

## Optimal Production Scheduling of Gases under Uncertainty with Flexibility Constraints

M. Paz Ochoa<sup>a\*</sup>, Hao Jiang<sup>a,b</sup>, Ajit Gopalakrishnan<sup>c</sup>, Irene Lotero<sup>c</sup>, Ignacio E. Grossmann<sup>a</sup>

<sup>a</sup>*Carnegie Mellon University, 5000 Forbes, Pittsburgh, PA 15213, U.S.A*

<sup>b</sup>*Tsinghua University, 30 Shuangqing Rd, Beijing 100084, P.R. China*

<sup>c</sup>*Air Liquide, 200GBC Drive, Newark, DE 19702 U.S.A*

*mchoa@andrew.cmu.edu*

### Abstract

In this work, we address the scheduling problem under uncertainties in electricity price and product demand in an air separation plant. The operation of the plant is represented by an efficient discrete-time MILP model as a process state transition network in order to deal with short-term production scheduling. On the one hand, uncertainties in electricity are addressed with stochastic programming techniques to find a schedule that minimizes expected cost over a proposed set of scenarios. On the other hand, uncertainties in product demand are tackled as flexibility constraints in order to ensure flexible operation over the entire range of variation of this uncertain parameter.

**Keywords:** Optimal schedule under uncertainty, power-intensive processes, two-stage stochastic programming, flexibility analysis.

### 1. Introduction

Demand side management is critical for maintaining profitability, especially in industrial power intensive processes where operating cost can be reduced by adjusting the production schedule to time-dependent electricity pricing schemes. However, uncertainty in these systems not only arises from electricity price but also from product demand.

Stochastic programming is the framework that models mathematical programs with uncertainty by optimizing the expected value over the possible realizations (Birge and Louveaux, 2011). The expected value is computed by integrating over the set of uncertain parameters. A simplification of this calculation involves a discretization of the uncertainty sets, where the realizations can be characterized with a finite number of scenarios. The most common stochastic programs that consider recourse is the Mixed-Integer Linear Programming (MILP) with continuous recourse in a second stage. The two-stage stochastic programming formulation considers two types of decisions: first stage, made before uncertainty reveals, and second stage, independent for each scenario.

Stochastic programming has found applications in process synthesis. For example, Halemane and Grossmann (1983) presented a two-stage approach for the design of flexible processes under uncertainty. The design problem is formulated to minimize a cost function and to guarantee feasible operation over a polyhedral uncertainty set.

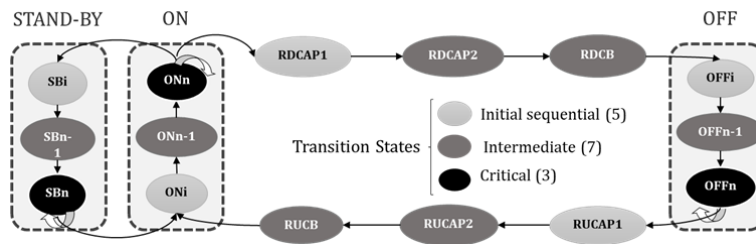
The design of robust or flexible chemical processes under uncertainty has been dominated by the concept of flexibility analysis, which was first proposed and then

further developed by Grossmann and co-workers, a description of its historical development can be found in Grossmann et al. (2016). Recently, Zhang et al. (2016) presented insights on the strong connection between flexibility analysis and robust optimization.

The basic idea of flexibility analysis is to consider explicitly uncertainties in chemical processes. In general, the study of the flexibility can be performed at different stages. First at the design stage, where the optimization models for process design explicitly include flexibility constraints. Then with fixed design variables, to evaluate if certain design can tolerate the uncertainties in a specified range, known as the flexibility test problem. Finally, to quantify the range of uncertainties that the design can tolerate, called the flexibility index problem.

In this work, we propose a novel approach for the optimal production schedule with flexibility constraints, an analogous approach for the design of flexible processes under uncertainty proposed by Halemane and Grossmann (1983). We deal with uncertainties in electricity price and product demand in a production scheduling model of an air separation plant (Basán et al., 2017). Operation is represented by a discrete-time MILP model as a process state transition network, a scheme of the states can be seen in Fig. 1. We propose to explore the use of stochastic programming to account for uncertainties in electricity price in order to find the optimal production schedule that minimizes expected cost over a given set of scenarios. A two-stage stochastic programming problem is formulated considering the plant state binary variables as first-stage and the operation variables, such as power consumption, production and inventory levels, as second-stage.

