SUPPLY RISK LIMITS FOR THE INTEGRATION OF PRODUCTION SCHEDULING AND REAL-TIME OPTIMIZATION AT AIR SEPARATION UNITS

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Abstract

In the optimization of liquid production from power-intensive Air Separation Units (ASU's), decisions need to be made at two time scales - week-ahead production scheduling to leverage fluctuations in electricity prices, and real-time decisions that optimize the entire plant operation, while capturing spot opportunities. Although methodologies exist for week-ahead production scheduling and real-time optimization of ASU's, integrating the two decisions has not been studied previously. In our work, we combine elements of flexibility analysis and robust optimization to propose a methodology to integrate production scheduling and real-time optimization. We illustrate the proposed methodology on a small multi-period inventory management example. The approach is generic and can be extended to any power intensive process with a variable production cost and inventory capacity.

Keywords

Air Separation Unit, Production Scheduling, Real-Time Optimization, Adjustable Robust Optimization, Flexibility Analysis

Introduction

Air Separation Units (ASU's) separate air into its constituent components (primarily Nitrogen, Oxygen & Argon) through cryogenic distillation. Most ASU's produce gaseous products that are delivered through pipelines, and liquid products that are stored in tanks and delivered to customers via trucks. Cryogenic temperatures at ASU's are achieved through multistage gas compressors that consume large amounts of energy. Due to the volatile nature of energy markets, there is significant opportunity to lower the costs by scheduling production of liquid products to coincide with the valleys in price curves and leveraging the inventory capacity at the plants.

Several papers have been published in the area of production scheduling for ASU's in the recent past (Ierapetritou et al. (2002), Karwan and Keblis (2007)). Mitra et al. (2012) propose a very efficient mixed-integer linear production scheduling formulation for ASU's, which was extended to a robust optimization (RO) formulation to address uncertainty in reserve markets by Zhang et al. (2016a). While Mitra et al. (2012) used a surrogate model that treated the plant as a single unit, Misra et al. (2016) proposed a state-task network representation in which all units of a plant are considered separately, providing more flexibility to capture real world constraints and limitations of an air separation plant.

With a wider scope, Marchetti et al. (2012) proposed a formulation to coordinate production and distribution from multiple ASU's in a basin. In all of the above approaches, significant cost savings were identified by scheduling production during periods of cheap electricity prices, and the savings were magnified when considering uncertainty or synergies between multiple plants in a basin.

Several papers and patents exist for real-time optimization (RTO) of ASU's. Huang et al. (2009) propose a nonlinear model predictive control (NMPC) formulation for the dynamic real-time optimization of ASU's, and Li et al. (2011) present a formulation for real-time optimization of a complex network of ASU's. The objective of the RTO formulations is to minimize cost while satisfying mass balance and purity constraints.

These models provide a detail plant representation but they are very computationally expensive and should not be used for making discrete decisions, such as turning on and off equipment.

The topic of integrating production scheduling and real-time decisions has been addressed differently depending on the community. While the scheduling community has focused on reactive or online scheduling (Gupta and Maravelias (2016)), the control community has looked into closed loop implementations for simultaneous scheduling and control (Zhuge and Ierapetritou (2012)). Instead of increasing the rescheduling frequency or developing a monolithic solution that results in an extremely challenging mixed integer dynamic optimization problems, our objective is increase the flow of information from the scheduling to the RTO; the later can react to disturbances without jeopardizing the schedule, while maintaining the hierarchical structure between them.

Traditionally, production schedules determined by a week-ahead optimization with an hourly discretization are passed to the plant as fixed production targets, and re-scheduling is done every day once the demand and electricity price forecasts are updated (rolling horizon). However, in the presence of high uncertainty at the sub-hourly time-scale, this approach can be sub-optimal. This is the case in highly volatile energy markets, where there are spot markets that offer significant cost incentives to modify the electricity consumption during periods of grid imbalance. This could also be the case for an Air Separation Unit that serves a highly volatile gas customer, and periods of unanticipated gas customer down-time could be opportunities to make liquid products at a lower cost. Both types of disturbances are hard to forecast and include within a production scheduler. This necessitates the development of RTOs that can deviate from the liquid targets when opportunities arise, without violating inventory limits for future time periods.

