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Scheduling optimization and risk analysis for energy-intensive industries under uncertain electricity market to facilitate financial planning

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ABSTRACT

The planning of energy-intensive processes is intrinsically uncertain due to their dependence on the volatile energy market, with scheduling having a vast impact on the final production cost of these plants. Traditional stochastic methods are mathematically very complex, which translates into a significant computational effort that might prevent a timely response to varying electricity prices. To encounter this uncertainty, we develop a reliable hybrid simulation-optimization approach for optimizing the production plant scheduling, combining scenario analysis with risk analysis. The proposed methodology is demonstrated with real data from a cryogenic air separation plant in Tarragona (Spain). This approach also informs decision-makers about risk or expected shortfall associated with the implied scenario. The generic methodology used here can be easily adapted to schedule facilities in other energy-intensive sectors such as cement, metallurgy or pulp and paper.

1. Introduction

The industrial sector requires a considerable amount of energy to manufacture ready-to-use products. Indeed, for energy-intensive industries (EIIs), the cost of electricity is the major factor in the operational costs and product pricing. EIIs represent an important share of the industrial sector (U.S. Energy Information Administration, 2016), with a direct impact on our daily life (e.g., chemical, refining, cement or mining). Amongst EIIs, the bulk chemical is the largest industry, representing over 27% of the energy consumption in the whole industrial sector ("Energy Use in Industry - Energy Explained, Your Guide To Understanding Energy - Energy Information Administration," n.d.).

One of the bulk chemical industries whose profit is greatly affected by the electricity prices is the air separation sector. Cryogenic air separation is the state-of-the-art technology for obtaining purified industrial gases (e.g., liquid oxygen, liquid nitrogen, and liquid argon) at large scale (Smith and Klosek, 2001). In these processes, electricity constitutes 31% of the total cost, evidencing the significance to obtain low-cost electricity (Ierapetritou et al., 2002).

Electricity prices are dictated by the regional/national electricity market, which is partly deregulated in most parts of the world. In deregulated markets, electricity is traded as a commodity for future and spot electricity consumption (Scharfhausen, 2009).

In the context of cryogenic air separation, some authors (Fernández et al., 2017) have optimized plant operations deterministically using their experience to predict future electricity prices and maximizing the expected profit. A similar approach has also been used for a variety of process industries such as cement production (Mitra et al., 2012), paper and pulp industry or metallurgy (Associates, 2005; Todd et al., 2009). Most works follow a deterministic approach (Sahinidis, 2004; Grossmann et al., 1999; Misra et al., 2017; Ierapetritou et al., 2002) and only to a limited extent include uncertainty (Charitopoulos and Dua, 2017; Finn and Fitzpatrick, 2014).

Due to the inherent fluctuations in electricity prices, all energy intensive plants operate under uncertainty and are susceptible to financial risks in practice. Uncertainties can be mainly due to exogenous and endogenous factors (Castro et al., 2018). For instance, the uncertainty generated from the electricity price fluctuation is an exogenous uncertainty, while uncertainty generated within the operation due to wear and tear of apparatus or intrinsic nature of the process/apparatus affecting the expected output presents endogenous uncertainty.

An inappropriate production scheduling can lead to financial depreciation with a negative effect on product pricing. Such negative

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Nomenclature

Process Units/Products

CBU conversion unit
CU compression unit
DCU distillation column unit
ECU external compression unit
EDCU external distillation column unit
FP final products
GANIP gas nitrogen intermediate product
GANP gas nitrogen product
GOXIP gas oxygen intermediate product
GOXP gas oxygen product
ILOXP industrial liquid oxygen product
LOXIP liquid oxygen intermediate product
LARIP liquid argon intermediate product
LARP liquid argon product
LINP liquid nitrogen product
LQU liquefaction unit
MILP mixed-integer linear programming
MLOXP medical liquid oxygen product
MX mixers
OGAN purchased gas nitrogen
OGOX purchased gas oxygen
PU pump unit
PTU pretreatment unit
SP splitters
T storage tank
U utility
VU vaporizer unit

