SHORT-TERM SCHEDULING OF CHEMICAL PROCESS INCLUDING UNCERTAINTY

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Abstract: This paper addresses the short-term scheduling of chemical process with uncertainty considerations. A multiobjective robust optimization method is proposed to identify Pareto optimal solutions, where Normal boundary intersection (NBI) technique is utilized in order to trace the Pareto optimal surface in the objective space, on which each point represents a trade-off between the various objectives. The issue is also addressed using parametric mixed integer linear programming (pMILP) analysis where uncertain parameters are present on the right hand side (RHS) of the constraints. For the case of multiple uncertain parameters, a new algorithm of multiparametric linear programming (mpLP) is proposed that does not require the construction of the LP tableaus but relies on the comparison between solutions at leaf nodes. Given the range of uncertain parameters, the output of this proposed framework is a set of optimal integer solutions and their corresponding critical regions and optimal functions.

Keywords: scheduling, uncertainty, robust optimization, parametric MILP.

1. INTRODUCTION

Substantial benefits can be achieved through the use of optimization techniques in plant operations by improving the resource utilization at different levels of decision making process. However, uncertainty exists in realistic manufacturing environment due to lack of accurate process models and variability of process and environment data. The presence of uncertainty can substantially reduce or eliminate the advantages of optimization approaches. Therefore, it is of great importance to develop systematic methods to address the problem of uncertainty in process operations.

Although there has been a substantial amount of work addressing the problem of design and planning under uncertainty, a detailed literature review of which can be found in Cheng et al. (2003), the issue of uncertainty in scheduling problems has received relatively little attention. Existing work mainly includes stochastic programming approaches involving chance constraints and two-stage programming (Bonfill *et al.*, 2005, Jia and Ierapetritou, 2004), as well as robust optimization methods (Basset *et al*., 1997; Lin *et al*., 2004; Vin and Ierapetritou, 2001). A brief overview of these approaches are presented here. Ierapetritou and Pistikopoulos (1996) addressed the scheduling of single-stage and multistage multiproduct continuous plants with a single production line at each stage when uncertainty in product demands is involved. They used Gaussian quadrature integration to evaluate the expected profit and formulated the problem as a MILP models. Lin et al (2004) proposed a robust optimization method to address the problem of scheduling with uncertain processing times, market demands, or prices. The robust optimization model was derived from its deterministic model considering the worst-case values of the uncertain parameters, and a certain infeasibility tolerance was introduced to allow constraint violations. Vin and Ierapetritou (2001) addressed the problem of multiproduct batch plant scheduling under demand uncertainty. They introduced a robustness metric based on deviations from the expected performance including the infeasible scenarios. Robust schedules are generated based on a multiperiod approach. Balasubramanian and Grossmann (2002) considered uncertain processing times in scheduling of multistage flowshop plants. They also proposed a multiperiod MILP model and proposed a special branch and bound algorithm with aggregated probability model to select the sequence of jobs with minimum expected makespan. Recently, Bonfill et al. (2005) used a two-stage stochastic approach to address the robustness in scheduling batch processes with uncertain operation times. The objective is to minimize a weighted combination of the expected makespan and wait times. Basset et al. (1997) proposed a framework considering uncertainties in processing times, equipment reliability, process yields, demands and manpower changes. They generate random instances by Monte Carlo sampling, and determine the schedules for these instances. The solutions are then analyzed to derive a number of operating policies. Orcun et al. (1996) presented an approach to deal with uncertain processing times in batch processes and utilized chance constraints to take into consideration the violation of operation time constraints under certain conditions. In our earlier work (Jia and Ierapetritou, 2004), we developed a branch-and-bound solution framework to determine a set of alternative schedules for a given range of uncertain parameters. The idea of inference based sensitivity analysis for MILP problems was employed that has the advantage of not substantially increasing the complexity compared with the deterministic formulation.

A number of problems from the area of process design and operations are commonly formulated as mixed integer linear programming (MILP) problems. One way to incorporate uncertainty into these problems is using MILP sensitivity analysis and parametric programming methods. The main limitation of most existing methods is that they can only be applied to problems with a single uncertain parameter or several uncertain parameters varying in a single direction. A number of approaches have been developed for parametric integer programming problems that involve a single parameter/scalar variation, basically including implicit enumeration methods (Roodman, 1972; Piper and Zoltners, 1976), branch and bound methods (Roodman, 1974}, Marsten and Morin (1977), Ohtake and Nishida (1985), and cutting plane methods (Holm and Klein, 1984), Jenkins and Peters, 1987), etc. A detailed literature review can be found in Jenkins (1990).

Jenkins' approach is extended by Crema (2002) for the multiparametric 0-1 integer linear programming (ILP) problem considering the perturbation of the constraint matrix, the objective function and the RHS vector. The proposed algorithm iteratively solves a nonlinear problem, which can be converted to an equivalent MILP formulation, in order to obtain a complete multiparametric analysis.

Acevedo and Pistikopoulos (1997) proposed a parametric programming approach for the analysis of linear process engineering problems under uncertainty. The procedure solves the multiparametric linear programming (mpLP) at each node of the B&B tree, then compares and identifies the different optimal integer solutions and their corresponding optimal value functions. Pertsinidis et al. (1998) developed an algorithm for MILP sensitivity analysis. At each iteration, the LP sensitivity analysis results and a cut that excludes the current integer solution are incorporated to a MILP problem so as to find the breaking point and the successor optimal integer solution. Their ideas were extended by Dua and Pistikopoulos (2000), by decomposing the mp-MILP into two subproblems and then iterating between them. The first subproblem is obtained by fixing the integer variables, resulting in a mpLP problem, whereas the second subproblem is obtained by relaxing the parameters as variables, leading to a MILP problem.

