PRO-ACTIVE SCHEDULING BY A COMBINED ROBUST OPTIMIZATION AND MULTI-PARAMETRIC PROGRAMMING APPROACH

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Abstract

In this work, we address short-term batch process scheduling under uncertainty in which the scheduling model is contaminated with uncertain data in the objective function, the right-hand side vector and in the constraint matrix, introduced by price, demand, and processing time or conversion rate uncertainty, respectively. We apply a two-stage robust optimization/multi-parametric programming procedure for the approximate solution of the scheduling model which translates into a multi-parametric mixed integer linear (mp-MILP) problem. We demonstrate that the proposed approach contributes to the construction of a pro-active scheduling strategy and show that it is an attractive alternative to the rigorous robust optimization approach in terms of providing a tight estimate of the optimal scheduling policy.

Keywords

Process Scheduling, Mixed Integer Linear Programming, Multi-Parametric Programming.

Introduction

The area of scheduling of chemical and pharmaceutical processes has received significant attention in industry and academia. For key contribution in this field we refer to the excellent reviews of Floudas and Lin (2004, 2005), Li and Ierapetritou (2008a) and Verderame et al. (2010). Most of the work is concerned with scheduling models in which all data are assumed to be available. In fact, processes may be subject to uncertainty arising from variations in the market demand, product prices, processing times, etc. Hence, the optimal scheduling policy related to the nominal values may not be optimal or even feasible anymore once a deviation from the nominal values has occurred. Pro-active scheduling is motivated by the need to address uncertainty upfront in order to avoid repetitive online optimization in response to disturbances. In the open literature, an approach to account for the presence of uncertainty in the model is robust optimization, which aims at finding scheduling policies that are feasible for all possible realizations of the parameters (Lin et al. (2004), Janak et al. (2007), Li and Ierapetritou (2008b)). On the other hand, multi-parametric programming has also found promising applications in process scheduling under uncertainty (Ryu et al. 2007, Ryu and Pistikopoulos (2007), Li and Ierapetritou (2007)) when the number of parameters is small. In this work, we employ a combined robust optimization and multi-parametric programming approach, also referred to as two-stage method (Wittmann-Hohlbein and Pistikopoulos (2011)), as a pro-active scheduling strategy for short-term batch processes. We show that the two-stage method (i) allows for the efficient treatment of all types of uncertainty in the underlying mathematical model and (ii) in comparison with a rigorous robust optimization approach is less conservative and also remains flexible towards the incorporation of the parameters once their actual values are known. For any instance, the close-to-optimal scheduling policy is then derived via function evaluation without any further need for optimization.

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Problem Formulation

We consider short term scheduling of batch processes. In particular, we use the unit specific event based model which is a continuous time formulation featuring the concept of event points (Ierapetritou and Floudas (1998)). Event points are time related instances at which tasks start in units. Binary variables that are introduced into the model denote the activation status of a task at a unit at an event point. The objective in scheduling is the maximization of profit although other criteria such as the minimization of make-span may also be considered. The scheduling formulation needs to account for material balances between all products produced and consumed, satisfy capacity and storage constraints, enforce allocation and sequencing constraints assigning tasks to suitable units, and fulfill time/duration constraints. Market demands must also to be met. The deterministic scheduling formulation which corresponds to a mixed-integer linear problem reads as follows:

$$\begin{split} \overline{z} &= \max_{x_{in}, s_{in}, s_{in}', s_{in}',$$

$$\begin{split} t^{s}_{ij(n+1)} \geq t^{s}_{ij'(n+1)} - H \ (1 - w_{ij'n}) \\ & i, i' \in I_{j,j'}, i \neq i', \ j, \ j' \in J, \ j \neq \ j', n \leq N^{\max} \ -1 \\ t^{s}_{ij(n+1)} \geq t^{s}_{ijn}, \ t^{f}_{ij(n+1)} \geq t^{f}_{ijn} \\ & i \in I, \ j \in J_{i}, n \leq N^{\max} \ -1 \\ t^{s}_{ijn} \leq H, \ t^{f}_{ijn} \leq H \\ \end{split}$$

