Optimization Concepts: II—A More Advanced Level

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Abstract Optimization subjects are addressed from both an introductory and an advanced standpoint. Theoretical subjects and practical issues are focused, conjugating Optimization basics with the implementation of useful tools and supply chain (SC) models. In the prior *Introductory* chapter on Optimization concepts, Linear Programming, Integer Programming, related models, and other basic notions were treated. Here, the *More Advanced* chapter is directed to Robust Optimization, complex scheduling and planning applications, thus the reading of the prior *Introductory* chapter is recommended. Through a generalization approach, scheduling and planning models are enlarged from deterministic to stochastic frameworks and robustness is promoted: model robustness, by reducing the statistical measures of solutions variability; and solutions robustness, by reducing the capacity slackness, the non-used capacity of chemical processes that would imply larger investment costs.

Keywords Robust Optimization · Batch scheduling · Process planning · Models generalization

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1 Introduction

Generalization approaches occur widely in Mathematics fields, namely, the enlargement of number sets, from the set of natural until the set of complex numbers, considering the set of integer, fractional, and real numbers. These successive enlargements occur also in the power operations, when the powers of natural, integer, fractional, real, and complex numbers are addressed. Or in certain functions, such as the Permutation function can be considered just a special case of Factorial function, the “complete factorial”, and the Factorial function just a restriction to non-negative integers of the Gamma function.

But generalizations occur also in Mathematical Programming (MP), since Linear Algebra solutions are considered in the Linear Programming (LP) feasible solutions space, the methods for Integer LP are using constrained-LP, deterministic LP are enlarged to Stochastic LP (SLP) and then to Robust Optimization (RO) models (Miranda and Nagy 2011). In fact, the analysis of the evolution of MP models, with quantitative and qualitative improvements, show successively extended models. Quantitative improvements are achieved when the objective function and/or space of admissible solutions are successively enlarged, and vice versa.

The study of several industry-based SC cases addressing petroleum refineries, fertilizers, pharmaceutics, chemical specialties, and paper production was developed in a first phase (Miranda 2007). The focus was on Mixed Integer Linear Programming (MILP) models that aim at chemical processes planning (PP), that is, long range investment planning.

Notice that in the chemical industry:

- Dedicated chemical processes, on one hand, use fixed proportions of products in all the time periods; for instance, in the Kellogg’s process for ammonia synthesis and in the electrochemical production of caustic soda;
- On the other hand, the flexible chemical processes that occur in petroleum refineries use different products along the various time periods.
- Process flexibility may occur in raw materials, namely, some refinery processes are suitable for several types of crude oil; and process flexibility may also occur in products; for instance, when producing several types of paper, considering different surface properties, various densities and colors.

The successive enlargement of models associated with the generalization approach was observed, with PP models treating dedicated processes, then flexible processes, and flexible processes through “production schemes”. Furthermore, robust planning with dedicated processes, and SC production planning with flexible processes were also treated, but not simultaneously in the same PP model.

Another focus on the industry cases was on MILP models aiming at the design and scheduling of chemical batch processes (here on this text: *Batch*, a *flowshop*-type problem), considering the production of tires, biotechnology, food industry, chemical specialties, pharmaceutics. The *flowshop* problem is a very well-known type of problem and addresses N tasks to be sequentially performed in M stages, assuming (Garey et al. 1976): (i) one machine is available in each stage; (ii) one task is performed in one machine at each allocation, without preemption; and (iii) one machine performs only one task at each time. Beyond the wide number of applications in manufacturing, and due to the high cost of equipment in chemical batch processes, either the maximization of equipment utilization or the make-span minimization are usually considered.

Like in the former PP cases, the evolution of *Batch* models is observed in two senses: (i) successively, more realistic formulations, integrating additional degrees of freedom and uncertainty treatment, which are making resolution more difficult; and (ii) usually, resolution procedures are considered at the very beginning of the modeling phase, and some issues of networks resolution, heuristics, and approximation schemes, were introduced. Due to its inherent difficulty, the *Batch* model at hand was treated only in a deterministic framework, and further developments except this generalization approach are not at our knowledge.

In order to obtain quantitative and qualitative improvements, then, a PP model and a *Batch* model are selected and generalized, aiming at the treatment of uncertainty and promotion of robustness. Simultaneously, these models also address the chemical processes designing and sizing, the material fluxes within such processes, and finally materials to purchase and products to sell.

2 Robust Model for Flexible Processes Planning

As an overview of the PP problem and considering the evolution of PP models during about a decade, a capacity expansion sub-problem was considered and, simultaneously, uncertainty is treated (Sahinidis et al. 1989), flexibility attributes are included (Norton and Grossmann 1994), and robustness is promoted (Bok et al. 1998).

The *Capacity Expansion* problem, in general, addresses the expansion of production capacities when products demand are expected to rise significantly. It considers economies of scale by modeling fixed and variable costs and, in particular, obsolescence (e.g., electronics manufacturing) or deterioration with increasing of operation and maintenance costs may be introduced. The improvements on operations (e.g., *learning curve*), introduction of multiple types of technology (e.g., energy production), the discrete enumeration of alternatives, and the long term uncertainty are being addressed through stochastic frameworks.