The problem of RHS multiparametric linear problem was first addressed by Gal and Nedoma (1972). Their algorithm is based on the Simplex algorithm for deterministic LPs. It starts with an initial optimal basis at a feasible point and moves to each of its possible neighbor bases by one dual step to determine the new optimal solution. This procedure is repeated until there is no optimal basis that still has unexamined neighbors. A geometric approach is proposed by Borrelli et al. (2003), which is based on the direct exploration of the parameter space and their definition of critical regions is not associated with bases but with the set of active constraints.

Our work towards addressing the problem of uncertainty in scheduling has been evolved around two different directions based on the variable information about uncertainty. For the cases where uncertainty is well characterized, robust optimization can be used to simultaneously optimize the different objectives in the face of uncertainty, such as expected profitability, flexibility, robustness. However, when there is not enough information, parametric programming can be employed to generate a set of alternative schedules to cover the whole uncertainty space.

This paper is organized as follows. Section 2 presents the multiobjective robust optimization model for short-term scheduling, whereas the details of the proposed parametric MILP approach for the cases of single and multiple uncertain parameters are presented in section 3. Section 4 is used to present the effectiveness of the proposed methods through the solution of one case study whereas section 5 summarizes the work and present some of the ideas for future developments.

2. ROBUST OPTIMIZATION

A wide variety of problems arising in design and operation of engineering systems require simultaneous optimization of more than one objective function. A solution that optimizes all the objectives most likely doesn't exist, thus we need to find out solutions that trade-off the different objectives.

This type of problems are known as multiobjective, multicriteria or vector optimization problems, which consist of two or more conflicting objective functions with a set of constraints taken into consideration. Optimization of these problems is to identify the set of Pareto optimal solutions.

A solution is Pareto optimal if improvement in one objective can only be achieved at the expense of some other objectives. In mathematical terms, for a general multiobjective optimization problem:

$$\min_{x\in C} F(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_n(x) \end{bmatrix} \qquad n \geq 2 \qquad \text{(MOP)}$$

where $C = \{x : h(x) = 0, g(x) \leq 0, a \leq x \leq b\}$

A point $x^* \in C$ is Pareto optimal (or non-dominated) for multiobjective optimization problem (MOP) if and only if there is no $x \in C$ such that $f_i(x) \leq f_i(x^*)$ for all $i \in 1,2,..,n$, with at least one strict inequality.

Classical approaches for MOP are the weighting method (1963) and the ε-constraint method (Haimes, 1973). Weighting method minimizes a positively weighted sum of the individual objectives, where the choice of appropriate weighting coefficients is left to the users. For this method the objective takes the following form:

$$\sum_i \alpha_i f_i(x), \qquad \alpha_i > 0, i = 1,2,...,n$$

where α_i are the weights for the different objectives. ε-constraint method (Haimes, 1973) minimizes a primary objective $f_p(x)$, and constrains the upper bounds for the remaining objectives as follows:

$$\min_{x\in C} f_p(x)$$

$$\text{subject to} \quad f_i(x) \leq \varepsilon_i \quad i = 1,..,n \quad i \neq p$$

Hillermeier (1995) proposed a homotopy method that considers the set of Pareto candidates as a differentiable manifold and constructs a local chart which is fitted to the local geometry of that Pareto manifold. New Pareto candidates are generated by evaluating the local chart numerically.

The normal boundary intersection (NBI) (Das and Dennis, 1998) method uses a geometrically intuitive parametrization to produce an even distributed set of points on the Pareto surface, even for poorly scaled problems. This method is utilized in this chapter to generate the Pareto surface of multiobjective scheduling problem. The details of this approach are provided in section 2.3 after the presentation of deterministic and robust scheduling in sections 2.1 and 2.2, respectively.

2.1 Deterministic Scheduling Formulation

In this section, the mathematical model for batch plant scheduling proposed by Ierapetritou and Floudas (1998) is adopted. It follows the main idea of event based continuous time formulation and involves the following constraints:

$$\min H \quad \text{or} \quad \max \sum_{s,n} price_s d_{s,n} \tag{1}$$

$$\text{subject to} \quad \sum_{i\in I_j} wv_{i,j,n} \leq 1 \tag{2}$$

$$st_{s,n} = st_{s,n-1} - d_{s,n} - \sum_{i\in I_j} \rho^P_{s,i} \sum_{j\in J_i} b_{i,j,n} + \sum_{i\in I_j} \rho^c_{s,i} \sum_{j\in J_i} b_{i,j,n-1} \tag{3}$$

$$st_{s,n} \leq st^{\max}{}_s \tag{4}$$

$$v^{\min}_{i,j} wv_{i,j,n} \leq b_{i,j,n} \leq v^{\max}_{i,j} wv_{i,j,n} \tag{5}$$

$$\sum_n d_{s,n} \geq r_s \tag{6}$$

$$Tf_{i,j,n} = Ts_{i,j,n} + \alpha_{i,j} wv_{i,j,n} + \beta_{i,j} b_{i,j,n} \tag{7}$$