The presence of uncertainty transforms the scheduling model into the general multi-parametric mixed-integer linear model (P),

$$\overline{z}(\theta) = \max_{x,y} (c + H\theta)^T x + (d + L\theta)^T y$$
s.t. $A(\theta)x + E(\theta)y \le b + F\theta$
 $x \in R^n, y \in \{0,1\}^p, \theta^{\min} \le \theta \le \theta^{\max},$
(P)

with all matrices and vectors having appropriate dimensions, $A(\theta) = A^N + \sum_{l=1}^{q} \theta_l A^l$ (analogously for $E(\theta)$), and $\theta \in R^q$ denoting the vector of parameters. For example,

price uncertainty introduces objective function coefficient (OFC) uncertainty, demand uncertainty affects the entries of the right-hand side (RHS) constraint vector b, and production time and conversion rate uncertainty affect the entries of the constraint matrices A and E, respectively, and introduce so called left-hand side (LHS) uncertainty into the model. For the explicit solution of (P), multiparametric programming techniques aim to derive the optimal solution without exhaustively enumerating the parameter space (Pistikopoulos (2009)). The presence of LHS-uncertainty poses a challenge in multi-parametric mixed integer linear programming. Therefore, we employ a combined robust optimization/multi-parametric programming procedure for the approximate solution of (P) as outlined in the next chapter.

Two-Stage Method for general mp-MILP Problems

In the first step of the two-stage algorithmic procedure, (P) is immunized against uncertainty in the constraint matrix A which yields a partially robust RIMmp-MILP problem featuring OFC- and RHS-uncertainty, as well as LHS-uncertainty related to the constraint matrix E, whereas in the second step the explicit optimal solution of the robust model is derived by applying a suitable multiparametric programming algorithm (Faísca et al. (2009)). The combined robust optimization/multi-parametric programming procedure is computationally efficient, providing a tight lower bound on $\overline{z}(\theta)$ of (P). Here, alongside the worst-case oriented formulation we also discuss an alternative robust model which allows controlling the degree of conservatism of the solution.

The worst-case oriented partially robust counterpart of (P)

The pair $(\overline{x}, \overline{y})$ is called a partially robust feasible solution of (P) if

$$\forall \,\overline{\theta} : \theta^{\min} \leq \overline{\theta} \leq \theta^{\max} \quad A(\,\overline{\theta}\,)\overline{x} \, + E(\,\theta\,)\overline{y} \leq b + F\,\theta \ (1)$$

for any feasible θ . Incorporating (1) into (P) yields the formulation of the partially robust counterpart (RC) of the general mp-MILP problem (P),

$$z(\theta) = \max_{x,y,u_{i}} (c + H\theta)^{T} x + (d + L\theta)^{T} y$$

s.t.
$$\sum_{j=1}^{n} a_{ij}^{n} x_{j} + \sum_{l=1}^{q} (\theta_{l}^{N} \sum_{j=1}^{n} a_{ij}^{l} x_{j} + \tau_{l} u_{i}^{l})$$
$$\leq b_{i} + \sum_{l=1}^{q} f_{il} \theta_{l} - \sum_{j=1}^{p} e_{ij}(\theta) y \quad i = 1,...,m$$
$$- u_{i}^{l} \leq \sum_{j=1}^{n} a_{ij}^{l} x_{j} \leq u_{i}^{l} \quad i = 1,..., m, l = 1,..., q$$
$$x \in R^{n}, y \in \{0,1\}^{p}, u_{i} \in R^{q}, \theta^{\min} \leq \theta \leq \theta^{\max},$$

where $\tau_i := (\theta_i^{\max} - \theta_i^{\min}) / 2, \theta_i^N := \theta_i^{\max} - \tau_i$ denote the range and the nominal value of $\theta_l, l=1, ..., q$, respectively. Every feasible solution of *(RC)* is a partially robust feasible

solution of (P). Note that the conventional worst-caseoriented robust counterpart of (P) corresponds to a fully deterministic MILP problem, see Lin et al. (2004) and Ben-Tal and Nemirovski (1998), respectively, whose solutions are immune against all data variations. Clearly, every feasible solution of the robust counterpart is also feasible for (RC), and consequently for (P).

