Addressing Product Demand Uncertainty: An Insight into an Ethylene Plant

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Abstract. The present work addresses the simultaneous planning of production and scheduling of the furnaces' maintenance shutdowns of an ethane-fed ethylene plant under demand uncertainty. The main processing units (eight parallel cracking furnaces) have decaying performance over time due to coke deposition inside the coils. The present Mixed Integer Nonlinear Programming (MINLP) model determines the furnaces run length between decoking procedures, as well as production and storage decisions. The objective function is to maximize the profit which includes sales, production costs, inventory costs and penalties for not meeting product demands. The higher the demand uncertainty, the more likely to unmeet the demand. Similarly, the risk of over-production rises, resulting in increased inventory requirements and costs. A two-stage stochastic programming strategy is employed with the probabilistic distribution of demands represented by a series of scenarios that are solved simultaneously.

Keywords: Optimization under Uncertainty, Stochastic Programming, Planning and Scheduling, Decaying Performance

1 Introduction

The efficient operation and the planning of the output level are crucial for surviving in competitive and changing environments. When product demand fluctuations are not accounted for properly, either unsatisfied customer demands (and loss of market share) or excessive inventory costs may occur. Therefore, a quantitative treatment of uncertain demand must consider the efficient use of the equipment and inventory which can be accomplished through simultaneously planning and scheduling. Conflicting decisions such as production and inventory levels, customer responsiveness and maintenance shutdowns must be addressed when aiming to avoid loss of market share, unnecessary inventory costs and customer demand unsatisfaction [1].

Ethylene production from ethane cracking involves cracking and quenching, compression and drying, and separation. Initially, an ethane-propane mix is cracked in furnaces to form ethylene, propylene, and other byproducts. The output is then quenched with water to prevent further reactions. The cracked gas is then compressed, cleaned, and dried. The dried gas is fed into a cold box to remove hydrogen and light hydrocarbons. The condensates from the chilling train are fed into separation columns where lights are removed and recycled, and polymer-grade ethylene is drawn as a side stream.

The cracking furnaces are the main operational units, and they present decreasing performance with time. Coke deposits on the internal coil walls during operation leading to higher heat duty requirements and/or lower conversion rates [2]. The furnaces must be frequently shutdown to perform cleaning tasks resulting in the total loss of furnace production during that period. Besides the furnaces decaying performance, an important ethane recycle also exists, both characteristics are challenges when modelling the complex interactions between the furnaces and the downstream processes (see Figure 1).

Few studies in the literature comprehensively address the optimization of decoking scheduling, operational conditions, and inventory management in the face of time-variant product demand. Schulz et al. [3] proposed a multistage MINLP model to streamline these elements in an ethylene plant operating 8 furnaces in parallel. However, their model was based on the limiting assumption of a cyclic schedule. Su et al. [4], in their work, employed a hybrid MINLP algorithm they developed earlier [5]. This algorithm facilitated faster convergence in large-scale problems compared to traditional MINLP methods. However, their model was based on basic assumptions such as constant operating flow rates and did not explore more complex models that could potentially increase the intractability of the MINLPs. Wang et al. [6] suggested a Lagrangian decomposition method to tackle the problem. Despite their algorithm yielding superior solutions compared to standard MINLP solvers, they acknowledged the challenges in achieving optimality due to the complexity of the formulation. Furthermore, this method is primarily applicable only when the underlying model exhibits a block angular structure. Lastly, Adloor and Vassiliadis [7] approached the problem from an optimal control perspective, thus avoiding the need for mixed-integer formulations and resulting in a more tractable NLP problem. However, in all these works, product demands are considered deterministic, meaning their values are perfectly known in advance.