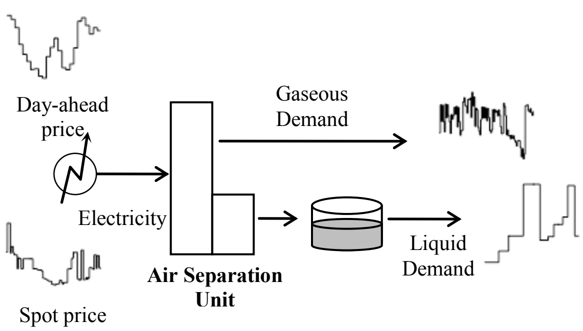


Figure 1. Schematic of various inputs affecting ASU operations at varying frequencies

For instance, Figure 2 shows the discrepancy between the day-ahead price (used in production scheduling) and spot price (used in real-time optimization) at an Air Liquide plant. The day-ahead price changes every hour but the spot price changes every 15 min. Between 9:00-15:00, since day-ahead price is high, a production scheduler would avoid production, but since the spot price is low (10 times lower than day-ahead in certain time periods), an RTO should be provided with room to deviate from the schedule and increase production.

However, deviating from the schedule could put inventory level constraints for future time periods at risk. In order to constrain the deviation from schedule, additional information needs to be provided to the RTO from the scheduling layer. We capture this information by performing a flexibility analysis on the system. We refer to these flexibility limits as 'supply risk limits', which provide a feasible region for the RTO that factors in future demand and supply constraints. The question of how much to deviate within the supply risk limits is a more complex optimization problem, and is outside the scope of this paper.

In the following sections we present the mathematical formulation to obtain the 'supply risk limits' following flexibility analysis (Grossmann et al. (1983) and Grossmann and Straub (1991)) and robust optimization approaches (Ben-Tal et al. (2009)). The formulations are applied to a simple example to illustrate the methodology. We close with conclusions and ideas for future work.

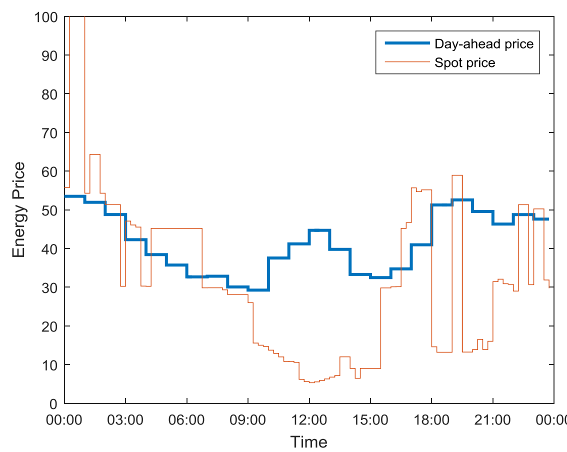


Figure 2. Day-ahead versus spot price at an Air Liquide plant.

Mathematical Formulation

Flexibility analysis focuses on how to design a process for guaranteed flexible/resilient operation, as well as to evaluate the process flexibility for a given design. A process is considered sufficiently flexible if feasible operation can be achieved for the entire range of the uncertain parameters. An example could be to determine whether a heat exchanger network design is feasible for any value (within a range) of the uncertain heat capacity flow-rate of one stream. Typically, the design variables correspond to the structure and equipment size of the plant, whereas the uncertain parameters are typically inputs or process parameters. For more detail information regarding flexibility analysis, we refer to the recent review by Grossmann et al (2014).

Within the classical flexibility analysis problem, the flexibility test problem deals with, for a given design d, determining whether by proper adjustment of the degrees of freedom available during operation z, the set of constraints that represent the system hold. The problem is posed as follows:

$$\mathcal{X}(d) = \max_{\theta \in \mathcal{U}} \min_{z \in \mathbb{R}^{n_z}} \max_{j \in \mathcal{J}} \; f_j(d, z, \theta)$$

where $d \in \mathbb{R}^{n_d}$ are the design variables, $z \in \mathbb{R}^{n_z}$ are the control variables, $\theta \in \mathbb{R}^{n_\theta}$ are the uncertain parameters and $\mathcal{J} = \{1,2,\dots,m\}$ is the set of constraints $f_j(d, z, \theta)$. If the flexibility function $\mathcal{X}(\mathrm{d})$ is less or equal to zero for a chosen d, then the design is feasible for all θ in the uncertainty set $\mathcal{U}$.

In the context of our problem, the supply risk limits are the extreme values of the design variable d (production at time period $t = k$), subject to the flexibility test problem for all time periods in the scheduling horizon. For any choice of production at time period k within the supply risk limits, the inventory constraints will hold for all future time periods for any demand within the uncertainty set. The production at time $t = k$ is a 'here-and-now' decision and the production for all time periods $t > k$ are recourse actions/control variables.

