretization of time

In order to investigate a planning horizon of up to 15 years and to cover the production at a level which is sufficiently detailed we use the time discretization scheme described by [13] using non-equidistant commercial and production time slices (periods); in most cases, the production schedule has a finer resolution than the commercial plans for sales and shipping. Different time scales allow to have smallest time slices relevant to production which may be of the order of just a few days while the commercial periods may cover even a few years. The entire planning horizon is therefore divided into N_s^K production slices of size D_t^P/U_{st} days, where D_t^P is the length of the t^{th} commercial period in days and U_{st} is the number of production slices embedded in that commercial period. Regarding delivery or sale, in typical operational planning, usually a commercial time scale of 12 periods (months) is chosen. Another possible scenario is, for instance, to cover a two year production plan with $N^T = 16$ periods: the first 12 with a length of about 30 days, and four additional ones with a length of 120 days. Commercial and production time slices are linked by the function

$$k_s(s,t) := \begin{cases} 0 & \text{, if } t = 1 \\ k_s(s,t-1) + U_{s,t-1} & \text{, if } t > 1 \end{cases} \quad \forall\{st\} \tag{1}$$

which gives the number (minus one) of the production slice starting at the beginning of commercial period t at site s, and, with u referring to a production slice embedded in the commercial time interval t. The function

$$k(s,t,u) := k_s(s,t) + u \quad \forall\{st\} \tag{2}$$

gives the absolute number $k(s,t,u)$ of the u^{th} production slice in the commercial period t within the production time scale referenced by t and u at plant s, and connects both time scales. For shortness, if sums cover the whole planning horizon, we use k rather than $k(s,t,u)$. Finally, we need the inverse function, $t_k(s,k)$,

$$t_k(s,k) := \min\{t \mid k_s(s,t) < k \leq k_s(s,t) + U_{st}\} \quad \forall\{st\} \tag{3}$$

returning the commercial period that covers the production slice k at plant s. It can be expressed in terms of the functions defined above: For further details on this topic we refer to [13]. A 5-year planning horizon in which the commercial data are available on an annual basis and production should be considered with a fineness of one month, leads to

$$N^T = 5 \quad ; \quad D_t^P = 360 \quad \forall t \quad ; \quad U_{st} = 12 \quad \forall\{st\} \tag{4}$$

while for asset evaluation over a time horizon covering 10 years with two production time slices per year is described by

$$N^T = 10; \quad D_t^P = 360 \quad \forall t; \quad U_{st} = 2 \quad \forall\{st\} \tag{5}$$

3.3 Limits and underlying assumptions

The limits of the model follow from its underlying assumptions which are further discussed in Section 7.1:

1. Only one mode change per production time slice is allowed as the model is formulated as a proportional lotsizing and scheduling problem (PLSP, [5, p.150] or [6]), *i.e.*, based on time-indexed formulations with at most one setup- or mode-change per period. This assumption seems not to be a very serious restriction for operational planning since a production time slice has a length of a week or a month and typically only one setup-change per month occurs. For the long term analysis the description of the mode changing reactors may not be accurate enough. But one should

keep in mind that the demand forecast and other input data are of limited accuracy as well; the client regarded the approach as sufficiently accurate and realistic.

2. Transport times are of the order of a few days. In the 12-month scenarios transport times are only considered using a probability assumption. In even longer term scenarios transport times are neglected.
3. Only variable inventory costs are considered. They are based on the capital tied up in inventories and interest rates.
4. Design reactors cannot be subject to intrinsic mode changes. In the current case this limitation did not cause any problems because the approximately 30 reactors subject to design decisions were single product reactors.
5. Production utilization rates and associated constraints refer to utilization per production slice. At present, the model does not include constraints enforcing global utilization aspects of the supply network.
6. In order to support net present value considerations all cost related data are discounted over time using a discount rate of $p\%$.

4 The mathematical model: the operational planning aspects

4.1 Plants, reactors and production

Each plant consists of one or two sets of reactors. While all reactors are subject to multi-stage production requirements and possible coproduction, some are multi-purpose reactors subject to mode changes. Topologically, at each plant, the reactors are arranged in chains, in which each reactor needs only one pre-product; however, the current model formulation does not exploit this features and can also be applied to convergent or divergent material flows and more general topologies. The reactors within a chain operate simultaneously and at different levels of the multi-stage production process. There exist capacity limits for each reactor and task, as well as capacities for the production of each product, and minimum production requirements. Some reactors in the chain are subject to mode changes lasting usually one or two days. Reactors obtain products from preceding reactors or from tanks, and charge the products through pipelines to tanks or to subsequent reactors.

Modeling production involves the concepts of multi-stage production, joint production (coproduction) and mode changes of the multi-purpose reactors. The description of the mode changes is based on [11, pp. 321]; the adoption of this approach to the current problem is as follows. The basic binary variables are the state variables

$$\delta_{srmk} = \begin{cases} 1 \text{ , if reactor } r \text{ is in mode } m \text{ at the end of period } k \\ 0 \text{ , otherwise} \end{cases} \tag{6}$$

It is one of the most fundamental assumptions in this model that there is at most one mode change per period. If the state variables take the values

$\delta_{srm_1k-1} = \delta_{srm_2k} = 1$ we have a mode change from mode m_1 to m_2 in time interval k.

Both, the continuity of modes and mode changes are tracked by the binary variables

$$\xi_{srkm_1m_2} = \begin{cases} 1 \text{ , if } \delta_{srm_1k-1} = \delta_{srm_2k} = 1 \\ 0 \text{ , otherwise} \end{cases} \qquad \forall\{srm_1m_2k\} \tag{7}$$

This variable is unity if at the end of period $k-1$ reactor $r \in \mathcal{R}_s \; \left| I_{sr}^{MC} = 1 \right.$ of plant $s \in \mathcal{S}$ is in mode $m_1 \in \mathcal{M}_{sr}$ and at the end of period $k \in \mathcal{K}$ it is in mode $m_2 \in \mathcal{M}_{sr}$. $\xi_{srkm_1m_2}$ is a variable not only describing whether a change-over occurs, but it also indicates whether production continues. If the reactor is in mode m both at the end of period $k-1$ and k then we have $\xi_{srkmm} = 1$.

The state variables and the mode-change variables will now be coupled by some additional binary variables: α_{srmk}, if reactor r at plant s spends some time in period k in mode m; β_{srmk}, if mode m is started on reactor r at site i in period k; and finally, γ_{srmk}, if mode m is terminated on reactor r at site i in period k. These binary variables are related to the mode changing variables by the constraints

$$\beta_{srmk} = \sum_{m_1 \neq m} \xi_{srkm_1m} \quad \forall(srmk) \tag{8}$$

and

$$\gamma_{srmk} = \sum_{m_1 \neq m} \xi_{skmm_1} \quad \forall(srmk) \tag{9}$$

The multi-stage production scheme looks as follows: at a site s a certain reactor r is connected to one (or possibly more) preceding reactors r'; it is assumed that transfer times between reactors are zero. The reactor topology is completely described by the indicator table $I_{sr'r}^{Topo}$ which takes the value 1 if reactor r' can charge to reactor r. Reactor r converts the product p' produced by preceding reactors r' into the product p, or possibly into several coproducts. Actually, this product p' can also be taken from the preceding reactor r' or from an intermediate tank. The total quantity $p_{srp'k}^U$ of product p' reactor r uses in period k is therefore

$$p_{srp'k}^U = u_{srp'k}^S + \sum_{r | I_{srr'}^{Topo} > 0 \wedge I_{sr'p'}^{SRP} = 1} p_{sr'rp'k}^D \tag{10}$$