Moreover, we address uncertainty in product demand so as to achieve robustness. We consider flexibility constraints to ensure flexible operation over the entire range of this parameter values. To obtain a flexible schedule with respect to product demand, the two-stage stochastic model evaluated at discrete electricity price scenarios with flexibility constraints need to satisfy the flexibility test. The test is evaluated with two different methodologies: affinely adjustable robust optimization and an iterative framework based on a dual-based flexibility analysis (Zhang et al., 2016). Once a flexible schedule is obtained, we calculate the flexibility index with both approaches to obtain a measure of the flexibility that can actually be achieved. We illustrate the application of the proposed models with a number of examples that show the effectiveness of the proposed approach for handling the uncertainties.



**Figure 1.** Process Transition Network (Basán et al., 2017).

## 2. Problem Statement and Methodology

The main objective is to minimize the expected value of the optimal cost function by selecting schedule variable  $s$  over the entire region  $T$ , which is the uncertainty set. First, the scheduling model corresponds to a MILP of the general form (see Basán *et al.*, 2017):

$$\min c^T x + d^T y \quad (1)$$

$$s.t. \quad Ax + By \leq d, x \geq 0, y = \{0,1\} \quad (2)$$

In order to represent the feasible region of operation, the model is expressed as:  $f(s, z, \theta) \leq 0$ , where  $s$  correspond to the 0-1 scheduling variables,  $z$  are the control variables and  $\theta$  the uncertain parameters. The problem of optimal schedule under uncertainty corresponds to a two-stage programming problem, leading to an infinite programming problem because the feasibility constraint must be satisfied for the whole range of variation of  $\theta$ .

$$\min_s \mathbb{E}_{\theta \in T} \left\{ \left( \min_z c(s, z, \theta) \mid f(s, z, \theta) \leq 0 \right) \right\} \quad (3)$$

$$s.t. \quad \forall \theta \in T \{ \exists z (\forall j \in J [f_j(s, z, \theta) \leq 0]) \} \quad (4)$$

The flexibility test problem states that for every point  $\theta \in T$  there must exist at least one value of the vector control variable  $z$  that gives rise to non-positive values for all the individual constraint functions  $j$ . This means that irrespective of the actual values taken by the bounded parameters  $\theta$ , the plant schedule  $s$  has the flexibility of operating to satisfy the specifications. A first simplification involves the discretization over the parameter space in order to approximate the expected cost by a weighted cost function. By using global maximum and minimum operators and inductive reasoning Halemene and Grossmann (1983), derived an equivalent multilevel optimization for the logical condition (4):  $\max_{\theta \in T} \min_z \max_{j \in J} f_j(s, z, \theta)$ .

The optimal schedule with flexibility analysis is then:

$$\min_{s, z_1, z_2, \dots, z_n} \sum_{i=1}^n \varphi_i \cdot c(s, z_i, \theta_i) \quad (5)$$

$$s.t. \quad f(s, z_i, \theta_i) \leq 0, i = 1, 2, \dots, n \quad (6)$$

$$\max_{\theta \in T} \min_z \max_{j \in J} f_j(s, z, \theta) \leq 0 \quad (7)$$

where  $\varphi_i$  are discrete probabilities or weights for the selected finite number of parameter points  $\theta_i$ . To solve the optimal schedule for the air separation plant with flexibility demand constraints we address two approaches: dual-based flexibility analysis (DFA) and adjustable robust optimization (AARO) following Zhang *et al.* (2016).

### 2.1. Schedule with Flexibility Constraints

Consider a set of  $m$  inequality constraints

$$f_j(s, z, \theta) = a_j s + b_j z + c_j \theta \leq 0 \quad \forall j \in J \quad (8)$$

where  $s \in \mathbb{R}^{n_s}$  are schedule variables,  $z \in \mathbb{R}^{n_z}$  are control variables and  $\theta \in \mathbb{R}^{n_\theta}$  are uncertain parameters,  $a_j$ ,  $b_j$  and  $c_j$  are row vectors, and  $J$  is the set of constraints.