$$Ts_{i,j,n+1} \geq Tf_{i,j,n} - U(1 - wv_{i,j,n}) \tag{8}$$

$$Ts_{i,j,n} \geq Tf_{i',j,n} - U(1 - wv_{i',j,n}) \tag{9}$$

$$Ts_{i,j,n} \geq Tf_{i',j',n} - U(1 - wv_{i',j',n}) \tag{10}$$

$$Ts_{i,j,n+1} \geq Ts_{i,j,n} \tag{11}$$

$$Tf_{i,j,n+1} \geq Tf_{i,j,n} \tag{12}$$

$$Ts_{i,j,n} \leq H \tag{13}$$

$$Tf_{i,j,n} \leq H \tag{14}$$

In the above formulation, allocation constraints (2) state that only one of the tasks can be performed in each unit at an event point (n). Constraints (3) represent the material balances for each state (s) expressing that at each event point (n) the amount $st_{s,n}$ is equal to that at event point (n-1), adjusted by any amounts produced and consumed between event points (n-1) and (n), and delivered to the market at event point (n). The storage and capacity limitations of production units are expressed by constraints (4) and (5). Constraints (6) are written to satisfy the demands of final products. Constraints (7) to (14) represent time limitations due to task duration and sequence requirements in the same or different production units. Parameters $\alpha_{i,j}$ and $\beta_{i,j}$ are defined as: $\alpha_{i,j} = \frac{2}{3}\overline{T}_{i,j}$, $\beta_{i,j} = \frac{2}{3}\overline{T}_{i,j} / (v^{\max}_{i,j} - v^{\min}_{i,j})$ wher $\overline{T}_{i,j}$ is mean processing time of task (i) in unit (j). This is based on the assumption that there is 33% variability of the processing time around the mean value to accommodate different batch sizes, although different processing times functions can be easily adapted. When $wv_{i,j,n}$ equals to 0, the last two terms in constraints (7) are equal to zero due to capacity constraints. Otherwise, the last two terms are added to $Ts_{i,j,n}$. Therefore, the duration of task (i) at unit (j) at event point (n) depends on the amount of material being processed. The remaining timing constraints (8) - (14) represent the production recipe constraints and should be satisfied to impose the correct task sequence.

There is a lot of discussion in the literature recently regarding different modeling attempts of the deterministic scheduling problem. Maravelias and Grossmann (2003) discussed different time representation schemes and proposed a general continuous time MILP formulation for the short-term scheduling of multipurposes batch plants. In this chapter, we select the above presented model since it has been shown to perform well for different case studies. However, the approach as presented in this paper to address the issue of uncertainty can be utilized independent of the scheduling formulation adopted.

2.2 Multiobjective Robust Optimization Model

In the proposed model, demand uncertainty is described by a number of scenarios (k), each of which is associated with probability p^k. The optimal schedule of the deterministic scheduling formulation presented in the previous subsection will be robust with respect to optimality if it remains close to the optimal solution for any realization of scenario $k \in K$. This solution is called *solution robust*. The schedule is also robust with respect to feasibility if it remains almost feasible for any realization of k, which is called *model robust*. Our aim is to find robust schedules in the face of uncertainty that can help the decision maker to select the optimal solution.

In order to incorporate these two objectives, a multiobjective robust optimization formulation is proposed, which has the following form for the case of uncertain demands:

$$\min \begin{bmatrix} \sum_k p^k H^k \\ \sum_{s,k} p^k slack_s^k \\ \sum_k p^k \Delta^k \end{bmatrix} \tag{15}$$

subject to $\sum_{i \in I_j} wv_{i,j,n} \le 1$ (16)

$$st_{s,n}^k = st_{s,n-1}^k - d_{s,n}^k - \sum_{i\in I_j} \rho_{s,i}^P \sum_{j \in J_i} b_{i,j,n}^k + \sum_{i\in I_j} \rho_{s,i}^c \sum_{j\in J_i} b_{i,j,n-1}^k \tag{17}$$

$$st_{s,n}^k \le st^{\max}{}_s \tag{18}$$

$$v_{i,j}^{\min} wv_{i,j,n} \le b_{i,j,n}^k \le v_{i,j}^{\max} wv_{i,j,n} \tag{19}$$

$$\sum_n d_{s,n}^k + slack_s^k \ge r_s^k \tag{20}$$

$$Tf_{i,j,n}^k = Ts_{i,j,n}^k + \alpha_{i,j} wv_{i,j,n} + \beta_{i,j} b_{i,j,n}^k \tag{21}$$

$$Ts_{i,j,n+1}^k \ge Tf_{i,j,n}^k - U(1 - wv_{i,j,n}) \tag{22}$$

$$Ts_{i,j,n}^k \ge Tf_{i',j,n}^k - U(1 - wv_{i',j,n}) \tag{23}$$

$$Ts_{i,j,n}^k \ge Tf_{i',j',n}^k - U(1 - wv_{i',j',n}) \tag{24}$$

$$Ts_{i,j,n+1}^k \ge Ts_{i,j,n}^k \tag{25}$$

$$Tf_{i,j,n+1}^k \ge Tf_{i,j,n}^k \tag{26}$$

$$Tf_{i,j,n}^k \le H^k \tag{27}$$

$$\Delta^k \ge H^k - \sum_k p^k H^k \tag{28}$$

$$\Delta^k \ge 0,\ H^k \le U \tag{29}$$

The first objective is minimizing the expected makespan, which is derived from the original objective in deterministic formulation. Model robustness is represented by the second objective that minimizes the expected unsatisfied demands, which is computed by introducing the artificial variables *slack^k(s)* in the demand constraints (20).