$$\forall \left\{ srp' \left| I_{srp'}^{PP} = 1 \wedge I_{sr}^{Pipi} = 1 \right. \right\} \quad \forall k \tag{11}$$

where $I_{srp'}^{PP}$ indicates whether reactor r uses p' as a pre-product at all. The indicator table $I_{sr'p'}^{SRP}$ controls which reactor r' at site s is able to produce product p', and $u_{srp'k}^S$ is the quantity of product p' taken by reactor r from the tank. Note that $I_{sr}^{Pipi} = 1$ means that reactor r is – via an input pipeline – connected to a tank and is able to extract material from that storage device; in the current case, each reactor needs exactly one pre-product, therefore I_{sr}^{Pipi} does not depend on the product as this is known a priori. $p_{sr'rp'k}^{D}$ is the quantity of product p' charged from reactor r' directly to reactor r and allows also to model convergent material flows if the topology is chosen appropriately. Note that $u_{srp'k}^{S}$ appears as a loss term in the stock balance equation (44). If p' is a raw material, which can only be purchased, (10) reduces to

$$p_{srp'k}^{U} = u_{srp'k}^{S} \quad \forall \left\{ srk \left| I_{srp'}^{PP} = 1 \wedge I_{sr}^{Pipi} = 1 \right. \right\} \tag{12}$$

because p' is not produced on any reactor, and therefore for all reactors r' we have $I_{sr'p'}^{SRP} = 0$. To model raw material availability it has to be ensured in the input data that $u_{srp'k}^{S}$ has no upper bound, or is consistent with the raw material availability, respectively. Finally, if the reactor is not connected to an input tank, (10) reduces to

$$p_{srp'k}^{U} = \sum_{r \mid I_{srr'}^{Topo} > 0 \wedge I_{sr'p'}^{SRP} = 1} p_{sr'rp'k}^{D} \quad \forall \left\{ srp'k \left| I_{srp'}^{PP} = 1 \wedge I_{sr}^{Pipi} \neq 1 \right. \right\} \tag{13}$$

The multi-stage production, *i.e.*, the quantity p_{srpk}^{P} of product p produced on reactor r at site s is described by recipe equations of the form

$$\sum_{p \in \mathcal{P} \left| I_{srp}^{SRP} > 0 \right.} R_{srp'p} p_{srpk}^{P} = p_{srp'k}^{U} \quad \forall \left\{ srp'k \left| I_{srp'}^{PP} > 0 \right. \right\} \tag{14}$$

It is a matter of taste whether to apply the recipe coefficient to p' or p. Note that reactor r produces several products p using p' simultaneously.

In addition to the multi-stage concept we also have to consider coproduction. If the conversion of product p' produces two products p_1 and p_2 in a fixed ratio $R_{srp_1p_2}^{FR}$, we have

$$p_{srp_1k}^{P} = R_{srp_1p_2}^{FR} p_{srp_2k}^{P} \quad \forall \left\{ srp_1p_2k \left| \exists R_{srp_1p_2}^{FR} > 0 \right. \right\} \tag{15}$$

So (15), means that for each mass unit that is produced of product p_2 one also gets $R_{srp_1p_2}^{FR}$ mass units of product p_1. The quantity p_{srpk}^{P} of product p which can be produced on reactor r at site s in period k is limited by the capacity R_{srp}^{P} specified in tons/day. With $P_{srpk}^{\min} := H_{srk} R_{srp}^{P\min} = H_{srk} R_{srp}^{U\min} R_{srp}^{P}$, where H_{srk} is the number of days available for production in period k and $R_{srp}^{U\min}$ specifies production utilization for reactor r at site s and product p in %, and the production capacity, $P_{srpk}^{\max} := H_{srk} R_{srp}^{P}$, of reactor r in tons in period k, we get the bounds

$$p_{srpk}^{P} \leq P_{srpk}^{\max} \quad \forall \left\{ srpk \left| I_{srp}^{SRP} = 1 \wedge I_{sr}^{MC} \neq 1 \right. \right\} \tag{16}$$

Some additional sets of constraints consider minimum production of a product at a plant over a specific time period. This may be quantified by $R_{srp}^{U\min}$, the production utilization for reactor r at site s and product p in %. If the minimum $P_{srpk}^{\min} := R_{srp}^{U\min} P_{srpk}^{\max}$ is not met, then no production is possible. Therefore, p_{srpk}^{P} is a semi-continuous variable or subject to the disjunctive constraints, resp.

$$p_{srpk}^{P} = 0 \quad \vee \quad P_{srp}^{\min} \leq p_{srpk}^{P} \leq P_{srp}^{\max} \quad \forall \left\{ srpk \left| \exists R_{srp}^{P} \right. \right\} \tag{17}$$

For those reactors subject to opening or shut-down decisions or belonging to plants which might be purchased the capacity balance reads

$$p_{srpk}^{P} = 0 \quad \vee \quad P_{srpk}^{\min}\theta_{sr} \leq p_{srpk}^{P} \leq P_{srpk}^{\max}\theta_{sr} \qquad \forall \left\{ srpk \left| \exists R_{srp}^{P} \wedge \exists I_{sr}^{D} \right. \right\} \tag{18}$$

where the indicator table I_{sr}^{D} indicates whether reactor r is a design reactor and the binary variable θ_{sr} specifies whether the reactor is available or not. It is also possible to apply global constraints enforcing that, if a design reactor falls below a certain minimum usage rate, it has to be shut down; however, due to the lack of space we do not present this feature here.

The quantity p_{srpk}^{P} of output product p is charged to a local tank (site inventory) or charged to subsequent reactors. This is expressed by the distribution equation

$$p_{srpk}^{P} = p_{srpk}^{T} + \sum_{r \in \mathcal{R} | I_{srr'}^{Topo} > 0} p_{srr'pk}^{D} \quad \forall \left\{ srpk \left| I_{srp}^{SRP} = 1 \right. \right\} \tag{19}$$

where p_{srpk}^{T} is the quantity of product p charged to the tank (site inventory) by pipeline, or by

$$p_{srpk}^{P} = \sum_{r \in \mathcal{R} | I_{srr'}^{Topo} > 0} p_{srr'pk}^{D} \quad \forall \left\{ srpk \left| I_{srp}^{SRP} = 1 \right. \right\} \tag{20}$$

if reactor r has no pipeline connection to an output tank.

4.2 Raw material modeling

Raw materials are in most aspects treated similarly to all other products, for instance, they fulfill the recipe equation (14). However, for raw materials we have to consider purchase cost C_{srp}^{RM} and the availability A_{srpk}^{RM} which describes how much raw material p is available in period k. Raw materials are fed to the reactors by a tank. Thus we model the availability exploiting the tank feature $I_{sr}^{Pipi} = 1$ and the variable u_{srpk}^{s} expressing how much of product p (in this case raw material) reactor r at site s takes from the tank. The variable u_{srpk}^{S} is subject to the availability constraint

$$u_{srpk}^{S} \leq A_{srpk}^{RM} \quad \forall \left\{ srpk \left| \exists A_{srpk}^{RM} \wedge I_{srp}^{PP} = 1 \right. \right\} \tag{21}$$

The notation $\exists A^{RM}_{srpk}$ reflects that an inequality is generated only if a table entry for A^{RM}_{srpk} exists. A more elaborated view of the raw materials, controlled by a site and raw material dependent flag $\mathtt{R}^{M}_{sp}$, takes the following features into account:

$\mathtt{R}^{M}_{sp}$	*description*
0	material requirement planning output; no constraints, no costs
1	take as much raw material as needed at a fixed price
2	take as much raw material as needed at a nonlinear price
3	take all available raw material (use or burn) at a fixed price

and generates all constraints only if a raw material tank has been declared, *i.e.*, if $\exists S^{SC}_{sp}$.
If $\mathtt{R}^{M}_{sp} = 0$ no raw material constraints or costs are considered. In the report we just print the raw material which would be required. For modeling the raw material features we introduce the following variables:

u^{R}_{spk} : usage (in tons) of raw material (product) p in period k
u^{RB}_{spbk} : usage (in tons) of raw material (product) p in segment b
b^{R}_{spk} : burned quantity (in tons) of raw material (product) p
μ_{spbk} : binary var. indicating $R^{BPV}_{spb-1k} \le u^{RB}_{spbk} \le R^{BPV}_{spbk}$ in period k,
ω_{spt} : binary var. indicating the use of raw material p in period t

If Y^{RM}_{spk} specifies the price per ton which can be obtained if the raw material is burnt, it can not be used otherwise, and thus converted into energy. For $\forall \left\{ spk \middle| \exists A^{RM}_{spk} \wedge \left(\exists r \text{ with } I^{PP}_{srp} = 1\right) \wedge \exists Y^{RM}_{spk} \right\}$ we apply the following bounds or constraints, resp.:

$$u^{R}_{spk} \le A^{RM}_{spk} \quad \text{if } \mathtt{R}^{M}_{sp} = 1 \tag{22}$$

$$u^{R}_{spk} + b^{R}_{spk} = A^{RM}_{spk} \quad \text{if } \mathtt{R}^{M}_{sp} = 3 \tag{23}$$

The case $\mathtt{R}^{M}_{sp} = 2$ is more difficult to model and requires the following data

R^{BPC}_{spbk} specific raw material cost in segment b
R^{BPV}_{spbk} raw material volume at break point b
R^{ACC}_{spbk} accumulated raw material cost at break point b
R^{FIX}_{spk} fixed cost (setup cost) if raw material p is chosen
R^{PEN}_{spk} penalty cost if raw material p is not used at all

where segment b refers to the range between break point $b-1$ and b, and thus to the interval $[R^{BPV}_{spb-1k}, R^{BPV}_{spbk}]$ the penalty cost R^{PEN}_{spk} apply to the situation that an annual contract with the raw material supplier has been established but the raw material is not used at all, $R^{ACC}_{sp1k} = 0$ and for $b = 2, \ldots, N^B$

$$R^{ACC}_{spbk} = R^{ACC}_{spb-1k} + R^{BPC}_{spbk}\left(R^{BPV}_{spbk} - R^{BPV}_{spb-1k}\right) \tag{24}$$

To select the appropriate segment or interval $[R^{BPV}_{spb-1k}, R^{BPV}_{spbk}]$ for the quantity of raw material purchased we exploit the binary variable μ_{spbk} which indicates that $R^{BPV}_{spb-1k} \leq u^{RB}_{spbk} \leq R^{BPV}_{spbk}$. The constraints

$$\sum_{b=1}^{N^B+1} \mu_{spbk} = 1 \quad \forall \left\{ spk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{25}$$

and

$$u^{RB}_{spbk} \geq R^{BPV}_{spb-1k} \mu_{spbk} \quad \forall \left\{ spk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{26}$$

$$u^{RB}_{spbk} \leq R^{BPV}_{spbk} \mu_{spbk} \quad \forall \left\{ spk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{27}$$

guarantee that u^{RB}_{spbk} falls exactly into one segment. Note that $\mu_{spN^B+1k} = 1$ is used to indicate that no raw material is used at all.

The real quantity u^R_{spk} of used raw material is coupled to the segment quantity by

$$u^R_{spk} = \sum_{b=1}^{N^B} u^{RB}_{spbk} \quad \forall \left\{ spk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{28}$$

As raw material is purchased on the basis of annual contracts, which might force that a certain quantity has to be purchased by the provider, we introduce the binary variable ρ_{spt} indicating whether any quantity of raw material p is used in the commercial period at all

$$\rho_{spt} \geq 1 - \mu_{spN^B+1k} \quad \forall \left\{ sptk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{29}$$

If no raw material is used at all, penalty cost may be applied by the provider.

An alternative, and in most cases superior formulation of these raw material aspects replaces (26) to (28) by

$$u^R_{spk} = \sum_{b=2}^{N^B} R^{BPV}_{spb-1k} \mu_{spbk} + \sum_{b=1}^{N^B} u^{RB}_{spbk} \quad \forall \left\{ spk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{30}$$

$$u^{RB}_{spbk} \leq R^{BPV}_{sp1k} \mu_{spbk} \quad \forall \left\{ spk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{31}$$

where u^R_{spk} has a slightly different meaning now, and

$$u^{RB}_{spbk} \leq \left(R^{BPV}_{spbk} - R^{BPV}_{spb-11k} \right) \mu_{spbk} \quad \forall \left\{ spk \left| \exists A^{RM}_{spk} \wedge \exists S^{SC}_{sp} \right. \right\} \tag{32}$$

The variable raw material cost are then given by

$$\sum_{s\in\mathcal{S}} \sum_{p\in\mathcal{P}} \sum_{b=2}^{N^B} \sum_{k=1}^{N^K_s} R^{ACC}_{spb-1k} \mu_{spbk} + \sum_{s\in\mathcal{S}} \sum_{p\in\mathcal{P}} \sum_{b=1}^{N^B} \sum_{k=1}^{N^K_s} R^{BPV}_{spbk} u^{RB}_{spbk} + \sum_{s\in\mathcal{S}} \sum_{p\in\mathcal{P}} \sum_{t=1}^{N^T} R^{PEN}_{spt} + \sum_{s\in\mathcal{S}} \sum_{p\in\mathcal{P}} \sum_{t=1}^{N^T} \left(R^{FIX}_{spt} - R^{PEN}_{spt} \right) \rho_{spt} \tag{33}$$

A special ordered set approach involving the μ_{spbk} variables has been tested as well, but did not turn out to be superior compared to the formulation in which the μ_{spbk} variables are just binary variables.

4.3 Transport

The model considers three types of transport: transport of products between production sites and transport of products from production sites to demand points; in some rare cases there is also transport between demand points. Transport costs depend on the source, destination and product, minimal quantities to be observed and transport times (typically a few days). Transportation quantities are expressed by non-negative, dimensionless semi-continuous *transport variables* specifying, when multiplied by the minimum transport quantity, T^M, the quantity of product p shipped:

$$\begin{array}{ll} \sigma^{DD}_{dd'pt} & : \ldots \text{ between demand points } d \text{ and } d' \\ \sigma^{SD}_{sdpk} & : \ldots \text{ shipped from site } s \text{ to demand point } d \\ \sigma^{SS}_{ss'pk} & : \ldots \text{ shipped from site } s \text{ to site } s' \end{array} \tag{34}$$

The semi-continuous variables, for instance, σ^{SD}_{sdpk} are defined

$$\sigma^{SD}_{sdpk} = 0 \ \vee \ 1 \leq \sigma^{SD}_{sdpk} \leq S^{+}_{sdpk} \quad \forall\{sdpk\} \tag{35}$$

with some upper bound S^{+}_{sdpk}, and they enter the inventory balance equation in the form $T^{MSD}_{sdpk}\sigma^{SD}_{sdpk}$ where T^{MSD}_{sdpk} is the minimum transport quantity.