In manufacturing processes, product demands are often uncertain at the outset of the scheduling horizon, even though many have a known distribution. It's crucial to factor in these uncertainties when formulating schedules. To preemptively address these uncertainties as the scheduling problem is solved offline, researchers have put forth various models based in robust optimization [8] and stochastic programming [9]. It is still an open question whether the incorporation of feedback and rescheduling is adequate to account for these uncertainties. In the online scheduling process that utilizes a deterministic model, the uncertainty is not explicitly modeled and it depends solely on feedback-based recourse [10]. In the case of a robust optimization model, the emphasis is on preserving feasibility, and typically, bounds on the uncertain parameters are employed, leading to conservative optimization decisions in the solution, regardless of the actual uncertainty realization. When employing the stochastic programming model, a set of scenarios is established based on the probability distributions of the uncertain parameters, and recourse is computed by either maximizing or minimizing an expectation function.

In this paper, optimal shutdown maintenance scheduling and process optimization under demand uncertainty in an ethylene plant has been considered through the formulation of a two-stage stochastic Mixed Integer Nonlinear Programming (MINLP) problem. The developed model facilitates midterm production planning over a 16-week period, while also scheduling maintenance shutdowns for eight parallel cracking furnaces. Based on Schulz *et al.* [3], the model represents ethane cracking furnaces and the separation train using surrogate models. These models are based on typical operational variables and are fitted with plant data. The model accounts for the declining performance of the furnaces due to coke deposition, represented by the inner coil roughness. The concept of relative inefficiency, as defined by Wu *et al.* [11], is used to model the equipment return to a 'good-as-new' condition after maintenance.



Fig. 1. Flowsheet of the ethane cracking plant

The proposed stochastic programming approach addresses parametric uncertainty through a two-stage optimization model [1]. The first-stage involves 'here-and-now' decisions made before the realization of uncertain parameters. The second-stage involves 'wait-and-see' decisions to be made after the uncertainty is resolved. The model uses a scenario-based approach to forecast and account for all potential outcomes. The first-stage decisions relate to manufacturing variables, while the second-stage decisions pertain to logistics.

The objective function aims to maximize the expected revenue value, subtracting production costs, the expected inventory costs and penalties for underproduction. The goal of the stochastic model is to maximize expected profit while avoiding both overproduction (thus, unnecessary production and inventory costs) and underproduction (missed sales and loss of market share).

2 Two-stage stochastic model

Sets			
i	components (hydrogen, methane, acetylene, ethylene, ethane, pro-		
J	pylene, propane, butylene, butane, pentane)		
f	final products (ethylene, propylene, propane, butane, gasoline)		
h	furnaces		
l	correlation terms (rug, rd, conv, Pf, Ff, FA)		
p	scenarios		
t, t'	time periods (weeks)		
и	units in separation train (demethanizer, deethanizer, debutanizer,		
Parameters	echane-echylene splitter, propane-propylene splitter)		
	slope of the roughness' linear function in time of furnace h		
$C3x_{1}$	coefficient for correlation term l for component i [Mmol/(wk·various units)]		
c_{f}^{inv}	inventory cost of final product <i>f</i> [\$/Mmol]		
fsin	separation factor for component <i>j</i> in separation train unit u		
Pr_{f}	sales price of final product f [\$/Mmol]		
prob	discrete probability of scenario p occurring		
Pty_f	penalty factor for unmet demand of final product f [\$/Mmol]		
rug ^{clean}	roughness of furnace h after cleaning		
Binary variables			
$y_{h,t}$	=1 if furnace h is shutdown at period t , = 0 if otherwise		
Positive variables			
$\Delta_{f,t,p}^{dmd}$	unmet demand of final product f at period t in scenario p [Mmol/wk]		
$A_{f,t,p}^{inv}$	average inventory of final product f at period t in scenario p [Mmol]		
$conv_{h,t}$	conversion rate in furnace h at period t		
cterm _{l,j,h,t}	correlation term l for component j in furnace h at period t [various units]		
$FA_{j,h,t}^{in}$	molar inlet flow of component j in furnace h at period t [Mmol/wk]		
$FA_{j,h,t}^{out}$	molar outlet flow of component j in furnace h at period t [Mmol/wk]		
$Ff_{h,t}^{in}$	total molar inlet flow of furnace h at period t [Mmol/wk]		
$Ff_{i,t}^{out}$	total molar outlet flow from furnaces of component <i>j</i> at period <i>t</i> [Mmol/wk]		
$QH_{h,t}$	heat consumption in furnace h at period t [MMBTU/we]		
Pty _f	demethanizer column pressure at period t [psi]		
$Pf_{h,t}^{out}$	outlet furnace h pressure at period t [psi]		
rd_t	dilution rate at period t		
Rl _t	ethylene-to-ethane ratio at the entrance of the separation train at period t		
$rug_{h,t}$	coil roughness in furnace h at period t [Mmol/wk]		
$Sls_{f,t,p}$	sales of final product f at period t in scenario p [Mmol/wk]		