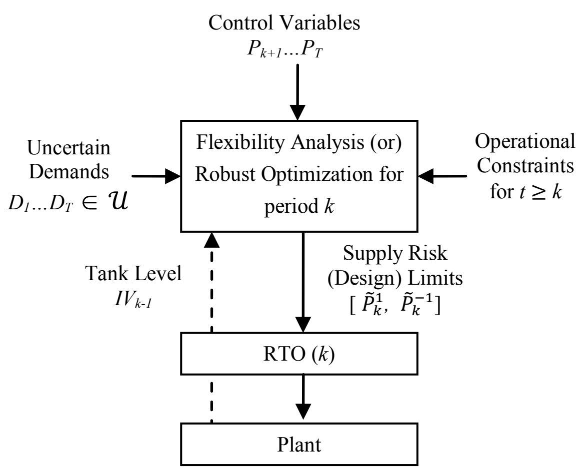


Figure 3. Flowchart showing the integration Supply Risk Limits and RTO

The calculation of the supply risk limits are shown in Figure 3 above. At time period k, the extreme values for production at $t = k$ are obtained by solving a Flexibility Analysis or Robust Optimization problem which factors in future uncertain demands and operational constraints, as well as past demand realizations. Along with liquid production targets, these limits are passed to the RTO and the solution of the RTO is communicated to the plant. Finally, information about the system's state is passed back to the next flexibility analysis through the tank level and the horizon is rolled forward.

The mathematical formulation describing the supply risk limits problem is given by:

$$\min \; \alpha \cdot P_k$$

s.t.

$$IV_t^{min} \leq IV_{ini} + \sum_{t'=k}^{t} (P_{t'} - D_{t'}) \leq IV_t^{max} \qquad \forall\, t \in T_k \qquad (1)$$

$$P_t^{min} \leq P_t \leq P_t^{max} \qquad \forall\, t \in T_k \qquad (2)$$

$$D_t \in \mathcal{U} \qquad \forall\, t \in T \qquad (3)$$

where P_t is the liquid production at time t, which is bound by P_t^{min} and P_t^{max}. D_t is the uncertain liquid demand belonging to uncertainty set $\mathcal{U}$, IV_{ini} is the initial inventory in the tank, IV_t^{min} and IV_t^{max} define the storage capacity, $T = \{1, \dots, H\}$ represent the planning horizon and T_k is a subset of T such that $T_k = \{k, \dots, H\}$. Eq. 1 is the result of combining mass balance in the tank (inventory level at time t is the inventory level at $t - 1$ plus the amount produced minus the demand) with bounds on inventory limits, and Eq. 2 defines the technical production limits. Eq. 3 represents a polyhedral uncertainty set for the demands, which for example may consist of an upper and lower limit for every D_t and correlations between them in the form of aggregated forecasts at various time levels:

$$\mathcal{U} = \{D_t \in \mathbb{R}^{|T|},\; h_{i,t} D_t \leq g_i \;\; \forall\, i \in I, t \in T\} \qquad (4)$$

where I is the set of linear inequalities defining the uncertainty set. The correlation between the uncertain parameters leads to non-trivial solutions for the supply risk limits. We will use this simplified version of an industrial production model for illustration purposes, but the methodology can be easily extended to more detailed formulations.

By setting $\alpha = 1$, we minimize production at $t = k$ and obtain lower supply risk limits, whereas if $\alpha = -1$, we maximize production at $t = k$ to obtain the upper supply risk limits.

Following the notation of flexibility analysis, the supply risk limit problem is formulated as:

$$\min \; \alpha \cdot P_k$$

s.t.

$$\mathcal{X}(P_k) = \max_{D_t \in \mathcal{U}} \min_{P_{t|t>k}} \max_{l \in \mathcal{L}} \; f_l\left(P_{t \in T_k}, D_{t \in T}\right) \leq 0 \qquad (5)$$

where P_k is the 'design variable', $P_{t|t>k}$ are 'control variables', D_t is the 'uncertain parameter' and $\mathcal{L} = \{(1), (2)\}$ is the set of constraints.