The various time scales in our model SSDOP force us to model transport time very carefully. The actual transport times are a few days, usually between 1 and 6 days. If the transport times are consistent with the time discretization, *i.e.*, the transport time is an integer multiple of the smallest time slice, the transport times can be considered in the index counting the time slice (see [11, Section 10.4]). Regarding the length of the planning horizon and the discretization of time we consider two model approaches to transport. In the 15-year planning horizon with half-year time slices and in the short term (operational planning) scenario covering three months the time resolution is one week. That fits transport times which will be reasonably approximated to be 0 or 1 week. In the one-year (operational) planning scenario with time slices of one month this is not accurate enough. We might use smaller time slices (leading to significantly increased CPU times) but in order to avoid this, we suggest to use the following approach based on a probability assumption (for clarity, we neglect some of the indices in this paragraph). The essential idea of this approach is to conserve the flow of materials but to distribute the shipment arrival to two adjacent time slices.

Let D^{PK}_{sk} be the length of the time period k at site s, Δ_{sd} be the time needed for transportation from site s to destination d and let us assume that $\Delta_{sd} \leq \min\left(D^{PK}_{k}, D^{PK}_{k+1}\right)$ for all k. If we assume that shipments during production period k leave site s with uniform probability in period k, the product will arrive at the destination d with probability

$$\omega_{sdk} := \frac{\Delta_{sd}}{D^{PK}_{sk}} = \frac{\Delta_{sd}}{D^{P}_{t}} U_t \tag{36}$$

in period $k+1$ and with probability $1-\omega_{sdk}$ in period k. Therefore, in the one-year planning scenario, we use the following heuristic approach to consider transport in the inventory balance equations. If p_{sd}^T is the quantity to be shipped (appears as a loss term at the site where transport origins) we consider (at the destination of shipment) $(1-\omega_{sdk})p_{sd}^T$ in the balance equation of period k and $\omega_{sdk}p_{sd}^T$ in period $k+1$ as source terms. This approach is not recommended if the planning tool is used operationally. But for long term, *e.g.*, annual planning, it should be perfectly suitable, especially, if there exists some minimum inventory level.

Let us now focus in more detail on products originating from site s in production period k arriving at demand point d in commercial period t. The time, Δ_{sd}, associated with this transport and the length, D_{sk}^{PK}, of the period allow us to compute ω_{sdk} from (36).

At first consider the short term scenario in which Δ_{sd} is an integer multiple of D_{sk}^{PK}, *i.e.*, $T_{sd} = \Delta_{sd}/D_{sk}^{PK}$. Then a shipment originating in period k arrives in period $k+T_{sd}$. If the commercial period t consists of U_{st} production time periods then all shipments originating in periods

$$\left\{k = 1, \ldots, N_s^K \,| t_k(s, k+T_{sd}) = t\right\} \tag{37}$$

arrive in that period.

In the long-term scenario transport is modeled using a probability assumption, *i.e.*, a fraction $1-\omega_{sdk}$ of the quantity $T_{sdpk}^{MSD}\sigma_{sdpk}$ arrives in period k at the destination d, *i.e.*, the arriving quantity of product p in period k is given by

$$(1-\omega_{sdk})\, T_{sdpk}^{Msd}\sigma_{sdpk} \quad \left\{k = 1, \ldots, N_s^K \,| t_k(s, k) = t\right\} \tag{38}$$

and the complementary fraction ω_{sdk} arrives in period $k+1$, *i.e.*,

$$\omega_{sdk'} T_{sdpk}^{Msd}\sigma_{sdpk'} \quad \left\{k' = 1, \ldots, N_s^K \,| t_k(s, k'+1) = t\right\} \tag{39}$$

Note that there might occur two terms containing the variable σ_{sdpk} (one associated with the $1-\omega_{sdk}$ term, and another one connected to $\omega_{sdk'}$ for the adjacent period), which in some modeling language may lead to complications (*column appears twice in a row*) if $U_{st} > 1$. This problem can be overcome by collecting all coefficients related to the same variable a priori.

4.4 Modeling inventories and stock balances

Inventories and related costs are considered for each product at both plants (inventories at sites) and regional warehouses (inventories at demand points). At demand points it is possible to lease some additional storage capacity.

4.4.1 Inventories at sites At present it is assumed that for each product p there is a dedicated tank available at a site. The stock, s^S_{spk}, for all $\{spk\}$, is described by the balance equation

$$s^S_{spk} = s^S_{spk-1} + p^{ES}_{spk} + \hat{S}^S_{spk} + u^R_{spk} - \sum_{r|I^{Pipi}_{sr}=1} u^S_{srpk} \tag{40}$$

$$+ \sum_{r\in\mathcal{R}\left|\left(I^{SRP}_{srp}=1\wedge I^{Pipi}_{sr}=1\right)\right.} p^T_{srpk} \tag{41}$$

$$- \sum_{s_d\in\mathcal{S}_{sdk}} T^{Mss}_{ss_d}\sigma^{SS}_{ss_dpk} - \sum_{d\in\mathcal{D}_{sdk}} T^{Msd}_{sd}\sigma^{SD}_{sdpk} \tag{42}$$

$$+ \sum_{s_s\in\mathcal{S}} (1-\omega_{s_ssk})\, T^{Mss}_{s_ss}\sigma^{SS}_{s_ssp,k-(1-\pi)T^{ss}_{s_ss}} \tag{43}$$

$$+ \sum_{s_s\in\mathcal{S}} \omega_{s_ssk} T^{Mss}_{s_ss}\sigma^{SS}_{s_ssp,k-\pi-(1-\pi)T^{ss}_{s_ss}} \tag{44}$$

in which the terms have the following meaning: s^S_{spk-1} is the stock level at the end of the previous period, p^{ES}_{spk} denotes external purchase [see Section 4.6], $\hat{S}^S_{spk}$

$$\hat{S}^S_{spk} := \sum_{s_s\in\mathcal{S}|\exists S^{SS}_{spk}} S^{SS}_{s_sspk} \tag{45}$$

denotes transport arriving in period k from shipment originating before the first period. The supply, u^R_{spk}, of raw material available in period k appears as a source term, the usage of the product, $\sum u^S_{srpk}$, as a loss term. The sum $\sum p^T_{srpk}$ represents the quantity of product charged from other reactors to this tank. The terms based on the σ-variables have been explained in Section 4.3 describing shipments to other sites and demand points as well as products received from other sites. The sets

$$\mathcal{S}_{sdk} := \left\{s_d \in \mathcal{S} \left| s_d \neq s \in \mathcal{S} \wedge k + T^{ss}_{ss_d} < N^K \right.\right\} \tag{46}$$

$$\mathcal{S}_{sk} := \left\{s_d \in \mathcal{S} \left| s_d \neq s \in \mathcal{S} \wedge k > T^{ss}_{ss_d} \right.\right\} \tag{47}$$

$$\mathcal{D}_{sdk} := \left\{d \in \mathcal{D} \left| k + T^{sd}_{sd} < N^K \right.\right\} \tag{48}$$

and

$$\mathcal{D}_{dk} := \left\{d_d \in \mathcal{D} \left| d_d \neq d \in \mathcal{D} \wedge t + T^{dd}_{dd_d} < N^T \right.\right\} \tag{49}$$

define the sets of sites or demand points which can be linked by transport to the current location s within the planning horizon.

For $k=1$ the term s^S_{spk-1} is replaced by the initial product stock S^{SS}_{sp}. The site-balance equation (44) for site inventories (also called local inventories) couples multi-stage production, intermediate storage space and transport (between sites, and between sites and demand points). p^{ES}_{spk} describes external purchase opportunity at site inventories. If no storage capacity is available the variables s^S_{spk} and s^S_{spk-1} drop out in (44).