**Table 1.** DFA and AARO formulation for the scheduling problem under uncertainty and for flexibility index.

Schedule problem with Dual-based Formulation	Schedule problem with AARO Formulation
$\chi(s) = \max_{\lambda, \bar{\lambda}, x} s^T A^T \lambda + \sum_{j \in J} \sum_{p \in \theta} c_{jp} [\lambda_j (\theta_p^N - \Delta \theta_p^-) + \bar{\lambda}_{pj} (\Delta \theta_p^+ + \Delta \theta_p^-)]$	$\eta = \min_{d, \bar{z}, p, Q, \mu, v} \hat{c}^T s + \sum_{i \in I} \varphi_i \bar{c}^T \bar{z}_i$
$s.t. \quad \begin{aligned} e^T \lambda &= 1 \\ B^T \lambda &= 0 \\ \bar{\lambda}_{pj} &\geq (\lambda_j - 1) + x_p \quad \forall p \in \theta, j \in J \\ \bar{\lambda}_{pj} &\leq \lambda_j \quad \forall p \in \theta, j \in J \\ \bar{\lambda}_{pj} &\leq x_p \quad \forall p \in \theta, j \in J \\ \lambda &\geq 0, \bar{\lambda} \geq 0, x \in \{0,1\} \end{aligned}$	$s.t. \quad \begin{aligned} As + B\bar{z}_i + C\bar{\theta}_i &\leq 0 \quad \forall i \in I \\ a_j s + b_j p + \{(\theta^U)^T \mu_j - (\theta^L)^T v_j\} &\leq u \quad \forall j \in J \\ \mu_j - v_j &= (b_j Q + c_j)^T \quad \forall j \in J \end{aligned}$
Flexibility Index with DFA	Flexibility Index with AARO
$FI(s) = \min_{\lambda, \bar{\lambda}, x} (-As - C\theta^N)^T \lambda$	$FI(s) = \max_{p, Q, \mu, \delta} \delta$
$s.t. \quad \begin{aligned} B^T \lambda &= 0 \\ \sum_{j \in J} \sum_{p \in \theta} c_{jp} [\lambda_j \Delta \theta_p^- + \bar{\lambda}_{pj} (\Delta \theta_p^+ + \Delta \theta_p^-)] &\geq 1 \\ \bar{\lambda}_{pj} &\geq (\lambda_j + 1) + x_p \quad \forall p \in \theta, j \in J \\ \bar{\lambda}_{pj} &\leq \lambda_j \quad \forall p \in \theta, j \in J \\ \bar{\lambda}_{pj} &\leq x_p \quad \forall p \in \theta, j \in J \\ \bar{\lambda}_{pj} &\leq 0, \lambda_j \leq 0, x_p \in \{0,1\} \end{aligned}$	$s.t. \quad \begin{aligned} \delta &\geq 0 \\ a_j s + b_j p + c_j (\theta^N - \delta \Delta \theta^-) + e^T \mu_j &\leq 0 \quad \forall j \in J \\ \mu_j &\geq (b_j Q + c_j \delta (\Delta \theta^- + \Delta \theta^+))^T \quad \forall j \in J \end{aligned}$

DFA is derived using LP duality theory, considering that solution must lie in the vertices, and then applying exact linearization to bilinear terms, leading to a MILP problem. Whereas, in the AARO approach the control actions are considered affine functions of  $\theta$ , i.e.  $z(\theta) = p + Q\theta$ , which allow some degree of recourse, but leading to a restricted problem. In this reformulation, it is also assumed that the solution lies in the vertices, which is true when the constraints are jointly convex. To obtain finally the affinely adjustable robust counterpart, a constraint-wise worst-case approach and LP duality theory are applied. An advantage of this approach is that it does not add any binary variable. The final formulation of both approaches is described in Table 1. Details of the reformulation steps for both approaches can be found in Zhang *et al.* (2016).

The flexibility function  $\chi(s)$  of schedule  $s$  with respect to the uncertainty set  $T$  represent the projection of the feasible region. If  $T$  is inscribed in the projection, then  $\chi(s) \leq 0$  meaning that a feasible schedule is obtained. When  $T$  is not completely constrained in the projection, then  $\chi(s) > 0$ .

The algorithm for the DFA is based on an iterative column-and-constraint generation approach, which relies on the fact that a schedule is feasible for all  $\theta \in T$  if it is feasible for the worst-case realization of the uncertainty, which lies at one of the vertices of  $T$ . It includes the following steps:

- 1) Set  $k=0$ . Choose an initial set  $\widehat{T}_0$  of  $N_0$  critical points
- 2) Solve:

$$\eta = \min_{s, \bar{z}, \bar{z}} \hat{c}^T s + \sum_{i=1}^n \varphi_i \cdot \bar{c}^T \bar{z}_i \quad (9)$$

(10)

$$\begin{aligned}
 s.t. \quad & As + B\bar{z}_t + C\bar{\theta}_t \leq 0, \forall i \in I && \text{Electricity Price Scenarios} && (11) \\
 & As + B\hat{z}_t + C\hat{\theta}_t \leq 0, \forall t \in \hat{T}_k && \text{Product Demand Vertices}
 \end{aligned}$$

To obtain  $s_k$

- 3) Solve Problem: Dual-based Flexibility Analysis with  $S = S_k$ , Obtain critical point  $\theta_k^c$ . If  $\chi(s) \leq 0$ , Stop. Else go to step 4.
  - 4) Set  $\hat{\theta}_{k+1} = \theta_k^c$ ,  $N_{k+1} = N_k + 1$ ,  $\hat{T}_{k+1} = \{1, 2, \dots, N_{k+1}\}$ ,  $k = k + 1$ . Go to Step 2.
- The algorithm converges in a finite number of iterations, since there is a finite number of vertices. Another difference between both approaches is that AARO does not require an iterative framework.