The Two-stage Stochastic Programming (2SSP) is widely used to address uncertainty. For instance, considering the *capacity expansion* problem: at the first stage, the capital and investment decisions must be taken, “here-and-now”; then, the project variables are obtained (project stage); in the second stage (recourse stage), the uncertainty is introduced through the set of foreseen scenarios and respective probability; this way, the control variables are calculated within a probabilistic character.

However, under uncertainty it is pertinent to promote robustness, either the *robustness on solution*—the solution remain “almost optimal” even when all scenarios are considered—and the *robustness in the model*—the optimal solution do not present high values to the excess/unused capacity or the unsatisfied demand. Usually a SLP objective function is modified in RO models by introducing penalization parameters on deviation, non-satisfied demand, capacity excess, or probabilistic restrictions are modified by enlarging/narrowing "soft" bounds.

Furthermore, using a theoretical approach and developing computational complexity studies of the PP problem, it is shown that most of the PP problems are NP-hard (Miranda 2007). Then, the necessity to develop heuristics may arise in case large instances are presenting. Nevertheless, it is suitable to solve instances of reasonable dimension using detailed knowledge about the models, by balancing their benefits and limitations. In the medium and large horizons, it is also pertinent to promote robustness in face of uncertainty. A generalization was then developed to properly address the "capacity production", to economically evaluate it, by considering flexible production schemes, and targeting robustness in 2SSP context. Logistics and financial subjects were not addressed in this generalization approach (e.g., inventory, distribution network, finance risk).

The purposes of the generalized model for processes planning thus are:

- To treat uncertainty and to promote robustness;
- To consider flexible processes, by integrating the production schemes formulation;
- To define the time implementation and the size of processes;
- To model economies of scale;
- To estimate the fluxes in the chemical processes, the raw materials' purchases, and the products sales.

The related nomenclature follows:

Index and sets

NC Number of components/materials j;
NM Number of markets l for purchase/sale materials;
NP Number of processes i;
NR Number of scenarios r;
NS Number of production schemes s;
NT Number of time periods t.

Parameters

$prob_r$ Probability associated with each scenario r;
λdsv, λzp Penalization parameters, respectively, for the solutions variability and the capacity slackness;
γ_{jlt}, Γ_{jlt} Unit prices for sale and purchase of the j materials, in market l, period t;
δ_{ist} Unit costs for the production processes i, at scheme s, period t;
α_{it}, β_{it} Variable and fixed costs for the capacity expansion of processes i, in each period t;
a_{jlt}, d_{jlt} Availabilities and demands of components and materials j, in market l, period t;

μ_{ijs}	Characteristic constants that associate the inflows and outflows of the various components within each process i;
ρ_{is}	Relative production rates at each process i, scheme s;
H_{it}	Upper value for the availability of production time, for process i during period t;
$PS(i)$	Set of production schemes s allowed for flexible process i;
$QE_{it\tau}^{acum}$	Upper bound for the capacities to expand, concerning the aggregated "demand of capacities" from period t until period τ.

Variables

ξ_r	Net Present Value (NPV) in scenario r;
$dsvn_r$	Negative deviation on the value of NPV in scenario r;
Sal_{jltr}	Products sales, for material j, in market l, period t and scenario r;
Pur_{jltr}	Materials purchases, for material j, in market l, period t and scenario r;
QE_{it}	Capacity expansion of process i in period t;
Q_{it}	Capacity of process i in period t;
y_{it}	Binary decision related to the expansion of process, in period t;
Zp_{itr}	Deviation by capacity slackness of process i, in period t at scenario r;
θ_{istr}	Amount of principal component j' being processed at scheme s of process i, at period t and for each scenario r.

Then the model ***ROplan_flex*** (adapted from Miranda and Casquilho (2008) along with some examples) in the relations set (RO.1-a–RO.1-l) considers and simultaneously conjugates the significant points of prior PP models;

- A robust objective function (RO.1-a); and
- The flexibility schemes within the processes planning frame are addressed on restrictions set (RO.1-b–RO.1-l).

These relations are synoptically described:

(a) Objective Function, aiming to maximize the expected Net Present Value (NPV), considering penalizations on variability around the expected value, and penalizations on capacity slacks (non-statistical measure);
(b) Definition of NPV;
(c) Definition of the solution variability through the negative linear deviation;
(d) Definition of capacity slacks;
(e) Upper bound to the investment budget;
(f) Logic bounds onto the expansion of processes;
(g) Balance to the process capacity 's "production";
(h) Mass balance onto the components;
(i) Upper bounds to the materials purchases;
(j) Upper bounds to components sales;
(k) Non-negativity restrictions;
(l) Binary variables definition.