Sets/indices

i set of process units indexed by i
p set of stream properties indexed by p
s set of streams indexed by s
t set of time intervals indexed by t
u set of utilities indexed by u

Subsets

EC set of units i whose electricity consumption is constant
EE set of units i with electrical consumption
EO set of external units i whose electricity consumption is accounted for
EV set of units i whose electricity consumption is variable
FCL set of streams s with maximum switch flow limitations in a time period
FP set of streams s which are final products
GP set of units i whose gasoil consumption is proportional to the input flow
MINCAP set of units i with a minimum input flow requirement
MO_i main output stream s of unit i
MS_i main input stream s of unit i
SI_i set of input streams s of unit i
SO_i set of output streams s of unit i
$SPTI_i$ set of units i which are splitters in which one output stream can only be used if the inventory level of the associated tank i is over VSINVi
SPW set of units i which are binary splitters (i.e., which cannot use more than one output stream simultaneously)
ST set of units i which are tanks
TVS set of tanks i which can send tankers to an associated storage plant
UPR2 set of units i which belong to supply process (i.e., downstream the main process)
UPR1 set of units i which belong to the main process
VS set of streams s which are tankers to a storage plant
GOCONS total gasoil consumption, L
$INV_{i,t}$ inventory of unit i in time period t, N m^3
$INVD_{i,t}$ disaggregated variable for inventory at level at which it can be depleted by means of tankers (inventory of unit i in time period t), N m^3
PROFIT profit, €
SALES sales, €
$UTCONS_{i,u,t}$ consumption of utility u in unit i in time period t, kWh
$Z_{i,d,t}$ auxiliary variable for Fs in interval d of piecewise equation for electricity consumption of unit i in time period t

Binary variables

$y_{i,d,t}$ binary variable (1 if interval d in piecewise equation for electricity consumption of unit i is active in time period t, 0 otherwise)
$yfc_{s,t}$ binary variable (1 if the flow of stream s is switched in binary variable (1 if the flow of stream s is switched in time period t, 0 otherwise)
$yi_{i,t}$ binary variable (1 if unit i is working in time period t, 0 otherwise)
$yinv_{i,t}$ binary variable (1 if inventory of tank i in time period t surpasses the minimum required for it to be depleted by means of tankers, 0 otherwise)
$yon_{i,t}$ binary variable (1 if unit i is switched on in time period t, 0 otherwise)
$yw_{i,t}$ binary variable that equals 1 or 0 depending on which output stream s is used in i in time period t

Parameters

η vaporizer efficiency
$a_{i,d}$ the slope of a straight-line equation in interval *d* of piecewise linear approximation for electricity consumption of unit i
$b_{i,d}$ independent term of a straight-line equation in interval *d* of piecewise approximation for electricity consumption of unit i
$CAPVOL_i$ maximum capacity allowed for input stream of unit i, N m^3/h
CF corrective factor between input and output streams in any unit
CF2 corrective factor between OGOX and OGAN in EDCU
$DEM_{s,t}$ demand for a product in stream *s* in time period *t*, N m^3/h
DISC supplier discount on outsourcing cost, €
DT idle time in liquefiers, h
$ECONCOST_t$ cost of electricity bought in advance for time period *t*, €/kWh
$ECOST_t$ electricity cost in time period *t*, €/kWh
GOCOST gasoil cost, €/L
GSCAP maximum flow allowed for a given stream, N m^3/h
HVAPN2 heat of vaporization of N_2, kJ/N m^3
$INVCAP_i$ capacity of unit i, N m^3
$INVini_i$ inventory of tank *I* at the beginning of the period scheduled, N m^3
$INVfin_i$ inventory of tank *i* requested for the end of the period scheduled, N m^3
LHVGO lower heating value of gasoil, MJ/L
$lo_{i,d}$ lower bound of interval *d* of piecewise equation for electricity consumption of unit i
MAINTCOST cost of maintenance applied in unit *i* when it is working in time period t, €/h
$MAXINV_i$ maximum inventory allowed for unit *i*,%
$MAXPR2_t$ maximum electricity that can be consumed in time period t by supply process, kW
$MAXPR1_t$ maximum electricity that can be consumed in time period