The MINLP stochastic model with discrete time representation (week periods) of an ethylene plant has been formulated based on nonlinear surrogate models. As previously mentioned, the optimal maintenance scheduling of the furnaces and the production planning are considered in the first stage decisions of the stochastic approach, while the sales logistics are allowed for in the second stage decisions. This is due to the complexity implied in the planning of the production that obliges to carry it out in advanced for the entire horizon. Besides, the storage of the final products decouples the stages and

buffers the production while the sales are conducted. The quantity of final product sold in each period cannot exceed what the market demands. However, many external factors may influence the consumer demands, not allowing its accurate prediction and, consequently, producing more than is required. Therefore, demand uncertainty not only has a direct impact in customer unmet demands, but also on the final products storage in each time period.

2.1 **Objective function**

The objective function is the maximization of the profit, defined as the difference between the sales and the costs and penalties (see Eq. (1a)). As explained above, production costs $(PC_{j,t})$ are first stage variables, while revenues $(RE(\theta_{j,t}))$, final product inventory costs $(IC(\theta_{j,t}))$ and unmet demand penalties $UD(\theta_{j,t})$ are second stage variables, since they depend on the uncertain demands $(\theta_{j,t})$ they are contemplated in the objective function by means of their expected values.

$$\max E\left[\sum_{t}\sum_{j}RE(\theta_{j,t}) - IC(\theta_{j,t}) - UD(\theta_{j,t})\right] - \sum_{t}\sum_{j}PC_{j,t}$$
(1a)

The uncertainty is herein included through sampling a normal probabilistic distribution of the stochastic demand, i.e. creating several scenarios (p) each of them with the corresponding variables for sales, inventory and unmet demand. All scenarios are solved simultaneously in the stochastic model and the objective function is expressed in terms of the expected values as follows:

$$\max \sum_{p} prob_{p} \sum_{t} \sum_{j} Pr_{f}Sls_{f,t,p} - c_{f}^{inv}A_{f,t,p}^{inv} - Pty_{f}\Delta_{f,t,p}^{dmd} - \sum_{t} \sum_{j} PC_{j,t}$$
(1b)

Where $prob_p$ is the probability of occurrence of scenario p. As a result, the optimization provides the first-stage variables' values and the best combination of expected revenue, inventory costs and penalties for unmet demands for the second-stage.

2.2 Furnaces' decaying performance

The expenses include raw material and furnaces cleaning costs, as well as furnaces' heat requirements that are strongly dependent on furnaces performance.