Model *ROplan_Flex:*

$$[\max]\Phi = \sum_{r=1}^{NR} prob_r \xi_r - \lambda dsv \sum_{r=1}^{NR} prob_r . dsvn_r - \lambda zp \sum_{i=1}^{NP} \sum_{t=1}^{NT} \sum_{r=1}^{NR} Zp_{itr} \quad \text{(RO.1-a)}$$

subject to

$$\begin{aligned} \xi_r = & \sum_{j=1}^{NC} \sum_{l=1}^{NM} \sum_{t=1}^{NT} \left(\gamma_{jlt} Sal_{jltr} - \Gamma_{jlt} Pur_{jltr} \right) \\ & - \sum_{i=1}^{NP} \sum_{s \in PS(i)}^{NS} \sum_{t=1}^{NT} (\delta_{ist} \rho_{is} \theta_{istr}) - \sum_{i=1}^{NP} \sum_{t=1}^{NT} (\alpha_{it} QE_{it} + \beta_{it} y_{it}), \quad \forall r \end{aligned} \quad \text{(RO.1-b)}$$

$$dsvn_r \geq \sum_{r'=1}^{NR} (prob_{r'} \xi_{r'}) - \xi_r, \quad \forall r \quad \text{(RO.1-c)}$$

$$\sum_{s \in PS(i)}^{NS} \theta_{istr} + Zp_{itr} = H_{it} Q_{it}, \quad \forall i, t, r \quad \text{(RO.1-d)}$$

$$\sum_{i=1}^{NP} (\alpha_{it} \, QE_{it} + \beta_{it} \, y_{it}) \leq CI(t), \quad \forall t \quad \text{(RO.1-e)}$$

$$QE_{it} \leq QE_{it}^{Upp} y_{it}, \quad \forall i, t \quad \text{(RO.1-f)}$$

$$Q_{it-1} + QE_{it} = Q_{it}, \quad \forall \, i, t \quad \text{(RO.1-g)}$$

$$\sum_{l=1}^{NM} Pur_{jltr} + \sum_{i=1}^{NP} \sum_{s \in PS(i)}^{NS} \mu_{ijs} \rho_{is} \theta_{istr} = \sum_{l=1}^{NM} Sal_{jltr}, \quad \forall j, t, r \quad \text{(RO.1-h)}$$

$$Pur_{jltr} \leq a_{jltr}^{Upp}, \quad \forall j, l, t, r \quad \text{(RO.1-i)}$$

$$Sal_{jltr} \leq d_{jltr}^{Upp}, \quad \forall j, l, t, r \quad \text{(RO.1-j)}$$

$$\xi_r, \, dsvn_r, \, Sal_{jltr}, \, Pur_{jltr}, \, \theta_{istr}, \, Zp_{itr}, \, QE_{it}, \, Q_{it} \geq 0, \quad \forall i, j, l, s, t, r \quad \text{(RO.1-k)}$$

$$y_{it} \in \{0, 1\}, \quad \forall i, t \quad \text{(RO.1-l)}$$

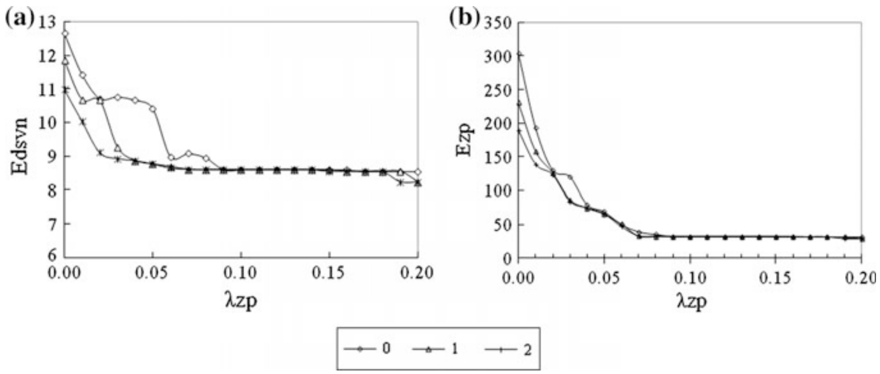

Fig. 1 Sensitivity of the objective function in face of the penalization parameters, showing solution robustness (**a**) and robustness in model (**b**)

Various examples were developed, and the sensitivity of the objective function considering the penalization parameters evolution is studied in the very first one. The graphs ***a*** and ***b*** in Fig. 1 consider:

(a) The variation of the expected value of the partial negative deviation, *Edsvn*, within the penalization parameters *λzp* and *λdsvn*, showing the solution robustness; for all the analyzed values of *λdsvn* on the 0–2 range (only three lines are presented for easier observation), the expected value measuring the solution variability, *Edsvn*, reduces rapidly with the *λzp* evolution and a flat level is reached;

(b) The variation of the expected value of capacity slacks, *Ezp*, within the penalization parameters *λzp* and *λdsvn* showing robustness on model; analyzing again the 0–2 range for *λdsvn*, the expected value measuring the capacity slackness, *Ezp*, also reduces rapidly with the *λzp* evolution onto a flat level.

In the second example, the issue of a reagent limitation is incorporated in the expansion of the existing dedicated process. Improvements of about 0.3 and 15 % due to the new two flexible processes are obtained, the superstructure and the average flows of the selected processes are presented in Fig. 2. Flexible processes are able to produce different components under different production schemes and different reagents, while only one configuration production-parameters-reagent is allowed on dedicated processes.