Standard Deviation (SD) is one of the most commonly used metrics to evaluate the robustness of a schedule. To evaluate the SD, the deterministic model with a fixed sequence of tasks $wv_{i,j,n}$ is solved for different realizations of uncertain parameters that define the set of scenarios k which results in different makespans H_k. The SD is then defined as:

$$SD_{avg} = \sqrt{\sum_k \frac{(H_k - H_{avg})^2}{P_{tot} - 1}}\ ,\ H_{avg} = \frac{\sum_k H_k}{P_{tot}}$$

where H_{avg} is the average makespan over all the scenarios, and p_{tot} denotes the total number of scenarios. A detailed discussion of different robustness metrics can be found in Samsatli et al. (1998). Vin and Ierapetritou (2001) proposed a robustness metric taking into consideration the infeasible scenarios. In case of infeasibility, the problem is solved to meet the maximum demand possible by incorporating slack variables in the demand constraints. Then the inventory of all raw materials and intermediates at the end of the schedule are used as initial conditions in a new problem with the same schedule to satisfy the unmet demand. The makespan under infeasibility H_{corr} is determined as the sum of those two makespans. Their proposed robustness metric is defined as: $SD_{corr} = \sqrt{\sum_k \frac{(H_{act} - H_{avg})^2}{P_{tot} - 1}}$ where $H_{act} = H_k$, if scenario k is feasible and $H_{act} = H_{corr}$, if scenario k is infeasible. The concept of upper partial mean (UPM) introduced by Ahmed and Sahinidis is used in the third objective function in order to optimize the solution robustness. They define the variance measure $\overline{\Delta}$ as follows: $\overline{\Delta} = \sum_k p^k \Delta^k \quad \Delta^k = \max\{0, H^k - \sum_k p^k H^k\}$

where Δ^k corresponds to the positive deviation of makespan under scenario k from the expected value.

The main advantage of using UPM instead of variance is that it can avoid introducing nonlinearities in the formulation. Thus, the resulting model remains a mixed-integer linear programming (MILP) problem.

Comparing to the deterministic problem, in this formulation, the binary variables $wv_{i,j,n}$ that represent the task sequences remain the same over all scenarios, while the continuous variables that correspond to the batch sizes, and the starting and finishing times can vary to accommodate the realization of different scenarios. Thus, the schedules obtained by solving this multiobjective optimization problem include robust assignments that can accommodate the demand uncertainty.

Note that this robust optimization model is written for a general batch plant scheduling problem where the objective is to minimize the makespan. However, other scheduling problems can have different objectives and constraints. In these cases, the above formulation has to be modified to accommodate the different objectives.

2.3 Normal Boundary Intersection

NBI is a solution methodology developed by Das and Dennis (1998) for generating Pareto surface in nonlinear multiobjective optimization problems. It is proved that this method is independent of the relative scales of the objective functions and is successful in producing an evenly distributed set of points in the Pareto surface given an evenly distributed set of parameters, which is an advantage compared to the most common multiobjective approaches - weighting method and the ε-constraint method.

The *anchor point* F_i*, is obtained when the *ith* objective is minimized independently, while f_i* represents the individual minima of the *ith* objective. The shadow minimum (utopia point) F*, is defined as the vector containing the individual global minima of the objectives, i.e. $F^* = [f_1^*, f_2^*, ..., f_n^*]^T$.

2.4 Robust Scheduling

The basic steps of NBI in the context of robust production scheduling are as follows:

Step 1: Determine the anchor points: The robust optimization model for scheduling problems as presented in section 2.2 has three objectives, which are the expected value of makespan, unsatisfied demand (model robustness), and the upper partial mean of the makespan (solution robustness). In order to determine the anchor points, the robust optimization formulation is solved with one objective function being minimized each time. The expected makespan, model robustness, and solution robustness is minimized with respect to constraints (16) - (29) individually, and the minimum value and the values of the other two objectives are saved. Since the makespan requirement is imposed through the inequality in constraint (27), when the problem is solved to minimize the model robustness or solution robustness, the makespan that corresponds to each scenario H^k obtained may not be equal to the finishing time of the last task. Thus, in order to get the optimal value of expected makespan at the anchor points, if model or solution robustness is optimized first, the following step is required.

Step 2: Tighten the anchor points: When model or solution robustness is minimized first, they are fixed at the optimal values and the problem of minimizing the expected makespan is solved again. Thus, the resulting points are the real anchor points that contain the optimal value of the expected makespan corresponding to the finishing time of the last performed task and utopia point F^* is correctly determined.

Step 3: Formulate and solve problem (NBI_ω) iteratively for different values of ω.