	t by main process, kW
MFCs	maximum flow change allowed in stream *s* in between two consecutive time periods, N m^3/h
$MINCAPVOL_i$	minimum flow rate required for input stream of unit i, N m^3/h
PCHT	product change time, h
MININVi	minimum inventory allowed for unit *i*,%
PCONt	Electricity purchased in advance for time period *t*, kW
PENINV	penalty for the deficit or excess of stored product in the last period time
PENYFC	penalty for changes in the flowrate of streams
PENYON	penalty for the numbers of times a unit is started
PENYW	penalty for the number of times external storage plant is used
PENMB	penalty for the breach of mass balances constraints
$PHTR_t$	electricity consumption in PTU heater in time period t, kWh
PLQ3t	electricity consumption limitation in time period t, kWh
$PRICE_s$	price of product in stream *s*, €/N m^3
PRODISC	unitary price discounted related with EDCU production, €/N m^3
RELATION	amount of product obtained by EDCU to apply the price discount
$SMINCAP_s$	minimum flowrate required for stream *s*, N m^3/h

effects can be counterbalanced to some extent by resorting to mathematical modelling and programming (Gebreslassie et al., 2009) considering uncertainty aspects. There are several approaches to incorporate different types of uncertainties into mathematical models: two-stage stochastic programming (Weskamp et al., 2019; Chen et al., 2020; Li et al., 2021a), parametric programming (Oberdieck et al., 2016), fuzzy programming (Wang et al., 2020), chance constraint programming (Wu et al., 2015), robust optimization techniques (Cao et al., 2020), and conditional value-at-risk (Rezaei et al., 2020) are some of the most used frameworks. Dynamic Response scheduling technique is another method which has been recently used in many case studies (Kelley et al., 2018; Kelley et al., 2020; Kelley et al., 2022) related to ASU and chemical plants. Cao et al. (2015) applied a framework in which they addressed the plant design limitation by optimizing the system performance under the electricity price fluctuation and demand uncertainty and concluded that the best achievable optimal solution is subjected to plant constraints. Building on the DR framework Cao et al. (2016) also addressed the problem of storage and excess production during the low peak hours of electricity pricing. In a similar approach Dias et al. (2018) focused on the model predictive control method to accommodate the scheduling changes based on DR feedback. A simulation-optimization methodology was used to predict the scheduling operation and a closed loop feedback tracking system was used later to integrate the required changes in previously optimized scheduling. Their methodology could not provide optimal solutions for discrete changes in the scheduling problem.

A detailed review of planning and scheduling under uncertainty for several sectors can be found in Verderame et al. (2010). All the above methodologies use random function to incorporate uncertainty. This typically provides an acceptable approximation for the real uncertainty, yet it fails to capture the temporal trend (i.e., rise vs decline) of electricity prices. On the other hand, and regardless of the approach followed, the inclusion of uncertainty in the problem formulation increases the model complexity and the computational effort required to solve it. For stochastic problems, in the area of planning and scheduling operations, the rolling horizon approach has been used to deal with this complexity (Mitra et al., 2012; Merkert et al., 2015; Zamarripa et al., 2016; Zhang et al., 2018). Analogously, Pattinson et al. (2017) used a moving horizon optimal scheduling approach for the scheduling of ASU with multiple assumptions of economic data forecasts and processes. They proposed multiple scheduling calculations over the scheduling time horizon and proposed changing the schedule if deemed necessary for optimal operation. In rolling horizon and moving horizon approach, the production targets and other internal variables change continuously after each rescheduling e.g. in rolling/moving horizon approach the horizon (Total time 'T') remains the same and this time 'T' (e.g. $T = 7$ days) is divided into 7 discrete time blocks i.e. t1, t2, …, t7 each representing one day. Now, at 't1', the forecasting and scheduling is done for total time 'T'. Then, at the end of day 1 i.e. 't1', the forecasting of the electricity prices performed again but this time the unknown variables corresponding to 't1' are known and are treated at as system constraints while the forecasting and scheduling is repeated again for the remaining period (T - t1). This process is repeated till the end of time horizon is met. Many process industries require short term scheduling (i.e., time horizons from 3 days to one week) and conventional approaches are not practically feasible due to the associated large computational time (Acevedot and Pistikopoulos, 1998). Hence, for complex problems where fluctuations of uncertain parameters can change on a daily to hourly basis, there is a need to adopt an approach trading-off the comprehensive analysis of all possible scenarios and the computational effort required to address it.