The superstructure represents a processes network with five continuous processes: the existing dedicated chemical process P3, produces high value component C7 using components C3 and C4, but component C3 has high price and short availability. The production of C3 is to be evaluated, and for that components C1 and C2 are to be purchased and transformed by chemical processes P1 and P2; these two processes are to be implemented if economically suitable. The flexible process P1 allows two production schemes, the first scheme presents similar parameters as

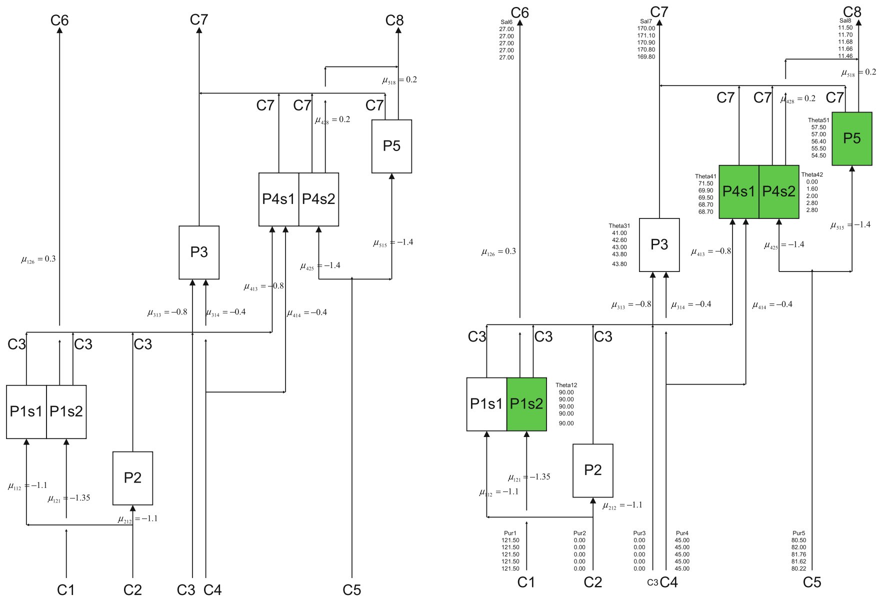

Fig. 2 Superstructure (*left*) and selection of flexible processes (*right*) for the numerical example on reagent limitation

dedicated process P2, but the second production scheme of P1 also allows the production of component C6. Component C6 presents high market value, so as components C7 and C8. In plus, the expansion of process P3 shall be evaluated too, and compared with the implementation of a flexible process P4 and/or the dedicated process P5: the parameters of the two production schemes on P4 are similar to the parameters of both dedicated processes P3 and P5. The uncertainty on components prices and demands along the time horizon is described by a discrete number of scenarios, and scenario probabilities are assigned.

A comparative study of the different production pathways can thus be developed, and the parameters that make economically preferable processes can be estimated. From the above, an alternative pathway for the production of component C7 is shown of interest, also including C8 production and using the replacement reagent C5. The self-production of limiting reagent C3 proved economically favorable too, preferably by the scheme that also produces C6 over the pathway which produces only C3. The selected processes are colored in the figure.

2.1 *Concluding Remarks on the Robust Process Planning*

The generalized process planning model, ***ROplan_flex***, integrated the risk policy of the decision maker. The model also integrates processes flexibility, the formulation of production schemes, and robustness without losing linearity. In addition, the expected values on deviation estimators, solution variability and capacity slacks fit the evolution the penalization parameters: consequently, the ***ROplan_flex*** model and the solutions are robust.

3 Robust Model for Design and Scheduling of Batch Processes

This section addresses the design of batch chemical processes and simultaneously considers the scheduling of operations. A model generalization is proposed, from a deterministic MILP model (Voudouris and Grossman 1992) to a stochastic 2SSP approach, this generalization being based on computational complexity studies (Miranda 2011a). The generalized model for design and scheduling of batch chemical process treats different time ranges, namely, the investment and scheduling horizons. Furthermore, the 2SSP framework allows the promotion of robustness solution, by penalizing the deviations; and the robustness in the model, with relaxation of the integrality constraints in the second phase variables.

In comparison with the evolution of PP models, a different way of evolution is observed for the design and scheduling problem (Miranda 2007). A realistic formulation was focused, with successive incorporation of freedom degrees, namely, extending the number of processes in each stage, the production and storage policies, and considering the economic charges on setups, operations, and inventories. Since the model becomes more and more difficult to solve, the solution procedures were adjusted in the early phases of modeling, and even network subjects were introduced to improve short term scheduling. Nevertheless, a minor impact of this case is noted, both in literature and industry applications.

In order to better select the equipment to purchase, the optimal production policy must also be found since it directly affects the equipment sizing. However, it involves the detailed resolution of scheduling subproblems where decomposition schemes are pertinent. These subproblems are focused in the second phase of 2SSP, where the control variables (recourse) occur. The integer and binary variables related to the scheduling and precedence constraints are disregarded as control variables, as they would make very hard the treatment of the recourse problem. Consequently, the second phase variables are assumed continuous (for example, the number of batches) and binary variables occur only in the first phase.