In each furnace, the molar output of each component j ($FA_{j,h,t}^{out}$) is calculated as a function of the dilution ratio (rd_t), the outlet furnace pressure ($Pf_{h,t}^{out}$), the furnace conversion ($conv_{h,t}$), the total furnace inlet flowrate ($Ff_{h,t}^{in}$), some components' inlet flows ($FA_{j,h,t}^{in}$) and the coil roughness ($rug_{h,t}$). The first three are typical operation variables of this kind of process. The dilution ratio, which is the process steam to hydrocarbon feed ratio, is an important optimization variable since the steam is added to the

ethane feed to minimize coke deposition on the coil walls. The model has been accurately fitted with real plant data.

$$FA_{j,h,t}^{out} = \sum_{l} C3x_{l,j} \cdot cterm_{l,j,h,t} \qquad \forall j, h, t$$
(2)

The coil roughness quantifies the decaying performance of the furnace due to the coke accumulated on the internal surface of a coil during operation and it is considered to increase linearly with time (see Figure 2). The initial state is different for each furnace and the roughness increases linearly with slope $C31_h$ until the furnace is shut down for a week to be cleaned, afterwards they resume operation with a minimum value of roughness (clean condition), rug_h^{clean} .



Fig. 2. Schematic of furnace roughness evolution

The heat duty in the furnaces $(QH_{h,t})$ is a function the furnace conversion $(conv_{h,t})$ and the total furnace inlet flowrate $(Ff_{h,t}^{in})$, as well as the coil roughness $(rug_{h,t})$. As coke is deposited on the coil walls and the surface roughness increases, the heat transfer towards the process stream diminishes. Consequently, the heat duty increases to uphold the conversion.

$$QH_{h,t} \ge f_{heat \ corr,h} \left(Ff_{h,t}^{in}, rug_{h,t}, conv_{h,t} \right) \qquad \forall h, t \tag{3}$$

The binary variable $y_{h,t}$ has been defined to take value 1 when furnace *h* is shutdown in period *t* and 0 otherwise. Roughness is reset to "as-good-as-new" condition [11] with Eqs. (4) and (5).

$$B_{h,t} + B_{h,t}^{dummy} = rug_{h,t-1} + C31_h - rug_h^{clean} \qquad \forall h,t$$

$$\tag{4}$$

$$rug_{h,t} = rug_{h,t-1} + C31_h - B_{h,t} \qquad \forall h,t \tag{5}$$

The Generalized Disjunctive Programming framework that nullifies the inlet and the outlet flows and the heat duty when furnace h is shutdown at period t is shown in Eq. (6). $f_{h,t}^{FAH}$ is the total furnaces feed of furnace h at period t.

$$\begin{array}{c} \neg y_{h,t} \\ \vdots \\ f_{h,t}^{FAH} \leq 1 \\ Ff_{h,t}^{in} \leq Ff_{h}^{in,max} \\ B_{h,t} = 0 \\ B_{h,t}^{dummy} \leq rug_{h}^{max} \\ QH_{h,t} \leq QH_{h}^{max} \end{array} \right| \lor \begin{bmatrix} y_{h,t} \\ \vdots \\ f_{h,t}^{FAH} = 0 \\ Ff_{h,t}^{in} = 0 \\ B_{h,t} \leq rug_{h}^{max} \\ B_{h,t}^{dummy} = 0 \\ cterm_{l,j,h,t} = 0 \\ QH_{h,t} = 0 \\ \end{array} \right| \lor h,t$$

Equation (6) combines with Eqs. (4) and (5) to model the evolution of roughness of a given furnace. When the furnace is working $B_{h,t}$ is zero per Eq. (6), except when a shutdown occurs. In such case $B_{h,t}$ is assigned the difference between the current roughness and the "as-good-as-new" value by Eq. (4), because $B_{h,t}^{dummy}$ is set to 0. Therefore, at the shutdown period, Eq. (5) forces $rug_{h,t}$ to return to clean state.