To that end, here, we develop a methodology to provide with optimized scheduling plan under electricity price uncertainty, for the given product demand and respective production period, to maximize the profit. Namely, we propose a tool combining mathematical modelling, time-series prediction, Monte-Carlo simulation and risk metrices, to facilitate the decision-making process for the management. The developed tool can handle the multi-period model simulation and the complexity involved in the prediction of electricity prices, with computational efforts that allow providing a timely response to varying electricity prices. The prediction accuracy of the model is found to be as high as 95%. The tool also presents a set of discrete electricity price scenarios for planning and scheduling strategies with estimated profit and associated risk. The applied methodology would reduce the over/under-estimation of the profit, intrinsic to any deterministic approach, while providing more realistic estimations.

As a test bed, we have demonstrated this methodology in an existing cryogenic air separation facility situated in Catalonia (Spain), where we maximize the profit under the volatility of electricity prices. Despite this, the methodology is general enough to be valid for any other energy-intensive sector. With this methodology, complex problems for short-term scheduling (e.g., 1 week for a 24 × 7 process industry) under uncertain electricity prices can be solved with little computational and programming effort allowing for a rapid response to changes in electricity prices. In this methodology we studied 100 different electricity price scenarios to assess the impact of uncertainty associated with electricity market and electricity price forecasting. We obtained a set of profit values for these scenarios which were then used to perform risk analysis in a similar manner as portfolio optimization in financial markets.

2. Problem statement

Energy intensive industries (EIIs) have a common functional framework as shown in Fig. 1. All EIIs are subjected to electricity price uncertainty and the demand uncertainty in general. The introduction of the uncertainty presents a planning dilemma for the management of these industries. The uncertainty of electricity prices is common to the EIIs while demand uncertainty can be managed by proper order book in most cases. Thus, the main uncertainty common to all EIIs is electricity price which affects the optimal planning. We are attempting to address this planning (scheduling and financial) problem through our methodology

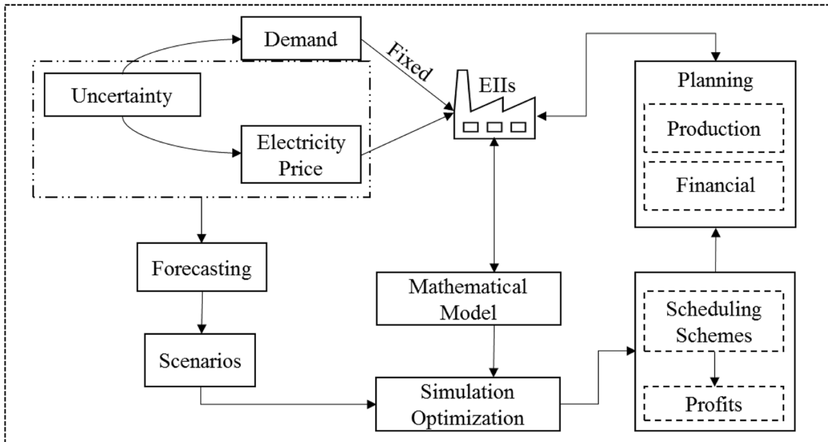

Fig. 1. Framework to facilitate financial planning of EIIs under uncertainty.

with real time data of an existing EII in the Tarragona region of Spain as a test bed.