The maximum stock levels for products read

$$s^S_{spk} \leq S^{CAP}_{sp} \quad \forall \left\{ spk \left| \exists S^{SC}_{sp} \right. \right\} \tag{50}$$

The product stock should never fall below the safety stock, S^{SS}_{sp},

$$s^S_{spk} \geq S^{SS}_{sp} \quad \forall \{spk\} \tag{51}$$

and a possible restriction, S^{LP}_{sp}, in the last period, *i.e.*, as forced by $\mathtt{I}^{RL}_{sp}$=4, is considered as

$$s^S_{spk} \geq S^{LP}_{sp} \quad \forall \{sp\} \quad , \quad k = N^K \tag{52}$$

The user selects different inventory constraints (here just verbally summarized) at the final period by the flag I^{RL}_{sp}

I^{RL}_{sp}	*description*
0	no condition at all
1	total inventory in final period equals total initial inventory
2	specific finished product stock equals the initial inventory
3	specific finished product stock equals pre-given target stock
4	specific finished product stock should be ≥ than target stock

4.4.2 Inventories at demand points At demand points there may exist a tank for an end-product p. If so, the stock balance equation reads

$$s^D_{dpt} = s^D_{dpt-1} + p^{ED}_{dpt} + \hat{S}^{DT}_{dpt} - \sum_{c=1}^{N^C} s^L_{dpct} - \sum_{d_d \in \mathcal{D}} T^{Mdd}_{dd_d} \sigma^{DD}_{dd_d} \tag{53}$$

$$+ \sum_{s \in \mathcal{S}} \sum_{\substack{k=1 | k+t_1(s,d) \leq K_s \\ t(k+t_1(s,d))=t}}^{K_s} \left(1 - \omega_{sdk}\right) T^{Msd}_{sd} \sigma^{SD}_{sdpk} \tag{54}$$

$$+ \sum_{s \in \mathcal{S}} \sum_{\substack{k=1 | k+t_2(s,d) \leq K_s \\ \wedge t(k+t_2(s,d))=t}}^{K_s} \omega_{sdk} T^{Msd}_{sd} \sigma^{SD}_{sdpk} \tag{55}$$

$$+ \sum_{d \in \mathcal{D} | t > t_1(d,d_d)} \left(1 - \omega_{dd_d t}\right) T^{Mdd}_{dd} \sigma^{DD}_{ddp,t-t_1(d,d_d)} \tag{56}$$

$$+ \sum_{d \in \mathcal{D} | t > t_2(d,d_d)} \omega_{dd_d t} T^{MDD}_{dd} \sigma^{DD}_{ddp,t-t_2(d,d_d)} \tag{57}$$

for all $\{sr | \exists S^{SC}_{dp}\}$and $t = 2, \ldots, N^T$, in which the terms have the following meaning: s^D_{dpt-1} is the stock level at the end of the previous period, p^{ED}_{dpt} denotes external purchase [see Section 4.6], $\hat{S}^{DT}_{dpt}$

$$\hat{S}^{DT}_{dpt} := \sum_{s=1 | \exists S^{PT}_{sdpt}}^{N^S} S^{DT}_{sdpt} \tag{58}$$

denotes transport arriving in period k from shipment originating before the first period, and the loss term, $\sum s^L_{dpct}$, due to the sales of finished products. The terms based on the σ-variables have been explained in Section 4.3 describing shipments to demand points as well as products received from other sites and demand points.

The functions

$$t_2(x,y) := t_1(x,y)+\pi \quad , \quad t_1(x,y) = (1-\pi)T^{xy}_{xy} \tag{59}$$

are used to select the appropriate indices in time; $\pi = 1$ indicates short term planning (in that case transportation times must correspond to the time discretization) and $\pi = 0$ indicates long term planning (in this case transport arriving is treated using a probability assumption). T^{SD}_{sd} denotes the minimum transport quantity and the time T^P_{sd} needed to ship products from site s to demand point d. Note that because T^P_{sd} is used in the index it is required that T^P_{sd} is measured in units of the period and that it is integral.

For the first period, $t = 1$, s^D_{dp0} is replaced by S^{DS}_{dp}, where S^{DS}_{dp} denotes the initial stock of product p at demand point d and

$$\hat{S}^{DT}_{dpt} := \sum_{s=1|\exists S^{PT}_{sdpt}}^{N^S} S^{DT}_{sdpt} \tag{60}$$

denotes transport arriving in period t from shipment not originating within the current planning horizon.

If no inventory is available and there exists a demand D_{dpct}, then the sales variables s^L_{dpct} are immediately coupled to the transportation variables and the terms s^D_{dpt} and s^D_{dpt-1} drop out in (57).

Stock must never exceed the storage capacity, *i.e.*,

$$s^D_{dpt} \le S^{CS}_{dp} + s^R_{dpt} \quad \forall\{dpt\} \tag{61}$$

where s^R_{dpt} gives the current additional tank capacity; sometimes it is possible to rent or lease a tank for a short while, *e.g.*, for a few months. The additional stock is usually bounded by

$$s^R_{dpt} \le S^{CR}_{dp} \quad \forall\{dpt \left| \exists S^{CR}_{dp}\right.\} \tag{62}$$

The safety stock bounds are

$$s^D_{dpt} \ge S^{DM}_{dp} \quad \forall \left\{spt \left| \exists S^{DM}_{dp}\right.\right\} \tag{63}$$

and the bounds for the last period are

$$s^D_{dpt} \ge S^{DE}_{dp} \quad \forall \left\{spt \left| \exists S^{DE}_{dp}\right.\right\} \tag{64}$$

Note that these bounds are only considered if the corresponding stock capacities or safety stocks exist.

4.5 Demand

There are 10 to 20 demand points for the products produced at the production sites located in various parts of the world. The demand points are thought of as regional warehouses. The demand at these points reflects mostly aggregate demand by several customers but also a few large individual customers. The demand for product p is characterized by volume and sales price. This input is generated from an independent sales forecasting model. Sales must not exceed the demand D_{dpct}, *i.e.*,

$$s^L_{dpct} \le D_{dpct} \quad \forall \{dpt \,|\exists D_{dpct}\} \tag{65}$$

where D_{dpct} indicates how much of product p at time t is required at demand point d.

In the “maximize contribution margin” scenario there is no need to satisfy demand completely. Therefore, this scenario provides the additional option that a lower limit, D^{LL}_{dpct}, on the demand is considered:

$$s^L_{dpct} \ge \min\left\{D^{LL}_{dpct}, D_{dpct}\right\} \quad \forall \left\{dpt \,\middle|\exists D^{LL}_{dpct} \wedge \exists D_{dpct}\right\} \tag{66}$$

In “satisfy demand” scenarios the demand has to be satisfied exactly, *i.e.*,

$$s^L_{dpct} = D_{dpct} \quad \forall \{dpct \,|\exists D_{dpct}\} \tag{67}$$

Due to lack of production capacity it may happen that not all of the demand can be covered by own production. Therefore, it is very important to provide the option to consider external purchase of products [see Section 4.6].

4.6 External purchase

External purchase of products helps to avoid running into situations of not being able to fulfil the demands. External purchase appears as source terms in the inventory balance equations for both site and demand points, and is characterized by the maximum quantity P^{ES}_{spk} $\left(P^{ED}_{dpt}\right)$ available for purchase and the costs/ton C^{ES}_{spk} $\left(C^{ED}_{dpt}\right)$. It is very important that these costs reflect the real business process, and that they are not considered as some artificial penalty costs. In addition to the upper bounds

$$p^{ES}_{spk} \le P^{ES}_{spk} \quad \forall \left\{spk \,|\exists\, P^{ES}_{spk}\right\} \tag{68}$$

$$p^{ED}_{dpt} \le P^{ED}_{dpt} \quad \forall \left\{dpt \,|\exists\, P^{ED}_{dpt}\right\} \tag{69}$$

there might be lower limit P^{ES-}_{spk} or p^{ED-}_{dpt}, resp. The external purchase variables might be interpreted as semi-continuous variables, *i.e.*,

$$p^{ES}_{spk} = 0 \;\vee\; p^{ES-}_{spk} \le p^{ES}_{spk} \le P^{ES}_{spk} \tag{70}$$

$$p^{ED}_{dpt} = 0 \;\vee\; p^{ED-}_{dpt} \le p^{ED}_{dpt} \le P^{ED}_{dpt} \tag{71}$$

if the supplier is willing to provide support but asks for a minimum quantity to deliver if support is requested.