The convex hull of individual minima (CHIM) has the following definition: let x_i^* be the respective minimizer of $f_i(x), i = 1, \ldots, n$ for $x \in C$. Let $F_i^* = F(x_i^*), i = 1, \ldots, n$, Φ be the $n \times n$ matrix whose i^{th} column is $F_i^* - F^*$. Then the set of points in ∂R^n that are convex combinations of $F_i^* - F^*$, i.e., $\{\Phi\omega : \omega \in \partial R^n, \sum_i \omega_i = 1, \omega_i \geq 0\}$ is referred to as the CHIM. The set of attainable objective vectors: $\{F(x) : x \in C\}$ is denoted by *Φ* so C is mapped onto *Φ* by F. The space ∂R^n which contains *Φ* is referred to as objective space. The boundary of *Φ* is denoted by $\partial \Phi$. NBI method determines the portion of $\partial \Phi$ which contains the Pareto optimal points solving problem (NBI_ω). The principal idea behind this approach is that the intersection point between the boundary $\partial \Phi$ and the normal pointing towards the origin ($\Phi\omega + t\hat{n}$, where ω is a convex weighting) emanating from any point in the CHIM (*Φω* is a point on the portion of $\partial \Phi$ containing the efficient points. This point is guaranteed to be a Pareto optimal point if the trade-off surface is convex. Each of the points represents a trade-off solution between the expected performance, feasibility and deviation from the mean.

3. PARAMETRIC MILP APPROACH

As mentioned in the introduction for the case where there is not enough information about uncertainty characteristics, parametric MILP can be used to generate alternative schedules that can be then evaluated in the face of uncertainty. In this section, the parametric MILP problem is discussed.

For the general mixed integer problem:

$$\min z = cx$$

$$\text{subject to} \quad Ax \geq \theta \qquad \text{(P1)}$$

$$x \geq 0, \quad x_j \text{ integer}, \ j = 1,..,k$$

Assuming a perturbation of problem RHS parameter values such that: $Ax \geq \theta + \Delta\theta$

The aim of is to investigate the effect of Δθ on the optimal solution *x* and objective value *z*.

3.1 Single Uncertain Parameter

For the case of single uncertain parameter, the proposed approach follows the basic ideas of the interactive reference point approach proposed by Alves and Climaco (2000) presented for multiple objective MILP problems. The proposed framework is shown in Figure 1.

First the problem is solved at the nominal values of the uncertain parameters using a branch and bound solution approach, and the dual information λ^p, z^p is collected at each leaf node.

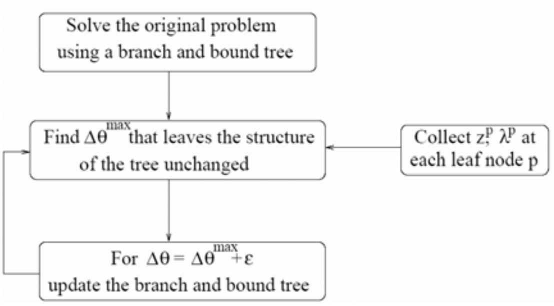

Figure 1. Flow chart of the proposed approach

Assuming that the optimal solution is found at node 0, the LP sensitivity analysis is then performed at node 0 to determine the range $\Delta\theta^{basis}$ within which the current optimal basis does not change.

We need to find the perturbation $\Delta\theta^{max}$ beyond which the structure of the branch and bound may not remain the same. $\Delta\theta^{max}$ can be found through the following equation: $\Delta\theta^{\max} = \min\{\Delta\theta^{basis}, \min\{\frac{z^p - z^0}{\lambda^0 - \lambda^p}\}\}$:

where z^0 and λ^0 are the objective value and dual multiplier at the optimal node 0, respectively. Note that only the positive $\frac{z^p - z^0}{\lambda^0 - \lambda^p}$ need to be considered, because the negative one means that node p can never provide a better solution than node 0 at a certain point.

3.2 Multiple Uncertain Parameters

This subsection presents the detailed steps (Figure 2) of the proposed approach to deal with the case of multiple uncertain parameters. Assuming for simplicity in the presentation that we want to investigate two parameters, θ_a and θ_b, changing in the range of $[a_0, a_0 + \Delta a]$ and $[b_0, b_0 + \Delta b]$. The MILP problem is first solved at (a_0, b_0) using branch and bound algorithm and the optimal solution is found at node 1 (Figure 3). Other leaf nodes of the B&B tree are denoted as node 2, node 3, ..., node n. Note that only the information at the leaf nodes is required.

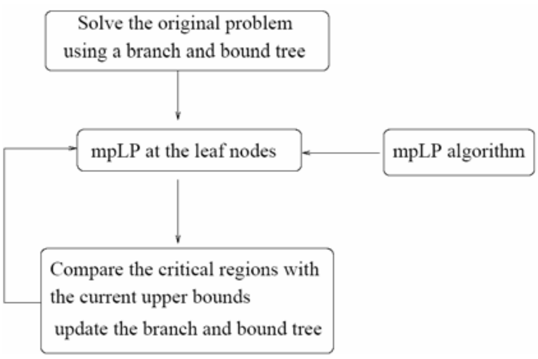

Figure 2. Flow chart of proposed approach for

multiple uncertain parameters case

This is true since if at another set of uncertain parameters (a', b'), there exists a new optimal solution, it can always be uncovered by checking or continuing the branching procedure on the current leaf nodes. Let's assume for example that the new optimal solution can be provided by a non-leaf node (node A). With the original data, the relaxed LP problem of node A must have a partial integer solution, otherwise it is a leaf node. With the perturbed data, the LP problem of node A gives the optimal integer solution. According to our proposed method, all the current leaf nodes are examined that include the subsequent nodes of node A (node 2 and 3). Apparently, if node A yields an integer solution, either node 2 or 3 should provide that solution too. Thus, it is true that only the leaf nodes need to be examined at each iteration.