The partially robust counterpart of (P) with an adjustable degree of conservatism of the solution

If in practice not all parameters are likely to change from the nominal value, then the worst-case oriented robust counterpart may be too restrictive. An approach that allows adapting the degree of conservatism of the solution is presented in Bertsimas and Sim (2003, 2004). Here, it is adapted to solely protect the solution against uncertainty in *A*. Assume that the entries of *A* are modeled as independent, symmetric and bounded random variables where $a_{ij}^{\ N}$ denotes the nominal value and $a_{ij}^{\ R}$ the range of a_{ij} for all *i*, *j*, respectively. We denote by J_i^a the set of uncertain coefficients of *A* that appear in the *i*-th constraint of (*P*). The parameter Γ_i^a is called the budget parameter, marking the trade-off between robustness of the solution and conservatism of the model. It holds

$$0 \leq \Gamma_i^a \leq |J_i^a| \quad i = 1,...,m$$
.

If Γ_i^a is an integer, which is a sufficient assumption in our framework, the solution is immune against up to Γ_i^a uncertain coefficients in the *i*-th constraint of A.

We say that the pair $(\overline{x}, \overline{y})$ is partially robust feasible with respect to Γ_i^a if

$$\sum_{j=1}^{n} a_{ij}^{N} \overline{x}_{j} + \max_{\{S_{i}^{a} \subseteq J_{i}^{a} \| S_{i}^{a} \| = \Gamma_{i}^{a}\}} (\sum_{k \in S_{i}^{a}} a_{ik}^{R} | \overline{x}_{k} |)$$

$$+ \sum_{j=1}^{p} e_{ij}(\theta) \overline{y}_{j} \le b_{i} + \sum_{l=1}^{q} f_{il} \theta_{l} \quad i = 1,..., m$$
(2)

for any feasible θ . Incorporating (2) into (P) yields the partially robust counterpart (RC_{Γ}),

$$z(\theta) = \max_{x,y,q^{a},p^{a}_{i},u} (c + H\theta)^{T} x + (d + L\theta)^{T} y$$
s.t.
$$\sum_{j=1}^{n} a_{ij}^{N} x_{j} + q_{i}^{a} \Gamma_{i}^{a} + \sum_{j \in J_{i}^{a}} p_{ij}^{a}$$

$$\leq b_{i} + \sum_{l=1}^{q} f_{il} \theta_{l} - \sum_{j=1}^{p} e_{ij}(\theta) y_{j} \quad i = 1,...,m$$

$$q_{i}^{a} + p_{ij}^{a} \geq a_{ij}^{R} u_{j} \qquad i = 1,...,m, \quad j \in J_{i}^{a}$$

$$q_{i}^{a} \geq 0, \quad p_{ij}^{a} \geq 0 \qquad i = 1,...,m, \quad j \in J_{i}^{a}$$

$$-u_{j} \leq x_{j} \leq u_{j} \qquad j = 1,...,n$$

$$x, u \in \mathbb{R}^{n}, y \in \{0,1\}^{p}, \quad \theta^{\min} \leq \theta \leq \theta^{\max},$$

which is also a RIM-mp-MILP problem. Note that setting $\Gamma_i^a = |J_i^a|$ reflects the most conservative model which is equivalent to the worst-case oriented approach as employed in (*RC*).

A decomposition algorithm for RIM-mp-MILP problems

We outline the steps of the algorithm presented in Faísca et al. (2009) for the solution of (*RC*) and, analogously, of (*RC*_{*l*}). The master problem (*M*) is derived from (*RC*) by treating the parameter θ as an optimization variable. The optimal integer node y^{opt} of (*M*) is input to (*RC*) which then yields mp-LP sub-problem (*S*). The critical regions of (*S*), each a subset of the feasible set of parameters in which a particular basis remains optimal are uniquely defined by the LP optimality conditions (Gal (1979)).

Between every master and sub-problem iteration the master problem is updated. A new MINLP problem is solved to global optimality for each one of the current critical regions. Integer cuts are introduced into the formulation of (M) in order to exclude previously visited integer solutions and parametric cuts ensure that only integer nodes that are optimal for (RC) for a certain realization of the parameters are considered. The cuts are given by

$$\sum_{i \in J^k :=\{ j \mid y_j^k = 1\}} y_j^k - \sum_{j \in \{ j \mid y_j^k = 0\}} y_j^k \le |J^k| \qquad k = 1, \dots, K$$

with K denoting the number of previously identified integer solutions in this region, and

$$(c + H\theta)^{T} x + (d + L\theta)^{T} y \ge s_{k}(\theta) \qquad k = 1, \dots, K$$

where $s_k(\theta)$ is the optimal objective value of (RC) at the integer node related to index k. The algorithm terminates in a region where the master problem is infeasible. We retain an *envelope of parametric profiles* (Dua et al. (2002)) and collect all integer nodes and corresponding continuous solutions that have been identified to be optimal for certain points within a critical region. Function evaluation and direct value comparison of the objective values for the parametric profiles stored in the envelope determine the optimal solution of (RC) at any parameter realization.