We are given the technical data of a cryogenic ASU (Air Separation Unit) located in the petrochemical complex of Tarragona (Spain). The plant (2,adapted from Fernández et al. (2017)) includes a pre-treatment unit (PTU), where impurities are removed from the atmospheric air input. After the PTU, the filtered air goes to the distillation column unit (DCU) where the air is split, under cryogenic conditions, into N_2, O_2, and Ar. Then, each component is either sent to their respective compressor (CUs) and to the customers via pipeline or, alternatively, liquefied and stored in tanks T1 – T4. Further details on the plant's topology and operation are provided elsewhere (Fernández et al., 2017).

Fernández et al., al.(2017) optimized the plant operation deterministically using single scenario forecast approach leaving it susceptible to suffer from the financial risks associated with the uncertain electricity price market. In this contribution, we also assume that liquid and gas demands are deterministic as they are known by the sales department one week in advance, whereas unexpected orders entailing large gas consumptions (i.e., deviating from average consumption or contracts) must be notified by the customers with sufficient anticipation. We are also given the price and the amount of electricity that has been bought from the futures market for (typically covering around 60% of the requirements). The remaining electricity (~40%) must be bought from the spot market, for which we consider the hourly variability of electricity prices and which represents the uncertainty source in this work. The aim is to develop a methodology that first predicts electricity prices in the spot market with accuracy and then optimizes the complex uncertainty scheduling problem in relatively low computational time, otherwise the solution will not be ready before the decision-makers need to make their decisions. To address this issue, we perform optimization for scheduling of the plant under electricity price uncertainty. Optimized scheduling plan for upcoming (next week's) production cycle provides us with speculated profit by calculating the expected incurring production cost and total sale (calculated by the preplaced orders). Then we calculate the associated risk of a shortfall for the optimized scheduling plan.

In this context, the objective is to determine the optimal operation of the plant (e.g., startup and shutdown times for process units, mass flow rates, product purchases from external manufacturers, etc.) under electricity price uncertainty that maximizes the expected profit while simultaneously provides a quantitative measure of the risk associated with this operation. To achieve this objective, we have also added the flexibility of selling the excess electricity back to the grid, provided by the market maker, in case we have surplus of contracted electricity for the contracted period (day, weekdays or weekend for Spanish electricity market) based on scheduling of plant.

3. Methodology

We have developed a hybrid two-step approach, as shown in Fig. 3. First, we use Monte-Carlo scenario generator (MCSG) for generating future electricity prices scenarios. MCSG uses ARIMA (Auto regressive integrated moving averages) to forecast the electricity prices and then it generates plausible scenarios for future electricity prices. In the second step, we introduce electricity price uncertainty by feeding the modified model for the ASU facility (Fernández et al., 2017) with the generated scenarios to calculate the potential outputs for each of the plausible forecasted electricity price scenarios independently. To some extent, even the most efficient forecasting models have prediction errors that can propagate through the model and lead to over or underestimation of the different variables, including the objective function. Therefore, with the aim of minimizing the risk of adopting an economically inefficient scheduling plan, we perform risk analysis for the obtained profit values to analyse the risk of deviating from the obtained profit values in each scenario. Thus, we have considered each scenario as a separate optimization problem and have used MILP to solve it. These steps are described in detail in the ensuing subsections.

3.1. Scheduling time horizon

The scheduling period (also known as time horizon) of a 24 × 7 operational plant is of utmost importance in scheduling problems. The production under the scheduling time horizon must match the customers' demand, and the operation and implementation aspects of the plant. Hence, as per the need in our case, we analysed hourly electricity price data for a period of one year to find a suitable time horizon for prediction and plant scheduling. To this end, we plot hourly electricity price data retrieved from Spanish electricity market operator OMIE for the year 2017 (Figs. 4& A.2.1).

Inspection of figures 4.1 and A.2.1 suggests electricity spot price follow a nonlinear weekly pattern, with weekends and working days showing different behaviors. This pattern, only altered for festivals (Christmas, regional holidays) and long holidays (Easter, summer and winter), calls for using a one-week time horizon for plant scheduling, which is also consistent with the status quo ordering policy for the plant. Also, in another study, Tsay et al. (2019) analysed the sensitivity of economic benefits achieved against the electricity price uncertainty and they found that cost benefits for multiday planning horizon were significantly better than the day ahead planning horizon.