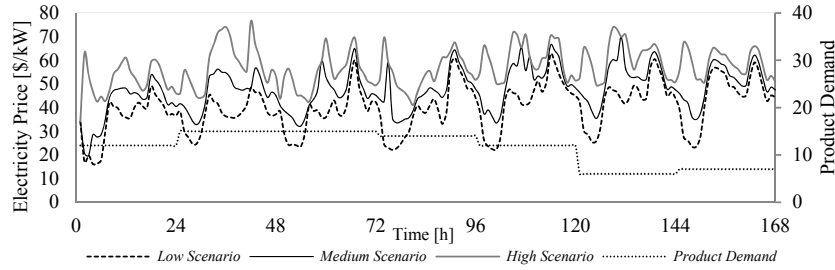
### 2.2. Flexibility Index

Consider the uncertainty set as  $T(\delta) = \{\theta: \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+\}$ , where  $\delta$  is a positive scalar,  $\Delta\theta^-$  and  $\Delta\theta^+$  negative and positive deviation from the nominal value. The flexibility index is a measure of how much flexibility can actually be achieved in the given schedule. The objective is to find the largest  $\delta$  such that by proper adjustment of control variables  $z$ , the inequalities  $f_j(s, z, \theta) \leq 0$   $j \in J$  hold for all  $\theta \in T(\delta)$ .

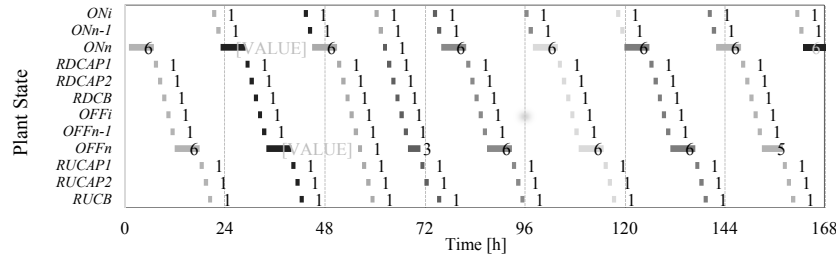
Following a similar reasoning as in the flexibility test, the flexibility index problem can be reformulated into the problems described in Table 1. If the value of  $FI > 1$ , then schedule exceeds the flexibility target, whereas when  $FI < 1$ , it does not meet the target.

## 3. Numerical Results

The presented methodology is applied to scheduling model of an air separation plant with a time horizon of 168 hours, proposed by Basán *et al.* (2017). First, the two-stage stochastic programming is applied considering the plant state (binary variables) as the first stage decision. Second stage decision are production level, inventory and power consumption. The different electricity price scenarios profiles proposed are shown in Fig. 2, together with the nominal demand profile. We should notice that vector  $\theta$  is partitioned into two subset,  $\theta_1$  for electricity prices and  $\theta_2$  for demand uncertainty.



**Figure 2.** Proposed electricity price scenarios and nominal product demand profile.



**Figure 3.** Optimal and flexible production schedule

**Table 2.** Scheduling under uncertainty with flexibility constraints and flexibility index results.

Problem	Approach	# of bin. variables	# of cont. variables	# of constraints	Result	Gap (%)	Solution Time (s)
Schedule under uncertainty	Dual-based	168	116,948	348,355	Cost 40814*	0	46
	AARO		247,218	116,779	40814		10.6
Flexibility Index	Dual-based	168	116,948	348,355	FI=1.083	0	10,739
	AARO		131,131	116,780	FI=1.083		135.6

(\*) The DFA problem converges in the first iteration.

DFA and AARO formulations lead to the same production schedule, shown in Fig. 3. In addition to, both approaches provide the same flexibility index value for the uncertain demand. This implies that the same level of flexibility can be achieved even when considering a restricted control variable as in the case of AARO. The solution time required by the AARO LP models is less compared to the DFA, especially in the case of the flexibility index with two orders of magnitude of difference, as detailed in Table 2.

#### 4. Conclusion

In this paper, we have addressed the scheduling problem under uncertainty. We proposed to deal with the uncertainty in electricity price stochastically and in product demand in a robust way by considering it as the uncertain parameter set of the flexibility constraint. We solved the problem with the dual-based flexibility analysis and affinely adjustable robust optimization formulations.

The proposed approach has allowed the efficient calculation of the optimal schedule for the expected value of electricity price profiles and feasible operation for the range of variation of product demand over a time horizon of 168 hours. In addition, flexibility indices were computed successfully with both formulations, providing a measure of feasibility of the obtained schedule. Both formulations led to the same results for the different problems, with shorter solution times for the AARO approach, in line with the results obtained by Zhang *et al.* (2016).

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