In flexibility analysis, a design is feasible if the flexibility function satisfies $\mathcal{X}(P_k) \leq 0$. Since we are looking for the extreme values of the design variables, we can replace the inequality in (5) with an equality sign and the inner min max problem can be reformulated applying the Karush–Kuhn–Tucker (KKT) conditions and an active-constraint strategy to convert the bi-level problems into single-level, mixed-integer problems as in Grossmann et al. (1987):

$$\min_{P,\lambda,s,y,D} \alpha \cdot P_k$$

s.t.

$$-IV_{ini} - \sum_{t'=k}^{t}(P_{t'} - D_{t'}) + IV_t^{min} + s_t^1 = 0 \quad \forall t \in T_k \quad (6)$$

$$IV_{ini} + \sum_{t'=k}^{t}(P_{t'} - D_{t'}) - IV_t^{max} + s_t^2 = 0 \quad \forall t \in T_k \quad (7)$$

$$-P_t + P_t^{min} + s_t^3 = 0 \quad \forall t \in T_k \quad (8)$$

$$P_t - P_t^{max} + s_t^4 = 0 \quad \forall t \in T_k \quad (9)$$

$$e^T\lambda = 1 \quad (10)$$

$$\sum_{\substack{t=k+1 \\ m\in\{2,4\}}} \lambda_t^m - \sum_{\substack{t=k+1 \\ m\in\{1,3\}}} \lambda_t^m = 0 \quad (11)$$

$$\lambda \leq y \quad (12)$$

$$s \leq M(e - y) \quad (13)$$

$$e^T y \leq n_{|T|-k} + 1 \quad (14)$$

$$P_t \in \mathbb{R}, \quad \lambda_t^m \in \mathbb{R}_+, \; s_t^m \in \mathbb{R}_+, \quad y_t^m \in \{0,1\} \quad \forall\, m \in \{1,\ldots,4\}, \; \forall t \in T_k \quad (15)$$

$$h_{i,t} D_t \leq g_i \quad \forall\, i \in I, \; \forall\, t \in T \quad (16)$$

where s is the vector of slack variables, λ denotes the vector of Lagrange multipliers, y is the vector of binary variables and M is a big-M parameter. For details on the reformulation refer to Grossmann et al. (1987).

Inspired by the connection made by Zhang et al (2016b) between flexibility analysis and robust optimization, we propose an adjustable robust formulation (Ben-Tal et al. (2004)) for this problem, in which the control variables are affine functions of the uncertain parameters:

$$\min_{P_k,a,b} \quad \alpha \cdot P_k$$

s.t.

$$\max_{D_t \leq \mathcal{U}} \left(-IV_{ini} - \sum_{t'=k}^{t}(P_{t'} - D_{t'}) \right) \leq -IV_t^{min} \quad \forall t \in T_k \quad (17)$$

$$\max_{D_t \leq \mathcal{U}} \left(IV_{ini} + \sum_{t'=k}^{t}(P_{t'} - D_{t'}) \right) \leq IV_t^{max} \quad \forall t \in T_k \quad (18)$$

$$\max_{D_t \leq \mathcal{U}} P_t \leq P_t^{max} \quad \forall t \in T_k \quad (19)$$

$$\max_{D_t \leq \mathcal{U}} -P_t \leq -P_t^{min} \quad \forall t \in T_k \quad (20)$$

$$P_{t|t>k} = a_t + \sum_{t'=t-\zeta}^{t} b_{tt'} D_{t'} \quad \forall t \in T_{k+} \quad (21)$$

where Eq. (21) represents the affine solution policy for production as a function of past demand realizations. Notice that a_t and $b_{tt'}$ are the decision variables instead of $P_{t|t>k}$.

Applying duality to the inner max problem in each constraint, we obtain a single-level problem in the space P_k, a_t, $b_{tt'}$ and the dual variables associated with the uncertainty set.

We used the solution from Robust Optimization for illustrative purposes below, although, as pointed out by Zhang et al. (2016) the Robust Optimization approach can lead to more conservative solutions compared to Flexibility Analysis due to treatment of recourse by the former method.

Regarding the computational complexity and scalability of the approach, Ben-Tal et al. (2004) showed that the affine adjustable robust counterpart problem of an uncertain LP is efficiently solvable if the uncertainty set is convex, compact and computationally tractable. However, the extensibility of the approach to an industrial application has not been addressed yet.

Illustrative Example

The following small example will be used to illustrate the methodology proposed to integrate scheduling information into an RTO. We consider a problem with 10 time periods with the following input data:

Table 1. Input data Illustrative Example

Parameter	Value
IV_{ini}	800
$[IV_t^{min}, IV_t^{max}]$	[725, 850]
$[P_t^{min}, P_t^{max}]$	[0, 30]
$[D_t^{min}, D_t^{max}]$	[0,15]
$D^{MIN} \leq \sum_{t=1}^{10} D_t \leq D^{MAX}$	[40, 120]

The last two rows in Table 1 contain the coefficients that characterize liquid demand uncertainty.