The study of existing models in the literature induces the enlargement of models and related applications (Miranda 2007), and this generalization of models simultaneously increases complexity and solution difficulties. A design and scheduling MILP model (Voudouris and Grossman 1992) that seems to have no improvements for more than a decade is addressed. Analytical results and computational complexity techniques were applied to the referred deterministic and single time MILP model, which is featuring multiple machines per stage, *zero wait* (ZW) and *single product campaign* (SPC) policy. That model was selected (Miranda 2007) because:

- For industrial applications with realistic product demands, multiple processes in parallel at each stage shall be considered, else numerical unfeasibility will occur;
- Due to modeling insufficiency, the option for the SPC policy arises from the difficulties to apply *multiple product campaign* (MPC) in a *multiple machine* environment;
- Assuming SPC, the investment cost will exceed in near 5 % the cost of the more efficient MPC policy; then, the SPC sizing is a priori overdesigned, and this will permit to introduce new products or to accommodate unforeseen growth on demands.

The generalized model ***RObatch_ms*** (adapted from Miranda and Casquilho (2011) along with some examples) includes the optimization of long term investment and also considers the short term scheduling of batch processes. Indeed, deterministic models do not conveniently address the risk of a wider planning horizon, and scheduling decision models often deal with certain data in a single time horizon. Thus, difficulty increases when the combinatorial scheduling problem is integrated with the uncertainty of the design problem. The following nomenclature is assumed:

Nomenclature

Index and sets

M	Number of stages i
NC	Number of components or products j
$NP(i)$	(Cardinal) number of processes $p(i)$ per stage
NR	Number of discrete scenarios r
$NS(i)$	(Cardinal) Number of discrete dimensions $s(i)$ in the process of stage i
NT	Number of time periods t;

Parameters

τ_{ij}	Processing times (h), for each product j in stage i
λdvt	Negative deviation on NPV penalization parameter
λqns	Non-satisfied demand penalization parameter
λslk	Capacity slack penalization parameter
c_{ips}	Equipment cost related to process $p(i)$ and size $s(i)$ selected in stage i
dv_{ij}	Discrete equipment volume in each stage
H	Time horizon
nc^{Upp}	Upper limit for disaggregated number of batches
$prob_r$	Probability of scenario r
$p(i)$	(Ordinal) Number of processes in stage i
Q_{itr}	Demand quantities (uncertain) for each product i

ret_{jtr} Unit (uncertain) values of return (net values) of the products j, in period t and scenario r
$s(i)$ (Ordinal) Number of process discrete dimensions in stage i
S_{ij} Dimension factor (L/kg), for each product j in stage i
V_{ij} Equipment volume (continuous value) in each stage;

Variables

ξ_r NPV value in scenario r
$dvtn_r$ Negative deviation on the value of NPV in scenario r
n_{jtr} Number of batches of product j, in period t and scenario r
nc_{ijsptr} Number of batches of product j, in period t and scenario r, disaggregated by process $p(i)$ and size $s(i)$ in each stage i
Qns_{jtr} Non-satisfied demand quantities of product j, in period t and scenario r
slk_{ijtr} Capacity slacks in each stage i, concerning totality of the *batches* of each product j, in period t and scenario r
$tcamp_{jtr}$ Campaign times (SPC) relative to each product j
W_{jtr} Global quantities produced of product j, in period t and scenario r
y_{isp} Binary decision related to process $p(i)$ and size $s(i)$ selected in stage i.

Then the model ***RObatch_ms*** in the relations set (RO.2-a–RO.2-m) considers a robust objective function (***a***) and the design and scheduling of batch plants with multiple machines and SPC policy are addressed on restrictions set (RO.2-b–RO.2-m) as follows:

(a) Objective Function, aiming to maximize the expected Net Present Value (NPV), considering penalizations of variability and capacity slackness;
(b) Definition of NPV—Each probabilistic part ξ corresponds to the NPV obtained at each discrete scenario r, and this part is obtained as the present amount of sales return less the investment costs;
(c) Definition of the solution variability through the negative linear deviation;
(d–e) The non-satisfied demand of each product, *Qns*, is related with the constraint slack, being a non-negative variable by definition;
(f) The global excess (*slk*) on the implemented production capacities results directly from the slacks of the constraints on the global quantities produced for each product;
(g–i) The disaggregated number of batches, *nc*, corresponds to the product-aggregation's variables (*n*. *y*), and the three logical sets of constraints consider: (g) upper bounds; (h) only one value is selected; and (i) the specification of its selected value;
(j–k) The campaign times, *tcamp*, must be determined to satisfy the time horizon, *H*, and are related to the number of batches, *nc*;
(l) Non-negativity restrictions;
(m) Binary variables definition.