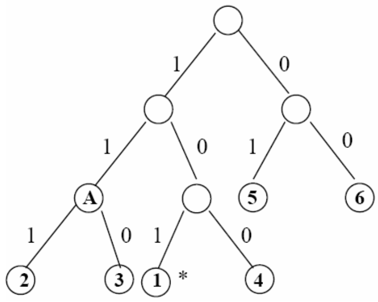

Figure 3. Branch and bound tree

Then the multiparametric linear programming is solved at each of the leaf nodes including node 1, so as to identify the optimal value functions and their corresponding critical regions in the region of $[a_0, a_0 + \Delta a]$ and $[b_0, b_0 + \Delta b]$. In this work, a new algorithm is proposed for the solution of mpLP. When the mpLP procedure is completed, the output will be a set of optimal functions $z = z^k + \lambda^k\theta_a + \beta_k\theta_b$, $k = 1, \ldots, K$, where K is the number of critical regions. For any point (θ_a, θ_b) in the range of $[a_0, a_0 + \Delta a]$ and $[b_0, b_0 + \Delta b]$, the objective value cx^* of the relaxed LP problem of that node can be expressed by $\max\{z^k + \lambda^k\theta_a + \beta_k\theta_b, k = 1, \ldots, K\}$. If the procedure is not complete, then there must exist a point (θ_a, θ_b), such that $\max_k\{z^k + \lambda^k\theta_a + \beta_k\theta_b\}$ is less than cx^*. Thus a bilevel programming problem is formulated as shown in problem (P2). It is proved that linear bilevel programming problems (BLPP) are strongly NP-hard (Bard 1998). In order to avoid solving a BLPP, we propose to first convert the relaxed LP problems (inner problem in (P2)) at the leaf nodes to its dual form, so that the uncertain parameters appear in the objective function and substitute the inner problem in problem (P1).

$$\max \quad \{\min cx \mid Ax \geq \theta\} - z \qquad \text{(P2)}$$

$$\text{subject to} \quad z \geq z^{(k)} + \lambda^{(k)}\theta_a + \beta^{(k)}\theta_b, k = 1,..K$$

$$a_0 \leq \theta_a \leq a_0 + \Delta a$$

$$b_0 \leq \theta_b \leq b_0 + \Delta b$$

In problem (P3), the objective function is to maximize the gap between the optimal objective value θy at any point in the uncertain range and the maximum value of the optimal function, which is $\max_k \{z^k + \lambda^k \theta_a + \beta_k \theta_b\}$. Note that the problem is nonlinear due to the bilinear term in the objective function. The constraints contain the original constraints and the current optimal functions $z = z^k + \lambda^k \theta_a + \beta_k \theta_b$, hence all the constraints are linear. If the objective value of the (P3) model is nonzero, it means that there exists at least one point (θ_a, θ_b) at which its real objective value cannot be represented by any of the current objective value functions. Therefore, the objective value function at that point is $z = z' + \lambda' \theta_a + \beta' \theta_b$ and should be included in the next iterations. This procedure terminates when the objective value for problem (P3) is 0, which means that the entire uncertain parameter range is covered by the existing objective value functions. Since (P3) is a nonconvex problem, a global optimization algorithm should be utilized such as GAMS/BARON (Sahinidis, 1996), which relies on *branch-and-reduce* algorithm. Therefore, by performing mpLP at each leaf node p, a number of critical regions (k), $CR_p^1, CR_p^2, \ldots, CR_p^K$ are identified and in each $CR_p^k, k = 1, \ldots, K$, the optimal value z_p^{*k} is expressed as $z_p^{*k} = z_p^k + \lambda_p^k \theta_a + \beta_p^k \theta_b$. The next step is to update the B&B tree. The main procedure involves to compare the critical regions of the leaf nodes with the current upper bounds and finally identify a set of new critical regions, and their corresponding objective function values and optimal integer solutions. At the beginning, the upper bounds CR_p^{UB} are set to be the critical regions of the current optimal node (node 1), which are $CR_1^{(1)}, CR_1^{(2)}, \ldots, CR_1^{(K)}$. Assuming that we want to compare critical regions CR_1^{UB} and CR_2^{UB}, which have intersection CR^{int}, the following constraint is defined: $z_1^{UB} \geq z_2^{*2}$ and a redundancy test for this constraint is solved in CR^{int} as shown in problem (P4) (Acevedo and Pistikopoulos 1997). The solution of this problem provides the optimal functional form in CR^{int}.

$$\max \ \theta y \qquad \text{(P3)}$$
$$\text{subject to} \quad A^T y \leq c$$
$$a_0 \leq \theta_a \leq a_0 + \Delta a$$
$$b_0 \leq \theta_b \leq b_0 + \Delta b$$
$$y \geq 0$$

$$\Downarrow$$

$$\max \ \theta y - z$$
$$\text{subject to} \quad A^T y \leq c$$
$$z \geq z^{(k)} + \lambda^{(k)} \theta_a + \beta^{(k)} \theta_b, k = 1, \ldots K$$
$$a_0 \leq \theta_a \leq a_0 + \Delta a$$
$$b_0 \leq \theta_b \leq b_0 + \Delta b$$
$$y \geq 0$$

At each iteration, the new leaf nodes in the updated B&B tree will be compared to the current upper bounds, so as to determine the new optimal functions in their intersected region. This procedure stops when no further branching is required and the uncertainty analysis of the entire uncertain space can be presented by a number of critical regions that contain their corresponding optimal functions and integer solutions.