5 The mathematical model: the design decisions

Since the network consists of several plants with different product streams it seems adequate to investigate whether it makes sense

- to open certain reactors at a site and to produce additional products,
- to shut-down certain reactors and thus not to produce some products at this site,
- or to buy whole sites.

One way to analyze such questions is to run different scenarios and to pick the best one. This simulation approach, however, might fail to identify the real good candidates and the optimal solution. The alternative approach is to model these questions or corresponding features appropriately and let the optimizer come up with optimal suggestions regarding the design of the production network.

5.1 A simple approach to include design decisions

A simple inclusion of the design features realized in the first phase of the project was to let the optimizer choose whether to open or shutdown a reactor once and for ever at the beginning of the planning horizon. That approach involves the following data: the total cost for buying a plant, C_s^B, the annual cost for buying a plant, C_s^{BA}, the fixed cost to operate a reactor, C_{sr}^{FIX}, the event value cost to open a reactor, C_{sr}^O, and the event value cost to shut down a reactor, C_{sr}^{SD}. The design costs to be included in a *net profit objective function* (contribution margin minus fixed costs minus design costs) has the form

$$-z^D := \sum_{s\in\mathcal{S}|\exists C_s^{BA}} C_s^{BA}\eta_s + \sum_{s\in\mathcal{S}} \sum_{r\in\mathcal{R}|\exists C_{sr}^{SDA}} \left(C_{sr}^{SDA} - C_{sr}^{FIX}\right)\varphi_{sr} + \sum_{s\in\mathcal{S}} \sum_{r\in\mathcal{R}|\exists C_{sr}^{SO}} \left(C_{sr}^{O} + C_{sr}^{FIX}\right)\mu_{sr} \tag{72}$$

where the binary variables η_s, φ_{sr} and μ_{sr} indicate whether a plant is bought, a reactor is shut down or opened.

An additional binary variable θ_{sr} is introduced if $I_{sr}^D = 1$;

$$I_{sr}^D = 1 \Leftrightarrow \left\{I_{sr}^{sR} = 1 \wedge \left(\exists C_s^{BA} \vee C_{sr}^{SD} \vee C_{sr}^{O}\right)\right\} \tag{73}$$

where I_{sr}^D indicates whether reactor r at site s is subject to design decisions; most cases we studied involved about 30 *design reactors*. θ_{sr} controls the available capacity of a reactor and is related to the other binary variables as follows:

$$\theta_{sr} = \eta_s \quad \forall \left\{sr\,|\exists\, I_{sr}^{sR} = 1 \wedge \exists C_s^{BA}\right\} \tag{74}$$

$$\theta_{sr} = 1-\varphi_{sr} \quad \forall \left\{sr\,|\exists\, I_{sr}^{sR} = 1 \wedge \exists C_{sr}^{SD}\right\} \tag{75}$$

$$\theta_{sr} = \mu_{sr} \quad \forall \left\{ sr \,|\exists\, I_{sr}^{sR} = 1 \wedge \exists C_{sr}^{O} \right\} \tag{76}$$

The relations (74) to (76) give us a hint on possible priorities (η_s,φ_{sr},μ_{sr},θ_{sr}) for the variables in the branching process. It is assumed that C_{sr}^{SD} and C_{sr}^{O} do not exist simultaneously.

The disadvantage of that approach, in a 10- or 15-year planning horizon, is that a reactor has to be opened or shut down in the first period of the planning horizon and stays in that status for the rest of the planning horizon. A more detailed view described in the next section allows for time dependent and temporary shutdowns and openings.

5.2 Time dependent and temporary shutdowns

In the course of the project it became obvious that more details regarding time resolution are necessary. Therefore, reactors, for which opening or shutdown cost are specified, will be treated as reactors subject to time dependent opening or shutdown decisions. These reactors are modeled similar as the reactors subject to mode changes. For each design reactor we assign two modes ($m = 1$ and 2 corresponding to *on* and *off*), and use the variables α_{sr1k} , β_{sr1k}, γ_{sr1k}, and δ_{sr1k} explained in ([11, Section 10.4]). Note that this model approach implies that the design reactors can not be subject to intrinsic mode changes which was not a problem in the current application. However, it is now possible that both C_{srk}^{SD} and C_{srk}^{O} may be different from zero. A further detail to be considered is that the opening decisions need some time to be put into reality. Therefore, a delay time K_{sr}^{FO} might specify which production time slice is the first one in which the reactor could be opened. This conditions, for $k = 1, \ldots, \max(1, K_{sr}^{FO} - 1)$, is realized by the bounds

$$\alpha_{sr1k} = \beta_{sr1k} = \delta_{sr1k} = 0 \quad \forall (sr) \in \mathcal{R}^{D} := \left\{ (sr) \left| I_{sr}^{MC} \neq 1 \wedge \exists I_{sr}^{IBR} \right. \right\} \tag{77}$$

for all design reactors which are not yet opened.

Although, the economical parameters may already prevent that reactors are opened and shut down wildly and very frequently it might be necessary for managerial reasons to introduce two parameters, K^O and K^C, which specify that if a reactor is opened in production time slice k, it has to be open for the next K^O time slices, and vice versa, if a reactor is shutdown in period k it has to stay closed for the next K^C time slices. These conditions tighten the model constraints by putting the variables α_{sr1k}, β_{sr1k}, γ_{sr1k} and δ_{sr1k} to zero for certain time slices in which a plant cannot operate and are enforced by

$$\sum_{\kappa=k+1}^{k+K^O} \gamma_{sr1k} \leq K^O - K^O \beta_{sr1k} \quad \forall (sr) \in \mathcal{R}^{D}, \quad \forall k \in \mathcal{K}_s^{O} \tag{78}$$

$$\sum_{\kappa=k+1}^{k+K^C} \alpha_{sr1k} \leq K^C - K^C \gamma_{sr1k} \quad \forall (sr) \in \mathcal{R}^{D}, \quad \forall k \in \mathcal{K}_s^{C} \tag{79}$$

$$\sum_{\kappa=k+1}^{k+K^C} \beta_{sr1k} \le K^C - K^C \gamma_{sr1k} \quad \forall (sr) \in \mathcal{R}^D, \quad \forall k \in \mathcal{K}_s^C \tag{80}$$

$$\sum_{\kappa=k+1}^{k+K^C} \delta_{sr1k} \le K^C - K^C \gamma_{sr1k} \quad \forall (sr) \in \mathcal{R}^D, \quad \forall k \in \mathcal{K}_s^C \tag{81}$$

$$\sum_{\kappa=k+1}^{k+K^O} \delta_{sr1k} \ge (K^O - 1)\beta_{sr1k} \quad \forall (sr) \in \mathcal{R}^D, \quad \forall k \in \mathcal{K}_s^O \tag{82}$$

$$\sum_{\kappa=k+1}^{k+K^C} \gamma_{sr1k} \le K^C - K^C \gamma_{sr1k} \quad \forall (sr) \in \mathcal{R}^D, \quad \forall k \in \mathcal{K}_s^C \tag{83}$$

$$\sum_{\kappa=k+1}^{k+K^C} \beta_{sr1k} \le K^O - K^O \beta_{sr1k} \quad \forall (sr) \in \mathcal{R}^D, \quad \forall k \in \mathcal{K}_s^O \tag{84}$$

with $\mathcal{K}_s^C := \{1, \ldots, \max(1, N^K(s) - K^C)\}$ and $\mathcal{K}_s^O := \{1, \ldots, \max(1, N^K(s) - K^O)\}$. Finally, when a reactor is open, *i.e.*, $\alpha_{sr1k} = 1$, it is ensured that a certain minimum quantity is really produced, *i.e.*,

$$p_{srpk}^P \ge P_{srpk}^{MIN} \alpha_{sr1k} \quad \forall \left\{ srpk \left| I_{sr}^{MC} \ne 1 \land \exists I_{sr}^{IBR} \land \exists I_{srp}^{SRP} \right. \right\} \tag{85}$$