2.3 Separation train

Downstream from the furnaces, the separation train is modelled through correlations and mass balances. It is a continuous process and thus there are no null flowrates. The outlet streams of the units in the separation train are represented with Eq. (7) as a function of the total furnaces production of individual components $(Ff_{j,t}^{out})$, the demethanizer column pressure (P_t^{dem}) , the ethylene-to-ethane ratio at the entrance of the separation train (Rl_t) , and a corresponding separation factors $(fs_{j,u})$ for each unit.

$$fs_{j,u,t} = f_{sep,u} \left(Ff_{h,t}^{in}, P_t^{dem}, Rl_t, fs_{j,u} \right) \qquad \forall j, u, t$$
(7)

2.4 Non-convex non-linearities

The model incorporates non-linearities that appear in three distinct sectors:

- a) The correlations for the components of the ethylene recycle are quadratically dependent on the molar ratio of ethane to ethylene in the feed to the deme-thanizer column.
- b) In each furnace and for each time period, the heat required to achieve the desired conversion is inversely proportional to the furnace's roughness. This indicates that a higher roughness necessitates more heat, influencing the decision on whether to clean a particular furnace or not.
- c) All flows are modeled as the sum of individual components' flow, a necessity for the correlations at the furnaces. Consequently, all mass balances at

separators transform into bilinear expressions, as illustrated in Equation (8). Here, fx_t^{sep} is a decision variable that determines the proportion of the incoming flow directed to the outgoing flow at time period t:

$$flow_{j,t}^{out} = fx_t^{sep} \cdot flow_{j,t}^{in} \quad \forall j,t$$
(8)

These non-linearities are all non-convex due to the following reasons: the correlations at the ethylene recycle involve quadratic equalities, the heat consumption calculations include a division, and the remaining expressions are bilinear. Moreover, the bilinear expressions in the separator preceding the furnaces significantly impact the solution performance.

3 Implementation and results

For the sake of simplicity, we are only considering demand uncertainty of the main product (ethylene) and it has been assumed to have a normal distribution with a mean of 190 Mmol per time period and a standard deviation of 10%.

The number of scenarios is crucial for a representative sampling of the uncertain parameters' probabilistic distribution. To have an adequate sample size, the stochastic model has been run multiple times varying the numbers of scenarios: 5, 50, 100, 250, 500 and 1000. Each scenario is generated by sampling the demand of all periods within the scheduling horizon, using the normal distribution specified before.

All instances were implemented in GAMS 43.6 software and solved with DICOPT 2, a local outer-approximation MINLP solver. CPLEX 22.1 and CONOP 3.17 were used as MILP and NLP sub-solvers, respectively. All computations were performed on an Intel Core i7 6700 computer with 8GB of RAM.



Fig. 3. Objective function value and resolution time vs. quantity of scenarios

Figure 3 shows that the value of the objective function stabilizes between 100 and 200 scenarios so instances with 250, 500, and 1000 scenarios adequately represent the

uncertain demands. However, the resolution time significantly increases beyond 500 scenarios. Further analysis for the case of 500 scenarios is provided below.

Table 1. Solution performance of the 500 scenarios instance

Concept	Value	Concept	Value
Variables (binary)	47738 (128)	Obj. Function [10 ³ \$]	551.50
Equations	55258	Production costs [10 ³ \$]	27699.03
CPU time [s]	1616.2	Expected sales [10 ³ \$]	32972.58
		Expected unmet demands [10 ³ \$]	2475.87
		Expected inventory costs [10 ³ \$]	2246.17

Table 1 shows the solution performance of the 500 scenarios instance. Although the size of the model is quite large in terms of variables and equations it can be solved in a reasonable time (less than 30 minutes). It must be observed that DICOPT is a local solver, and the solution obtained may not be the global optimum, primarily due of the presence of bilinear expressions.



Fig. 4. Coil roughness in each furnace vs. time

Figure 4 shows the coil roughness of each furnace as a function of time (weeks) for the case with 500 scenarios. The cleaning periods are located where the roughness decreases vertically. Evidently, cleaning most furnaces early in the domain of time favors the operation of the cracking units since they are closer to their optimal conditions. Despite the seven maintenance shutdowns, the plant successfully keeps up a consistent production level of all the final products along the time horizon (see Figure 5).