$$\max \ \varepsilon \qquad \text{(P4)}$$
$$\text{subject to} \quad z_1^{UB} = z_2^{*(2)} + \varepsilon$$
$$z_1^{UB} = z_1^{UB} + \lambda_1^{UB} \theta_a + \beta_1^{UB} \theta_b$$
$$z_2^{(2)} = z_2^{(2)} + \lambda_2^{(2)} \theta_a + \beta_2^{(2)} \theta_b$$
$$b_0 \leq \theta_b \leq b_0 + \Delta b$$
$$\theta_a, \theta_b \in CR^{ubt}$$

Comparing to the existing approach (Acevedo and Pistikopoulos 1997), the proposed method solves the mpLP at only the leaf nodes in the B&B tree instead of every node during the branch and bound procedure, and consequently reduces the computational efforts significantly as will be shown in the preliminary results in the next section. Moreover, the new mpLP approach can efficiently determine the optimal function with respect to the uncertain parameters and the critical regions without having to retrieve the optimal tableaus and investigate the neighboring bases.

4. CASE STUDY

In this section a case study is presented and the results evaluated to assess the viability and efficiency of the proposed approach. High quality solutions were found efficiently, which provides confidence that the proposed approach will also be effective on new problems and extensions.

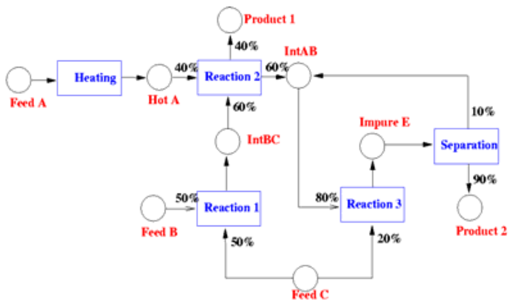

Figure 4. STN for example problem

To present the main steps, the first example is considered here as described through the STN representation in Figure 4. The data for this example can be found in Ierapetritou and Floudas (1997). The problem is solved at the initial demand value (50). A branch and bound tree is constructed to determine the optimal schedule, which is found to be schedule 1 with makespan 7.04 hours. It is provided by two nodes 1A and 1B that represent equivalent schedules. Performing linear sensitivity analysis on the optimal nodes, we get $\Delta\theta^{max} = 6.92$ which is the change allowed in the demand for which the B&B structure remains the same. For a slight change in $\Delta\theta = \Delta\theta^{max} + \varepsilon = 7$, nodes 1A(B) still yield optimal solution with objective value of 7.08 hours, but the basis changes. For the second iteration, LP sensitivity analysis is performed on nodes 1A(B). This results in $\Delta\theta^{basis}$=26.03, which is the value of change of demand where the basis remains unchanged, and there is no leaf node at which this value is intersected which is determined by examining the value of $(z^p - z^0)/(\lambda^0 - \lambda^p)$ where z^p is the objective value at node p and λ^p the corresponding lagrange multiplier, and found to be larger than 26.03 for all leaf nodes. Therefore $\Delta\theta^{max} = 26.03$. For a small perturbation away from this value $\Delta\theta = \Delta\theta^{max} + \varepsilon = 27$, the tree is updated and the optimal solution is provided by nodes that correspond to equivalent schedules 2A(B, C, D). Nodes 2A(B, C, D) are intersected by another two nodes 3A(B) in the next iteration, then nodes 3A(B) continue to provide the optimal schedule but with a different basis in the following iteration. After that, the problem becomes infeasible when the demand is greater than 87.5. The three operations schedules are presented in Figure 5 and Figure 6 presents how the makespan and optimal schedule change with the demand.

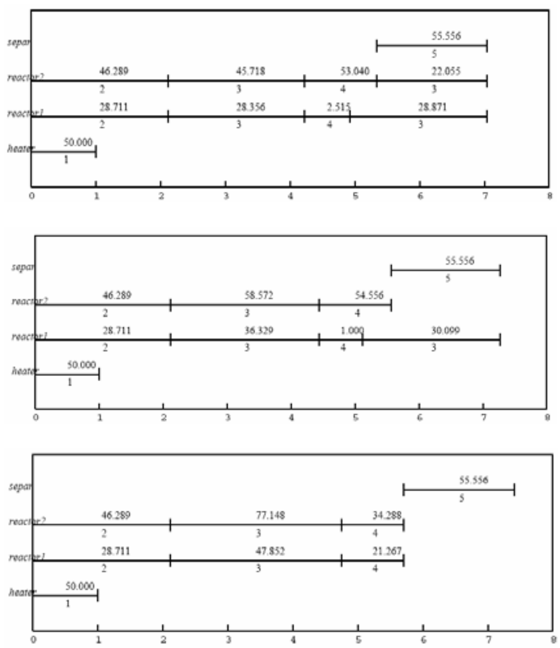

Figure 5: Gantt charts of schedules 1,2,3

For the multiobjective approach, the nominal demand for both products 1 and 2 is 80 and is assumed to exhibit a variability of ±50%. 5 scenarios (40, 60, 80, 100, 120) are selected to represent the uncertain demand for each product and thus result to a total of 25 scenarios. 10% demand satisfaction is also assumed for this example.