Note that the critical regions of (RC) obtained by the decomposition algorithm are polyhedral convex and that the solutions stored in the envelope are piecewise affine functions. The number of regions is influenced by the number of integer nodes and constraints. For a thorough study of the computational complexity of the algorithm, the reader is referred to Faísca et al. (2009).

Computational Studies

Example 1. The production process whose STN-representation is given in Figure 1 consists of three tasks that take place in three separate units. The final product S3 and its purified version, S4, are sold off to the market. We assume price, demand, and processing time uncertainty for the mixing task. The data for Example 1 are presented in Table 1.

Employing the two-stage method, the partially robust model (RC) enforces feasibility of the solution for all scenarios of the variable terms of the processing time. The

corresponding partially robust duration constraint reads as follows:

$$t_{mix, 1,n}^{f} \ge t_{mix, 1,n}^{s} + \frac{2}{3}(4.5 + \theta_{2}) w_{mix, 1,n} + \frac{2}{300} 5b_{mix, 1,n}$$
$$n \in N$$

The partially robust counterpart (RC) with 5 event points over a time horizon of 12 hours involves 185 constraints and 15 integer variables. The decomposition algorithm requires the solution of 9 MINLP master problems solved to global optimality and 3 mp-LP subproblems. Three integer nodes have been identified to be optimal for certain regions of the feasible parameter space. The critical regions are depicted in Figure 2 and the objective function values associated to the solutions stored in the envelope of parametric profiles are given in Table 2. For the lack of space the solutions stored in the envelope are not given. In all but one critical region the optimal partially robust scheduling policy has been identified. In region CR_1 , the envelope contains two candidate solutions among which, for every parameter realization, the optimal partially robust schedule of Example 1 is always included.

For example, consider $\theta^* = (0.5, -0.5)^T \in CR_1$. At this point, function evaluation yields $z_1 = 128.6$ associated with the first profile and $z_2 = 116$ with the second profile, respectively, Direct comparison identifies the first profile to be the optimal partially robust scheduling policy at θ^* . The corresponding Gantt-Chart of the optimal partially robust scheduling policy at θ^* is presented in Figure 3. In comparison, the exact optimal value of Example 1 at θ^* is z=144. The deterministic worst-case oriented robust counterpart of Example 1, however, is infeasible.



Figure 1. STN-Representation of Example 1

Unit	Capacity	Task		Processing Time (τ)	
Unit 1	100	Mixing	5	$4.5+\theta_2$	
Unit 2	75	Reaction	on	3.0	
Unit 3	50	Separation		1.5	
State	Storage	Initial	Price	Demand	
	Amount				
S 1	-	-	0	-	
S2	100	0	0	-	
S 3	100	0	0.7	-	
S4	-	0	$1+\theta_I$	$50-20\theta_I$	
		θ_{I}		θ_2	
Range		-1≤θ₁≤0.5		$-0.5 \le \theta_2 \le 0.5$	

Table 1. Data for Example 1



Figure 2. Critical Regions of Example 1 with Two-Stage Method

 Table 2. Envelope of Partially Robust Profits
 of Example 1

	Critical Region	Profit
CR_1	$\{0 \le \theta_1 \le 0.5, -0.5 \le \theta_2 \le 0.5\}$	$-8.3\theta_1\theta_2 + 62.2\theta_1 - 20.6 \ \theta_2 + 84.9$ $50\theta_1 - 16\theta_2 + 83.9$
CR_2	$\{-0.19 \leq \theta_1 \leq 0.5, -0.5 \leq \theta_2 \leq 0.5\}$	$-8.3\theta_1\theta_2+62.2\theta_1-20.6\ \theta_{2+}84.9$
CR ₃	$\{-\theta_1+0.4\theta_2 \le 0.62, \\ \theta_1 \le -0.19, -0.5 \le \theta_2 \le 0.5\}$	$-20{\theta_1}^2 + 46{\theta_1} - 19{\theta_2} + 82.4$
CR ₄	$\{-\theta_1+0.9\theta_2\leq 0.7, -1\leq \theta_1, \\ \theta_1-0.4 \ \theta_2\leq -0.6, -0.5\leq \theta_2\}$	$-20{\theta_1}^2 + 50{\theta_1} - 16{\theta_2} + 86.4$
CR5	$\{\theta_{1}-0.9\theta_{2}\leq-0.7,-\theta_{1}+\\0.8\theta_{2}\leq0.9,-1\leq\theta_{1},\theta_{1}-0.4\theta_{2}\leq\\-0.6,\theta_{2}\leq0.5\}$	$-20{\theta_1}^2+50{\theta_1}-16{\theta_2}+86.4$