Model *RObatch_ms*:

$$[\max]\Phi = \sum_{r=1}^{NR} prob_r \xi_r - \lambda dvt \sum_{r=1}^{NR} prob_r.dvtn_r - \lambda qns \sum_{r=1}^{NR} \frac{prob_r}{NC.NT} \left(\sum_{j=1}^{NC} \sum_{t=1}^{NT} Qns_{jtr} \right) - \lambda slk \sum_{r=1}^{NR} \frac{prob_r}{M.NC.NT} \left(\sum_{i=1}^{M} \sum_{j=1}^{NC} \sum_{t=1}^{NT} slk_{ijtr} \right) \tag{RO.2-a}$$

subject to,

$$\xi_r = \sum_{j=1}^{NC} \sum_{t=1}^{NT} ret_{jtr} W_{jtr} - \sum_{i=1}^{M} \sum_{s=1}^{NS(i)} \sum_{p=1}^{NP(i)} c_{isp} y_{isp}, \quad \forall r \tag{RO.2-b}$$

$$dvtn_r \geq \sum_{r'=1}^{NR} (prob_{r'} \xi_{r'}) - \xi_r \geq 0\,, \quad \forall r \tag{RO.2-c}$$

$$W_{jtr} + Qns_{jtr} = Q_{jtr}\,, \quad \forall j,t,r \tag{RO.2-d}$$

$$Qns_{jtr} \geq 0\,, \quad \forall j,t,r \tag{RO.2-e}$$

$$S_{ij} W_{jtr} + slk_{ijtr} = \sum_{s=1}^{NS(i)} \sum_{p=1}^{NP(i)} dv_{is} nc_{ijsptr}, \quad \forall i,j,t,r \tag{RO.2-f}$$

$$nc_{ijsptr} - nc_{ijsp}^{Upp} y_{isp} \leq 0\,, \; \forall\, i,j,s,p,t,r \tag{RO.2-g}$$

$$\sum_{s=1}^{NS(i)} \sum_{p=1}^{NP(i)} y_{isp} = 1, \quad \forall i \tag{RO.2-h}$$

$$\sum_{s=1}^{NS(i)} \sum_{p=1}^{NP(i)} nc_{ijsptr} - n_{jtr} = 0, \quad \forall i,j,t,r \tag{RO.2-i}$$

$$\sum_{s=1}^{NS(i)} \sum_{p=1}^{NP(i)} \left(\frac{\tau_{ij}}{p(i)} nc_{ijsptr} \right) - tcamp_{jtr} \leq 0, \quad \forall i,j,t,r \tag{RO.2-j}$$

$$\sum_{j=1}^{NC} tcamp_{jtr} \leq H, \quad \forall t,r \tag{RO.2-k}$$

Table 1 Numbers of parameters, variables and constraints corresponding to examples solved assuming: NC = 4; M = 3; NS = 5; NP = 3; NT = 1

Numerical examples	Parameters *NR*	Continuous variables	Constraints
EX1	1	209	226
EX2	3	603	672
EX3	7	1391	1564
EX4	15	2967	3348
EX5	30	5922	6693
EX6	100	19712	22303

$$\xi_r, dvtn_r,\ slk_{ijtr}, nc_{ijsptr},\ n_{jtr}\ ,\ Qns_{jtr},\ tcamp_{jtr}, W_{jtr} \geq 0, \quad \forall i, j, s, p, t, r \qquad \text{(RO.2-l)}$$

$$y_{isp} \in \{0; 1\}, \quad \forall i, s, p \qquad \text{(RO.2-m)}$$

The application of the generalized model ***RObatch_ms*** for the robustness promotion is illustrated through various numerical examples, as indicated in Table 1.

For that, numerical instances of uncertain demands on a unique time period (“static”) are addressed, and the generalization of the deterministic problem to the minimization of investment costs in a stochastic and robust formulation is considered. Through the usual reasoning of polynomial reduction of problem instances, the following is assumed: (i) only one time period; and (ii) zero value of return in products.

Considering one single time period, the unsuitability of NPV maximization must be noticed: NPV is usually addressed in a multiperiod horizon (dynamic problem) due to high investment costs that do not allow payback at one single time period. Furthermore, supposing ret_{jtr} = 0, then the NPV variables ξ are representing only the investment costs because there are no cash flows returning:

$$\xi = \xi_r = -\sum_{i=1}^{M} \sum_{s=1}^{NS(i)} \sum_{p=1}^{NP(i)} c_{isp} y_{isp}, \quad \forall r \qquad \text{(RO.3)}$$

There is no variability at this instance: NPV variables ξ are scenario independent and a null deviation, $dvtn_r$ = 0, is observed in all scenarios. And aiming to satisfy the uncertain product demands, the penalization of capacity slacks is not being considered (λslk = 0). The objective function in equation RO.2-a is thus reduced to the robust minimization of investment costs, assuming only the penalization of non-satisfied demand:

$$
\begin{aligned}
[\max]\Phi &= \xi.\sum_{r=1}^{NR} prob_r - \lambda qns\sum_{r=1}^{NR}\frac{prob_r}{NC.NT}\left(\sum_{j=1}^{NC}\sum_{t=1}^{NT} Qns_{jtr}\right)\\
&= -\sum_{i=1}^{M}\sum_{s=1}^{NS(i)}\sum_{p=1}^{NP(i)} c_{isp}y_{isp} - \lambda qns\sum_{r=1}^{NR}\frac{prob_r}{NC.NT}\left(\sum_{j=1}^{NC}\sum_{t=1}^{NT} Qns_{jtr}\right)
\end{aligned}
\tag{RO.4}
$$

or,

$$
[\min]\Psi = \sum_{j=1}^{M}\sum_{s=1}^{NS(i)}\sum_{p=1}^{NP(i)} c_{isp}y_{isp} + \lambda qns\sum_{r=1}^{NR}\frac{prob_r}{NC.NT}\left(\sum_{j=1}^{NC}\sum_{t=1}^{NT} Qns_{jtr}\right)
\tag{RO.5}
$$

The model defined in the relations set (RO.2-a–RO.2-m) is being restricted, and the following can be neglected: the time period index, t, because only one time period is considered; the constraint sets concerning the definition of the probabilistic variables, ξ, which will have a constant and scenario-independent value; and, the same for the deviation definitions, *dvtn*, which consequently will be null and useless. The various examples (EX1 to EX6) are described in Table 1.