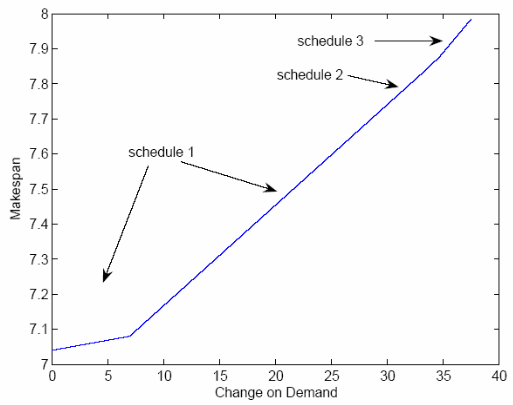

Figure 6. Parametric solution for example problem

Following the proposed approach presented in Section 3.2, the individual minimum points are obtained as follows: $f_1(x^*) =$ (5.005, 143.65, 0.045), $f_2(x^*) =$ (10.56, 0, 0.696), $f_3(x^*) = (5.236, 143.55, 0)$. Therefore, the utopia point is $F^* = (5.055, 0, 0)$ and the matrix $\Phi = \begin{pmatrix} 0 & 5.501 & 0.181 \\ 143.65 & 0 & 143.55 \\ 0.045 & 0.696 & 0 \end{pmatrix}$. In order to generate different values of ω, let's assume that for a n-objective problem, δ_j is the uniform spacing between two consecutive ω_j values for $j = 1, \ldots, n-1$. The possible values that can be taken by ω_1 are: $[0, \delta_1, 2\delta_1, \ldots, 1]$. Given a particular value of ω_1, $i = 1, \ldots, j-1$, the possible values of ω_j, $j = 1, \ldots, n-1$ are: $[0, \delta_j, 2\delta_j, \ldots, k_j\delta_j]$ where $k_j = I\left[\frac{1 - \sum_i \omega_i}{\delta_j}\right]$. The last component of ω_n is defined as: $\omega_n = 1 - \sum_i \omega_i$. For this example the step sizes are chosen to be $\delta_1 = 0.1$ and $\delta_2 = 0.05$, and NBI_ω problem is formulated and solved for different values of ω. The resulting Pareto optimal surface is shown in Figure 7, which contains 8 different schedules. Taking a closer look at the optimal Pareto solutions, a number of interesting observations can be made. For example, focusing on two points A and B as shown in Figure 6 point A which is obtained with ω= (0, 1, 0) is in the area of solutions that prefer model robustness. The three objective values for this point are 10.56, 0, 0.70 for expected makespan, model robustness, and solution robustness, respectively. On the other hand, point B represents the optimal solution for ω = (0.6, 0.4, 0), which corresponds to a different schedule. Comparing to the schedule A, this solution corresponds to a decision that favors the expected makespan and solution robustness, the values of which are 6.82 and 0.25, respectively, at the expense of low model robustness, which is 64.39. For the nominal demand of (80, 80), schedule A requires 9.83hr and schedule B prefers having a shorter makespan of 8.46hr. However, at the maximum demand value (120, 120), schedule A focuses more on meeting the demands and can produce the required amount within 13.32hr, while schedule B results in an unsatisfied amount of 33.33 units for product 1 and 32.25 units for product 2.

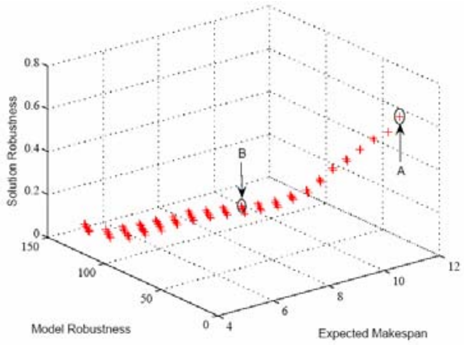

Figure 7. Pareto set of solutions for example 1

These results indicate that the proposed methods can be extended to meet all research objectives. The parametric analysis generates alternative solutions to cover the uncertainty space whereas the multiobjective optimization provides solutions according to decision maker's position towards risk.

5. CONCLUSIONS AND FUTURE WORK

A multiobjective robust optimization model is proposed to deal with the problem of uncertainty in scheduling considering the expected performance, model robustness and solution robustness. NBI technique is utilized to solve the multiobjective model and successfully produce Pareto optimal surface that captures the trade-off among different objectives in the face of uncertainty.

The issue is also addressed through parametric MILP analysis. An integrated framework is developed that allows the parameters in the RHS of the MILP formulation to vary independently. It mainly consists of two steps: LP/mpLP sensitivity analysis and updating the B&B tree. For the case of mpLP, a novel algorithm is proposed which solves a set of NLP problems iteratively using the commercially available global optimization solver BARON.

The work can be further extended to investigate the cases where preferences exist among the objectives, so as to generate more meaningful Pareto optimal solutions. This will help reducing the computational complexity of the proposed approach. In addition, there are cases that instead of unique anchor points, anchor curves are found due to the fact that the objectives are not entirely conflicting with each other. For these cases, it will be of interest to study how the selection of anchor points can affect the Pareto surface.

The parametric MILP approach can be further developed to enable the analysis of uncertainty in the constraints coefficients and the case that uncertainty exists in the objective function coefficients, constraints coefficients and the RHS parameter at the same time. In that case, a linear bilevel programming problem, which is similar to (P2), will be formed and solved using appropriate algorithms.

Acknowledgement

The authors gratefully acknowledge financial support from the National Science Foundation under the NSF CAREER program CTS-9983406.

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