Figure 3. Gantt-Chart of the Optimal Partially Robust Scheduling Policy of Example 1 at $\theta^* = (0.5, -0.5)^T$

Example 2. The process involves the production of two final products and several intermediate products as depicted in the STN-representation, Figure 4.The reaction tasks R1, R2 and R3, respectively, take place in one of two units, U1 and U2, and there are separate units for heating and separation. Because of the lack of space, for the data of Example 2 we refer to Ierapetritou (1998). The prices and the demands of the final products S8 and S9 vary and there is uncertainty in the production rates of S8 and the intermediate product S7:

$$\begin{split} C_{ss} &= 10 + 10\,\theta_1, \quad R_{ss} = 50 - 40\,\theta_1, \quad 0 \le \theta_1 \le 1, n \in N \\ C_{sy} &= 15 + 5\theta_2, \quad R_{sy} = 60 - 20\,\theta_1, \quad 0 \le \theta_2 \le 1, n \in N \\ \rho_{ss,i}^p &= 0.4 - 0.1\theta_3, \quad \rho_{s7,i}^p = 1 - 0.2\theta_4, \quad 0 \le \theta_{3,4} \le 1, i = U1, U2. \end{split}$$

Furthermore, we know that at most one of the production rates for S7 and S8, respectively, in U1 and U2 is likely to change from the nominal value. Hence, within the two-stage method we embed the partially robust model (RC_{Γ}) with an adjustable degree of conservatism of the solution. Conversion rate uncertainty affects the constraints accounting for the material balances. The amount of a state (raw, intermediate, or final product) at any event point has to be less than the maximum storage capacity and, naturally be always non-negative. For every triplet $sn \overline{n}, s \in \{S7, S8\}, 2 \le n \le N^{\max}, 2 \le \overline{n} \le n$ we introduce the budget parameter $\Gamma_{sn(\overline{n}-1)}$. The corresponding storage constraint, immunized against conversion rate uncertainty, reads as follows:

$$\begin{split} sti_{s} &- x_{s1} - \sum_{i \in I_{s}} \rho_{si}^{c} \sum_{j \in J_{i}} b_{ij1} + \\ &\sum_{\overline{n} \le n, \overline{n} \ge 2} (-x_{s\overline{n}} - \sum_{i \in I_{s}} \rho_{si}^{c} \sum_{j \in J_{i}} b_{ij\overline{n}} + \sum_{i \in I_{s}} \rho_{si}^{pN} \sum_{j \in J_{i}} b_{ij\overline{n}} + \Gamma_{sn(\overline{n}-1)} q_{sn(\overline{n}-1)} \\ &+ \sum_{i \in I_{s}} \sum_{j \in J_{i}} p_{sn(\overline{n}-1)ij}) \le ST_{s}^{\max} \qquad 2 \le n \le N^{\max}, s \in \{S7, S8\} \\ q_{sn(\overline{n}-1)} + p_{sn(\overline{n}-1)ij} \ge \rho_{si}^{pR} b_{ij(\overline{n}-1)} \\ &i \in I_{s}, j \in J_{i}, 2 \le n \le N^{\max}, 2 \le \overline{n} \le n, s \in \{S7, S8\} \end{split}$$