The effect related to the utilization of distinct numbers of discrete scenarios is analyzed in the generalized stochastic model, which conceptually reduces to the deterministic model when considering one single scenario. Although the number of binary variables is kept constant and equal to 45 for all the six examples, both the number of continuous variables and the number of constraints vary linearly with the number of scenarios, *NR*.

(a) Variation of robust costs (10^5 €) versus the penalty values on non-satisfied demand, λqns, for various numerical examples.
(b) Variation of the expected value for non-satisfied demand, *Ensd* (10^3 kg), with the evolution of λqns, for various numerical examples.

Graphical representations are shown for the variation of different estimators (robust cost, ψ, expected value of the non-satisfied demand, *Ensd*, expected value of the capacity slacks, *Eslk*, non-robust cost, *Ecsi*), with the conjugated increase of the number of scenarios, *NR*, and the penalization for non-satisfied demand, λqns. Due to the near coincidence of the different lines represented, from $NR = 1$ (EX1) to $NR = 100$ (EX6), only three lines are shown in these graphs.

Considering the graphs at Fig. 3, two key subjects are observed:

(i) the behavior of the numerical instances is similar even when different number of scenarios is considered, *NR* from 1 to 100; and
(ii) the model robustness, with adequate sensitivity of technical estimators to the evolution of the non-satisfied demand penalization parameter, λqns; for all the scenarios number on the 1–100 range, the expected values associated with robust cost, ψ, and the non-satisfied demand, *Ensd*, alter rapidly with the λqns evolution and a flat level is reached in both cases.

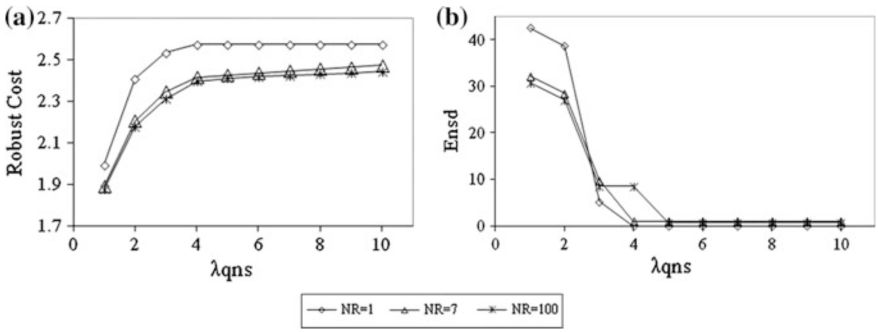

Fig. 3 Sensitivity of the objective function in face of the penalization parameters, showing solution robustness (**a**) and robustness in model (**b**)

Table 2 Significant values of the robust optimization considering distinct instances of numerical example EX3 (for *NR* = 7)

λqns	Costs	Ord(s)	Sum(dv)	%Eslk	%Ensd
0	124,596.08	1/1/1	3451.47	21.0	54.1
1	156,737.60	1/3/3	6087.68	11.7	21.0
2	163,661.91	1/3/4	6659.83	11.5	18.6
3	205,467.00	2/5/5	9366.59	11.1	6.3
4	237,689.36	3/5/5	10,298.62	13.6	0.6
5	237,689.36	3/5/5	10,298.62	12.0	0.6
	(…)		(…)		(…)
10	237,689.36	3/5/5	10,298.62	13.2	0.6
			(…)		(…)
20	237,689.36	3/5/5	10,298.62	12.7	0.6
21	257,332.14	4/5/5	10,929.24	13.3	0.0
	(…)		(…)		(…)
40	257,332.14	4/5/5	10,929.24	12.8	0.0

In Table 2, significant values for instances of EX3 are shown, in which instances are considered with seven scenarios, but whose variation with the growth of the penalization on the non-satisfied demand, λqns, is similar to all the other examples with different numbers of scenarios. These significant values are the values associated to alterations in the optimum configuration. Table 2 relates the penalty parameters λqns and the (non-robust) costs, showing:

- the order of the discrete dimension (size, *s*) selected in each stage, *Ord*(*s*); for example, "4/7/2", indicates that the fourth dimension was chosen at the first stage, the seventh dimension at the second stage, and the second dimension at the third stage; these values come directly from the binary solution;

- the sum of the discrete dimensions or equipment volumes selected, *Sum*(*dv*); this measure is important for slackness analysis, due to the interest of appreciating *Eslk* in relative terms at each example;
- the percentage of non-satisfied demand expected value, *%Ensd*; for each example, the reference value (100) is the expected value of uncertain demand;
- the percentage of capacity slacks expected value, *%Eslk*; for each example, the reference value for the calculation of this estimator is the discrete volumes sum, *Sum*(*dv*).