Note that (85) cannot be applied to reactors which are design reactors and are already open at the beginning of the planning horizon. The reason is that for such reactors we necessarily have $\alpha_{sr1k} = 1$. However, if such a reactor is subject to a shutdown decision it may be not even able to produce and thus cannot meet the minimum production requirement (85).

The basic cost terms are the costs for shutdown and opening adjusted for discounted cash flows and depreciation (see below), *i.e.*, terms such as

$$c^{D_1} := \sum_{(sr) \in \mathcal{R}^D} \sum_{k=1}^{N_s^K} C_{srk}^{SD} \gamma_{sr1k} \quad , \quad c^{D_2} := \sum_{(sr) \in \mathcal{R}^D} \sum_{k=1}^{N_s^K} C_{srk}^{O} \beta_{sr1k} \tag{86}$$

The improved design model also considers the residual book value V_{srk} [see Equation (90)] of an opened reactor, *i.e.*, a reactor which caused opening cost) at the end of the planning horizon. This adds the term

$$z^{D_2} := - \sum_{\{sr\} \in \mathcal{R}^D} \sum_{k=1}^{N_s^K} V_{srk} \beta_{sr1k} + \sum_{\{sr\} \in \mathcal{R}^D} \sum_{k=1}^{N_s^K} V_{srk} \gamma_{sr1k} \tag{87}$$

to the objective function. V_{srk} is based on the *net present value* and on the depreciation. At present we apply a linear depreciation rate. The discounted opening cost in production time slice k are D_t^P / U_{st}

$$C_{srk}^O = C_{sr}^O / D^{k-1} \quad , \quad D := 1 + \frac{p}{100 U_{st}} \tag{88}$$

where p is the discount rate in percent. The calculation of the depreciation depends on the opening time and thus we obtain the depreciation factor

$$F_s^D := 1 - \frac{N_s^K - k}{U_{st} T^D} \tag{89}$$

where T^D denotes the depreciation time in years; a typical value is $T^D = 15$ years. Formula (89) for the computation of the depreciation factor assumes that the depreciation time is measured in units of the commercial time scale; typically the discretization of the commercial time periods is one year and so the depreciation time is also given in years. Based on these assumptions, if the opening occurs in period k the residual book value is

$$V_{srk} = C_{sr}^O / D^{k-1} \left(1 - \frac{N_s^K - k}{U_{st} T^D}\right) \tag{90}$$

If we assume that a reactor which causes opening cost is not shut down, *i.e.*, it is opened at most once, the term added to the objective function is

$$\sum_{\{sr\} \in \mathcal{R}^D} \sum_{k=1}^{N_s^K} V_{srk} \alpha_{sr1N_s^K} \beta_{sr1k} = \sum_{\{sr\} \in \mathcal{R}^D} \sum_{k=1}^{N_s^K} V_{srk} \beta_{sr1k} \tag{91}$$

Therefore, the total contribution of β_{sr1k} to the design term in the objective function representing the opening cost and the residual book value is

$$z^{D_2} := \sum_{\{sr\} \in \mathcal{R}^D} \sum_{k=1}^{N_s^K} \left(V_{srk} - C_{srk}^O\right) \beta_{sr1k} \tag{92}$$

An additional cost term is included to describe reactors that are subject to a shutdown decision in the first period but require continuation cost C_{sr}^{CNT}, *e.g.*, for maintaining or upgrading existing facilities, if the reactor is not shut down in the first period. This feature is considered by the binary variable

$$\sigma_{sr} \quad \forall \left\{ sr \,\middle|\, (sr) \in \mathcal{R}^D \wedge \exists C_{sr}^{CNT} \right\} \tag{93}$$

the constraint

$$\sigma_{sr} \geq 1 - \gamma_{sr11} \quad \forall \left\{ sr \,\middle|\, (sr) \in \mathcal{R}^D \wedge \exists C_{sr}^{CNT} \right\} \tag{94}$$

and the costs term

$$c^{D_3} := \sum_{(sr) \in \mathcal{R}^D | \exists C_{sr}^{CNT}} C_{sr}^{CNT} \sigma_{sr} \tag{95}$$

in the *net profit* objective function.

The total contribution of the design reactors to the objective function is

$$z^D := -c^{D_1} + z^{D_2} - c^{D_3} \tag{96}$$

6 The mathematical model: the objective functions

The model covers eight different objective functions invoked by `OBJTYPE`=n, where n is a number between 1 and 8:

1. "max. contribution margin" ([11, Section 10.4])
2. "max. contribution margin while guaranteeing minimum demand"
3. "min. cost while satisfying full demand" ([13])
4. "max. total sales neglecting cost" ([13])
5. "max. net profit" (the detailed and full design problem)
6. "multi-criteria objectives" (maximize profit & minimize transport)
7. "max. total production"
8. "max. total production of products for which demand exists"

Only the fifth one exploits all design features; all other assume a fixed design. The first one maximizes the contribution margin, $y - c$, and includes the yield, y, calculated on the basis of production and the associated sales prices and the sum of all variable cost c. The second one minimizes the variable cost, c, while satisfying demand. In the cases 1 to 6 the following variable cost are involved: variable production cost, change-over cost, transport between sites, between sites and demand points, and between demand points, inventory cost for products, and cost for external purchase of products; in case 5 these cost terms are discounted according to Section 5.2 which leads to the *net profit* objective function

$$\max z \quad , \quad z := y - c + z^D \tag{97}$$

The objective functions 7 and 8 are used in an initial phase to test the data and to derive the theoretical capacity of the production network. The total net profit objective function contain the design cost terms which have quite different scaling characteristics compared to the standard production planning terms. Using variable directives in the B&B scheme, *i.e.*, prioritizing the design decisions, it was possible to cope with this problem. The multi-criteria objectives scenario is solved by a goal programming approach as described in [9].

7 Computational issues, implementation and results

The model has been coded and the MILP problem has been solved using Dash's modeling language and MILP-solver `XPRESS-MP` 10.60 ([2], [3] and [4]). During some first numerical experiments it was observed that the objective function in the scenarios 4, 7 and 8 was dually degenerated. Thus, a significant speed-up was achieved using the primal Simplex algorithm to solve these scenarios. Some DOS-based procedures have been programmed to automate the process of accessing the data from an `EXCEL` spreadsheet, generating the matrix, solving the problem and returning the results into the `EXCEL` spreadsheet. Especially, some batch files developed enabled us to pass appropriate command streams to the solver depending on the objective function scenario.