where the superscripts N and R denote the nominal value and the range, respectively, of the production rate. In a similar way we are able to derive the robustified constraints related to the non-negativity of the amounts of S7 and S8 at every event point. Note that the uncertain coefficients of the constraint matrix are, in fact, not independent. Therefore, a sensible choice of the budget parameters is necessary to ensure consistency between different constraints and event points in order to derive a meaningful robust model, i.e. $\Gamma_{sn(\overline{n}-1)} = \Gamma_{sn'(\overline{n}-1)}, n \neq n'$. Enforcing that the solution is protected against the derivation of at most one production rate from the nominal value, we set $\Gamma_{s_1(\overline{n}-1)} = 1$. The two-stage method applied to Example 2 with 5 event points over a time horizon of 8 hours requires the solution of 7 MINLP problems and one mp-LP problem. The solutions of the partially robust model are independent of θ_3 and θ_4 . In total 6 critical regions have been identified which are depicted in Figure 5. In each of the regions one solution is stored. Therefore, the optimal partially robust scheduling policy of Example 2 has been determined and we depict the overall partially robust profit in Figure 6.

Note that setting $\Gamma_{sn(\overline{n}-1)} = 2$ resembles the worst-case oriented approach, i.e. all production rates are likely to change from the nominal values, whereas by setting $\Gamma_{sn(\overline{n}-1)} = 0$ no deviation is supported. In comparison, the rigorous worst-case oriented robust MILP model of Example 2 yields a profit of z=615.32 which is a lower bound on the optimal partially robust profit with respect to $\Gamma_{sn(\overline{n}-1)} = 1$, as depicted in Figure 6, but also on the optimal partially robust profits for $\Gamma_{sn(\overline{n}-1)} = 0, 2$.



Figure 4. STN-Representation of Example 2 with Nominal Conversion Rates



Figure 5. Critical Regions of Example 2 with Two-Stage Method



Figure 6. Optimal Partially Robust Profit (Surface Plot) and Optimal Worst-Case Oriented Robust Profit (Grid Plot) of Example 2

Conclusions

In this work, we have addressed short-term batch process scheduling contaminated with uncertainty in the data using a two-stage method which combines state-ofthe-art robust optimization and multi-parametric programming techniques. We obtain an optimal partially robust scheduling policy that yields a tight lower bound on the overall profit and is less conservative than the rigorous robust optimization approach. The two-stage method is able to deal with all types of uncertainty in the scheduling model, in particular with disturbances in the entries of the constraint matrices which are the most challenging types of uncertainty in multi-parametric mixed-integer linear programming. The benefit of multi-parametric programming as a tool for pro-active scheduling is that the model is solved offline with the parametric profiles being stored in a look-up table. Hence, once the true values of the parameters are known, the optimal partially robust scheduling policy is readily obtained via function evaluation from the profiles stored in the look-up table. Within the two-stage method, as an alternative to the worst-case oriented partially robust model we presented the formulation of a partially robust model that allows controlling the robustness of the model and conservatism of the solution which then has been applied to batch process scheduling as studied in Example 2.

Acknowledgments

Financial support from EPSRC (EP/G059071/1, EP/I014640/1) and from the European Research Council (MOBILE, ERC Advanced Grant, No 226462) is gratefully acknowledged.

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Appendix

Notation

Н	Time horizon		
$i \in I, I_{j,}I_s$	Tasks, tasks performed in unit j/processing state s		
$j \in J, J_i$	Units, units suitable for performing task i		
$s \in S$	States		
$n \in N$	Event points		
X sn	Amount of state s sold to market at event point n		
st _{sn} , sti _s	Amount of state s at event point n, initial amount		
b_{ijn}	Amount of material undertaking task i in unit j at		
	event point n		
t_{ijn}^{s}, t_{ijn}^{f}	Starting/finishing time of task i in unit j related to		
	event point n		
W_{ijn}	Activation status of task i in unit j at event point n		
C_s	Price of state s		
R_{s}	Demand of state s		
$\rho_{s}^{c}, \rho_{s}^{p}$	Proportion of state s consumed/produced during		
	task i		
ST_{s}^{\max}	Maximum storage capacity of state s		
$V_{ij}^{\mathrm{\ min}}$, $V_{ij}^{\mathrm{\ max}}$	Minimum/maximum capacity for task i in unit j		
$ au_{ij}$	Mean processing time of task i in unit j		
α_{ij}, β_{ij}	Constant/variable term of processing time for task i		
	in unit j with		
	$\alpha_{ij} := \frac{2}{3} \tau_{ij}, \beta_{ij} := \frac{2}{3} \frac{\tau_{ij}}{V_{ii}^{\max} - V_{ij}^{\min}}$		