Fig. 5. Production of final products in each week

Figure 6 shows the time evolution of each term of the objective function in Eq. (1a). The shaded area represents the range covered by the values of the sum of the secondstage terms considering the 500 scenarios. In the final period, there is a noticeable reduction in the sum of the second-stage terms. As evident from the graph, this is attributed to penalties incurred due to a larger proportion of demands remaining unfulfilled. The probable cause of this trend is that by the final period, the ethane reservoir is nearly depleted. Consequently, the plant's production capacity alone is insufficient to meet all the demands.



Fig. 6. Evolution of the terms in the objective function: the solid line represents first-stage term owing to production costs) and the dotted lines correspond to the expected value of the second-stage terms. The shaded area indicates the range covered by the sum of the second-stage terms.

4 Conclusions

A two-stage stochastic model capable of managing uncertainty in the final product demands has been formulated for optimal midterm planning of an ethane-fed ethylene plant. The model successfully determines the production and inventory planning and the optimal shutdown schedule for the furnaces' maintenance, despite the complex behavior of the plant due to large recycle streams, nonlinear surrogate models for the production and the decaying performance of the furnaces. The solution provides the best expected value for the profit which is comprised by the production costs (firststage variables) and the revenues, the final products inventory costs and the penalties for unmet demands (second-stage variables). The normality assumption has been invoked for the demand uncertainty, sampling a large number of scenarios to assure a proper representation of the probabilistic distribution. Nevertheless, the problem could be solved within a reasonable timeframe, at least with a local optimization solver.

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References

- Li, C., Grossmann, I.E.: A Review of Stochastic Programming Methods for Optimization of Process Systems Under Uncertainty. Front. Chem. Eng., 2, Article 62224 (2021).
- Jain, V, Grossmann, I.E.: Cyclic scheduling of continuous parallel-process units with decaying performance. AIChE J., 44, 7, 1623-1636 (1998).
- Schulz, E.P., Bandoni, J.A. and Diaz, M.S.: Optimal Shutdown Policy for Maintenance of Cracking Furnaces in Ethylene Plants. Ind. Eng. Chem. Res., 45, 2748-2757 (2006).
- Su L., Tang, L., Grossmann, I.E.: Scheduling of cracking production process with feedstocks and energy constraints. Comput. Chem. Eng., 94, 92-103 (2016).
- 5. Su L., Tang, L., Grossmann, I.E.: Computational strategies for improved MINLP algorithms. Comput. Chem. Eng., 75, 40-48 (2015).
- Wang, Z., Li, Z., Feng, Y., Rong, G.: Integrated short-term scheduling and production planning in an ethylene plant based on Lagrangian decomposition. Can. J. Chem. Eng., 94, 1723-1739 (2016).
- Adloor, S.D., Vassiliadis, V.S.: An optimal control approach to scheduling maintenance and production in parallel lines of reactors using decaying catalysts. Comput. Chem. Eng., 142, Article 107025 (2020).
- Lin, X., Janak, S.L., Floudas, C.A.: A new robust optimization approach for scheduling under uncertainty: I. Bounded uncertainty. Comput. Chem. Eng., 28, 1069-1085 (2004).
- Bonfill, A., Espuña, A., Puigjaner, L.: Addressing robustness in scheduling batch processes with uncertain operation times. Ind. Eng. Chem. Res., 44, 1524-1534 (2005).
- Gupta, D., Maravelias, C.T.: Framework for studying online production scheduling under endogenous uncertainty. Comput. Chem. Eng., 135, Article 106670 (2020).

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 Wu, Y., Maravelias, C.T., Jiang, Y., Fan, J., Wenzel, M., Elbsat, M., Turney, R.: Optimization Methods for Predictive Maintenance Scheduling of Building Heating/Cooling Equipment with Performance Decay. In: International High Performance Buildings Conference. Paper 273 (2018)