7.1 Model assumptions and validation

The first step of model validation was to review and summarize the assumptions and limitations of our mathematical model. They are already given in Section 3.3 but in this practical case, only the implementation of the model showed that they have been reasonable and acceptable. The model was carefully validated by the client, *i.e.*, by an experienced production planner and a financial expert running the model and the software under different circumstances. Especially, the opening and shut-down of reactors were carefully traced and subject to plausibility checks by the financial planners, for instance, taking into account the contribution margin related to a newly opened reactor compared to its investment cost. It was interesting to inspect solutions in which a reactor which was no longer profitable was shut-down immediately, after a reactor based on a new technology was opened. Transport between sites and demand points was an issue which sometimes lead to solutions non-intuitive to the people responsible for the production planning in single plants, and usually needed clarification.

7.2 Computational issues

To give an example of the problem size and some solution characteristics we quote a typical scenario (S_5) with about 30 design reactors covering 10 years with 10 commercial and 20 production time slices, for which we derived production and design plans maximizing total net profit. Using Dash's MILP-solver `XPRESS-MP` 10.60 ([2], [3] and [4]) for a problem with $n_c = 26941$ continuous, $n_c = 5100$ binary and $n_{sc} = 1100$ semi-continuous variables and $c = 28547$ constraints, we got the following results (including the integer solution number IP, number of nodes n_n, run time τ on a 266 MHz Pentium II PC in minutes, best upper bound z^U, best lower bound z^L and integrality gap $\Delta := 100\frac{z^U - z^L}{z^L}$):

	IP	n_n	τ	z^U	z^L	Δ
S_5	1	218	4	140.8	137.5	2.4
S_5	2	1794	34	138.4	138.4	–

The first feasible integer solution is usually found within 10 minutes after exploring about 300 nodes in the B&B tree. Usually, for pure operational planning, this solution is accepted and the tree search is terminated. This heuristic is justified if Δ is of the order of a few percent (well within the error associated with the input data) because it eliminates the need for the time consuming complete search for the absolute optimal solution via the B&B algorithm. In the SSDOP approach this is only valid, if Δ is less or equal, say, 1%.

It is remarkable that this model even when all design features are exploited is able to find the first feasible integer solution, usually after 200 or

300 nodes, within a few minutes (integrality gap between 1 and 3 percent) and is able to prove optimality in most cases within 30 minutes (3000 nodes typically). If all design features are fixed, the problem is solved to optimality within a few minutes (1000 to 2000 nodes).

In order to carry out sensitivity analyses of the solution with respect to the input data, especially to the demand data and costs or sales prices, it is important that we are able to conduct the complete search via the B&B algorithm or to get an integrality gap Δ less than one percent. The sensitivity analysis was carried out by the client by varying the input data by up to 20 percent and inspecting the objective function value and the design decisions.

7.3 Commercial results, benefits and experience

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.

The results obtained with the use of the design feature allowed the business team to clearly demonstrate the value of its investment plan to senior management. The comprehensive results obtained from the model allowed the team to focus its recommendation on facts and quickly address questions concerning product flows, production sourcing, capacity constraints, and working capital needs in addition to investment capital requirements. 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.

It was vital to the project that on the client's side people responsible for the operational planning and colleagues from the financial planning department cooperated with each other. It was very interesting during the modeling phase to see how know-how from quite separate areas merged and lead to a complex model providing just the right degree of detail to satisfy all parties involved.

8 Conclusions

We have developed and applied a model that combines operational planning with strategic aspects having consequences for years. The decisions determine the infrastructure and aggregate production plans for a horizon up to 15 years. It is important that realistic and detailed demand forecast, and, possibly, cost and sales prices are available, and also that a sensitivity analysis is performed showing how stable the optimal solution is with respect to changes in these input data. Especially, for problems with such a long planning horizon and great financial impact it is vital that the optimality of a solution can be proven, or that at least some safe bounds can be specified.

As far as good modeling practice is concerned, we learned from the discussion and communication with the client during the model building phase that great attention has to be paid to achieving a good balance of details entering the model. Some focus had also to be given to the structure of the objective function which might contain terms of very different size, and thus may lead to bad scaling. A useful extension of the model might be to include tax and depreciation related features considering special rules for specific countries and their tax rates.

Provided that optimality is proven or safe bounds are derived, combining strategic or design aspects with operational planning is an elegant approach taken by some chemical companies; it can save huge quantities of money and also supports an analysis related to the stability of solutions.

Last but not least we want to stress one crucial fact learned from two projects (one described in this paper, for the other one see [9, Section 9.2]): the simultaneous strategic/design & operational planning approach requires that the departments being responsible for the strategic or design decisions and the planning/scheduling cooperate; our experience is that this problem is by far more difficult to solve than the mathematical or technical ones, especially in large companies and their cultural and organizational structures. But especially, in large organizations, for instance, if new sites are established in otherwise nonindustrial areas (*e.g.*, the construction of new plants in South East Asia) or new structures have to be embedded into existing sites, appropriate models combining operational planning with strategic or design planning almost certainly lead to great financial savings, and therefore, the simultaneous approach should be attractive to many other, especially large companies.

References

1. J. Ahmadi, R. Benson, and D. Supernaw-Issen. Mixed-Integer Nonlinear Programming Applications. In T. A. Ciriani, S. Gliozzi, E. L. Johnson, and R. Tadei, editors, *Operational Research in Industry*, pages 199–231. Macmillan, Houndmills, Basingstoke, UK, 1999.
2. R. W. Ashford and R. C. Daniel. LP-MODEL XPRESS-LP's model builder. *Institute of Mathematics and its Application Journal of Mathematics in Management*, 1:163–176, 1987.
3. R. W. Ashford and R. C. Daniel. Practical aspects of mathematical programming. In A. G. Munford and T. C. Bailey, editors, *Operational Research Tutorial Papers*, pages 105–122. Operational Research Society, Birmingham, 1991.
4. R. W. Ashford and R. C. Daniel. *XPRESS-MP Reference Manual*. Dash Associates, Blisworth House, Northants NN73BX, http://www.dash.co.uk, 1995.
5. W. Domschke, A. Scholl, and S. Voß. *Produktionsplanung*. Springer, Heidelberg, 2nd edition, 1997.

6. A. Drexl and K. Haase. Proportional lotsizing and scheduling. *Int J of Prod Econ*, 40:73–87, 1995.
7. J. Kallrath. Diskrete Optimierung in der chemischen Industrie. In A. Bachem, M. Jünger, and R. Schrader, editors, *Mathematik in der Praxis - Fallstudien aus Industrie, Wirtschaft, Naturwissenschaften und Medizin*, pages 173–195. Springer Verlag, Berlin, 1995.
8. J. Kallrath. Mixed-Integer Nonlinear Programming Applications. In T. A. Ciriani, S. Gliozzi, E. L. Johnson, and R. Tadei, editors, *Operational Research in Industry*, pages 42–76. Macmillan, Houndmills, Basingstoke, UK, 1999.
9. J. Kallrath. *Gemischt-Ganzzahlige Optimierung: Modellierung und Anwendungen*. Vieweg, Wiesbaden, Germany, 2002.
10. J. Kallrath. Planning and scheduling in the process industry. *OR Spectrum*, in print, 2002.
11. J. Kallrath and J. M. Wilson. *Business Optimisation Using Mathematical Programming*. Macmillan, Houndmills, Basingstoke, UK, 1997.
12. R. Kuik, M. Solomon, and L. N. van Wassenhove. Batching Decisions: Structure and Models. *European Journal of Operational Research*, 75:243–263, 1994.
13. C. Timpe and J. Kallrath. Optimal Planning in Large Multi-Site Production Networks. *European Journal of Operational Research*, 126(2):422–435, 2000.