The model was implemented in AIMMS 3.14, and the commercial solver CPLEX 12.6.1 was applied to solve the LPs on a Intel® Core^{TM} i5-5300U machine at 2.30 GHz with 4 processors and 16 GB RAM running Windows 7 Enterprise. Since the example has only an illustrative purpose, the size of the model is very small: 442 constraints and 257 variables. The walk-clock computation time to optimality is barely 0.02 seconds.

Figure 4 shows the supply risk limits (dashed lines upper figures) in three different production scenarios for the same demand realization (lower figures). The middle row shows the progress of the inventory level profile as the horizon rolls.

Scenario 2 represents the nominal production from a scheduling tool, Scenario 1 represents an extreme scenario in which the RTO deviates from the target by cutting back production to 0 (e.g., in periods of high spot prices where it is profitable to sell back to the grid), and in Scenario 3 production overpasses the targets filling the tank (e.g., when spot prices are significantly lower).

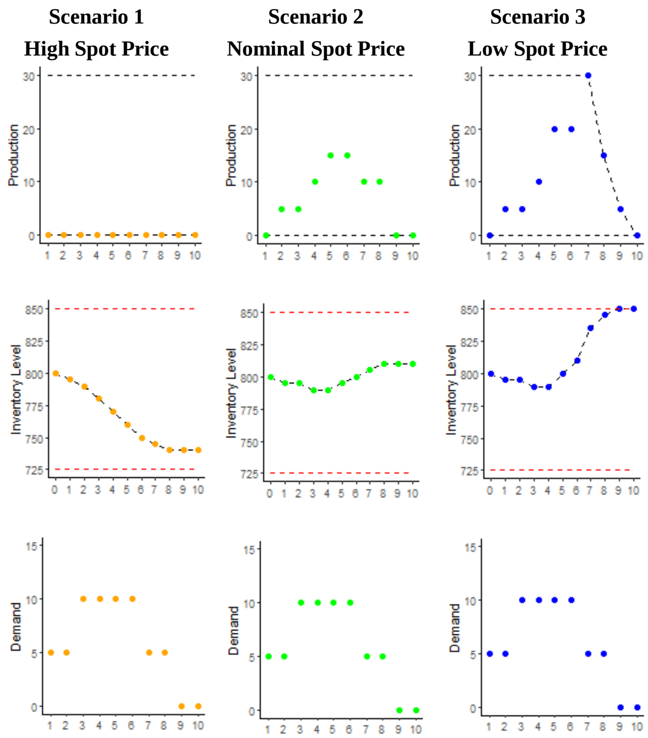
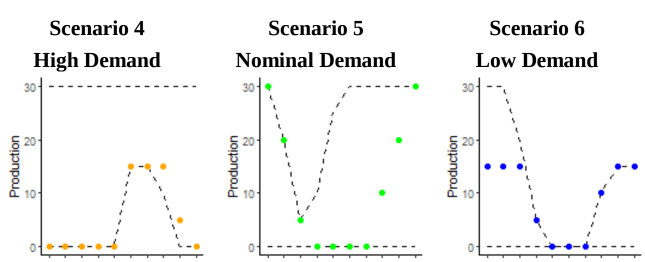


Figure 4. Three production scenarios for same demand realization

While Scenario 1 does not show modification of the flexibility of the system (the supply risk limits coincide with those of the nominal case), Scenario 3 shows modification of the maximum production limit passed to the RTO to prevent upper inventory level violations.

A second example is shown in Figure 5 for three demand realizations. In the high demand case (Scenario 4) coupled with high spot prices, the RTO could still choose to reduce production to 0 for the first 5 time periods, but the lower supply risk limits will force production in time periods 6-8 in order to maintain the inventory levels.

In the nominal case (Scenario 5), the production and demand follow opposite profiles. The upper supply risk limit will constrain production during the first time periods so as to keep the inventory within bounds, but the system recovers its full flexibility after period 6.