In Table 2, a progressive increase on costs is observed, due to the corresponding increase of the orders of dimension, *Ord*(*s*), and the increasing sum of volumes, *Sum*(*dv*). But in percentage of the expected value of the capacity slacks, *%Eslk*, it is verified that this one is kept in a strict range of values, between 11 % and 13 %. In absolute terms, the expected value for the slack, *Eslk*, is increasing for the first values of the penalty, λqns, but then attains a stable value. This permits to confirm the inherence of a residual value for the capacity slacks in this type of problem, where multiple products are processed in the same equipment. Focusing the effect of non-satisfied demand penalization, λqns, on the related percent expected value, *%Ensd*:

- if the penalization parameter is large, all the demand will be satisfied, *Ensd* and *%Ensd* tend to be null; the selected dimensions and the related costs are also large, but notice that one single scenario with tiny probability can drive such a large sizing;
- instead of full demand satisfaction, if the requirement of non-satisfied demand is relaxed to 1 %, the investment costs are reduced in about 8 %; and assuming more flexibility, if the non-satisfied demand is allowed to reach up to 6 %, the cost reduction is about 20 %;
- this kind of reasoning is realistic, since the model and the numerical examples are based on SPC policy; and if SPC is considered instead of MPC in the design and scheduling models studied, a relative overdesign of about 5 % in investment costs is foreseen (Miranda 2007).

3.1 Concluding Remarks on Robust Design and Scheduling

The MILP model featuring SPC and multiple machines (Voudouris and Grossmann 1992) was found to be the most promising from a computational standpoint (Miranda 2011b), and it was generalized toward a stochastic model ***RObatch_ms***. Its results point to a significant reduction (8–20 %) on the investment costs in comparison to the deterministic non-relaxed case. If the MPC policy is adopted or if a slight relaxation is made to the impositions on the uncertain demands (respectively, of 1–6 %), the demand relaxation does not cause real losses: model ***RObatch_ms*** assumes the lower efficient SPC policy and an overdesign in about

5 % on investment cost is thus expected (Miranda 2007). And remark also the ***RObatch_ms*** model robustness, with estimators responding adequately to the variation of the penalty parameter for non-satisfied demand, λqns.

4 Conclusions

The study of optimization cases and models from the literature allowed a detailed overview, and permitted to conjugate realistic subjects both in formulation and solution procedures. Developing theoretical studies, the various models at hand are detailed and insight is gained, their benefits and limitations are balanced, and robust generalization is developed. In addition, the studies on computational complexity along with the computational implementation fostered the construction of heuristics, such as local search procedures.

Based on the generalization approach described in prior paragraph, two problems are addressed:

- The PP problem—beyond the uncertainty treatment it is also considered the formulation of flexible production schemes, the robustness on solution and on model, and the processes parameters were economically evaluated.
- The *Batch* problem—the treatment of uncertainty also considered the problems' specificities; the short term scheduling and the multi-period horizon were simultaneously addressed, the deterministic approach from the literature is generalized onto a stochastic one, and economic parameters of interest were evaluated.

Further developments include modeling issues and solution methods, while the development of Decision Support Systems will foster the application to industrial cases.

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Appendix 1: Technical and Economic Estimators

The non-robust NPV expected value:

$$Ecsi = \sum_{r=1}^{NR} prob_r \xi_r \tag{A.1}$$

The negative deviation expected value:

$$Edvt = \sum_{r=1}^{NR} prob_r.dvtn_r \tag{A.2}$$

The non-satisfied demand expected value:

$$Ensd = \sum_{r=1}^{NR} \frac{prob_r}{NC.NT} \left(\sum_{j=1}^{NC} \sum_{t=1}^{NT} Qns_{jtr} \right) \tag{A.3}$$

The capacity slack expected value:

$$Eslk = \sum_{r=1}^{NR} \frac{prob_r}{M.NC.NT} \sum_{j=1}^{NC} \sum_{t=1}^{NT} \left\{ \sum_{i=1}^{M} \sum_{s=1}^{NS} \sum_{p=1}^{NP} p(i).y_{isp}. \left(dv_{js} - S_{ij}. \frac{W_{jtr}}{n_{jtr}} \right) \right\} \tag{A.4}$$

The percentage non-satisfied demand expected value:

$$\%Ensd = \frac{Ensd}{Qmed}.100, \quad \text{with} \quad Qmed = \sum_{r=1}^{NR} \frac{prob_r}{NC.NT} \left(\sum_{j=1}^{NC} \sum_{t=1}^{NT} Q_{jtr} \right) \tag{A.5}$$

The percentage capacity slack expected value:

$$\%Eslk = \frac{Eslk}{Vtotal}.100, \quad \text{with} \quad Vtotal = \sum_{i=1}^{M} \sum_{s=1}^{NS} \sum_{p=1}^{NP} \left(y_{isp}.dv_{is} \right) \tag{A.6}$$

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