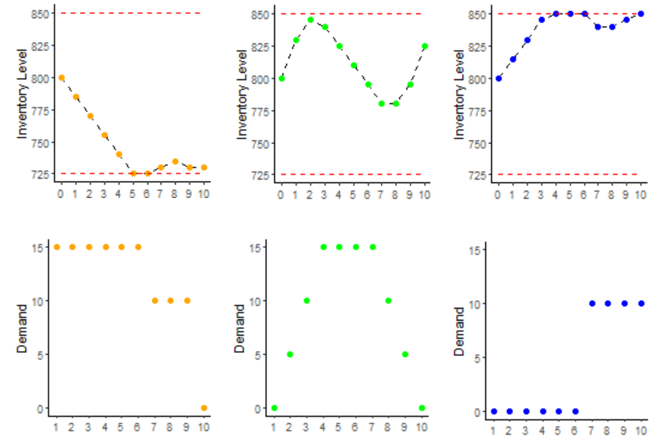


Figure 5. Three production scenarios for three demand realizations

In the low demand case (Scenario 6), the demand happens only at the end of the horizon. For this scenario, the RTO solution is to keep production at 15 units. The inventory can accept this production rate until period 3 but the upper supply risk limits will force a reduction in production at the middle of the horizon.

The supply risk limits are not trivial or already implied in the RTO model, especially when considering uncertainty correlations. An RTO solution without supply risk limits would always be at either minimum (maximum) production when the objective is to minimize cost (maximize profit), as the inventory in the tank is considered ‘free’ for use to satisfy the mass balance for the current time instant. By replacing the mass balance constraint with the supply risk limits coming from a flexibility analysis of the system over a scheduling horizon, the RTO decisions can be constrained to maintain feasibility of the system for future time periods.

Conclusions and Future Work

In this work, we have presented a methodology to integrate mid-term uncertain demand information and real-time optimization for production of storable products with varying production cost. We achieve the integration by using the solution of two multi-period optimization problems under uncertainty as bounds for production at the RTO level. We describe how to formulate the problems as single-level deterministic mathematical programs, using approaches from Flexibility Analysis and Adjustable Robust Optimization.

We apply the methodology to an illustrative example consisting of 10 time periods. We generate different demand and production scenarios to show different profiles for the supply risk limits. We observe that these limits are not trivial even in this simple example and that, at the RTO level, the mass balance constraint should be replace by bounds on production obtained from a flexibility analysis on the system.

Future work will focus on how to set the objective function of the RTO for storable products to accurately determine how much to deviate from the schedule to capture spot opportunities. We would also like to examine the possibility of obtaining the supply risk limits off-line, i.e. before the start of the horizon, eliminating the need to solve a potentially complex optimization problem before every run of the RTO. The challenge here is that at any time $t = k$, not only demand is uncertain but production at $t < k$ would be uncertain since it would be the result of the RTO decision at a previous time period.

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Nomenclature

Indices

j	constraints (flexibility analysis)
l	inventory and production constraints
i	inequalities that define $\mathcal{U}$
t	time periods
k	current time period

Sets

J	constraints (flexibility analysis)
T	time periods
T_k	subset of time periods, $T_k = \{k, \dots, H\}$
$\mathcal{U}$	uncertainty set
I	set of inequalities that define $\mathcal{U}$
$\mathcal{L}$	constraints in supply risk limit problem

Deterministic Parameters

H	horizon length
P_t^{max}	maximum production in time period t
P_t^{min}	minimum production in time period t
IV_{ini}	initial inventory
IV_t^{min}	minimum inventory in time period t
IV_t^{max}	maximum inventory in time period t
α	sign of objective function
$h_{i,t}, g_i$	demand uncertainty characterization
M	big-M parameter
$n_{\|T\|-k}$	maximum number of non-zero y_t^m
e	column vector of appropriate dimensionality where all entries are 1
ζ	extent of recourse
D_t^{min}	minimum demand in time period t
D_t^{max}	maximum demand in time period t
D^{MIN}	minimum total demand
D^{MAX}	maximum total demand

Uncertain Parameters

θ	uncertain parameters (flexibility analysis)
D_t	liquid demand in time period t

Continuous variables

d	design variables (flexibility analysis)
z	control variables (flexibility analysis)
P_t	liquid production in time period t
IV_t	inventory in time period t
$\tilde{P}_k^{\alpha}$	(α)-supply risk limit at time period k
s_t^m	slack variables
λ_t^m	Lagrange multipliers
a_t	coefficient decision rule (adj. robust opt)
$b_{tt'}$	coefficient decision rule (adj. robust opt)

Binary Variables

y_t^m

Functions

$\mathcal{X}$	flexibility function
f_j, f_l	problem constraints