3.2. Scenario generation model

The mathematical model (explained in detail in Section 3.3) for the air separation plant is a multi-period model that requires hourly

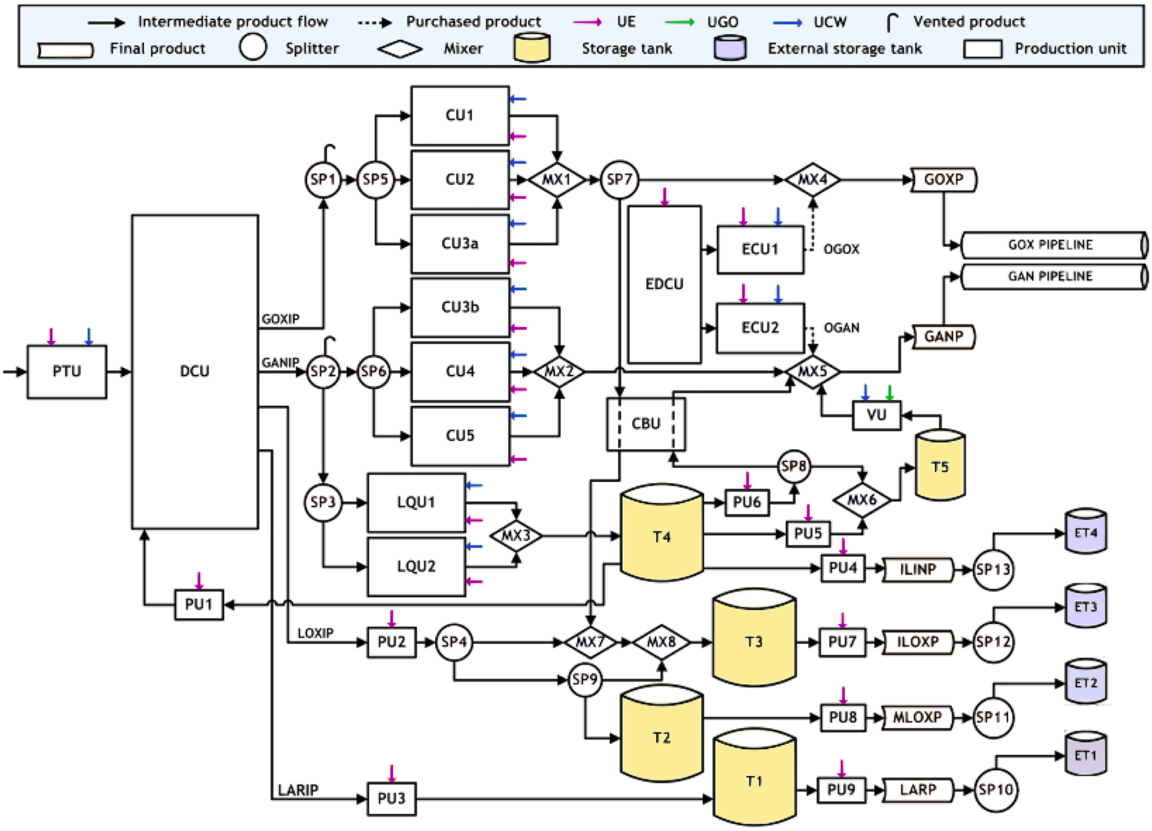

Fig. 2. Process network configuration of the air separation unit adapted from Fernández *et.al.*(Fernández et al., 2017), PTU: pretreatment unit; DCU: distillation column unit; PU_i: pump units;, SP_i: splitter; CU_i: compressor units; MX_i: mixer units; T_i: tanks; LQU_i: liquefier; CBU: conversion unit; EDCU: external distillation column unit; ET_i: external tanks; VU: vaporizer unit. LOX: liquid Oxygen; GOX: gaseous Oxygen; LAN; liquid Nitrogen; GAN: gaseous Nitrogen; LAR: liquid Argon.

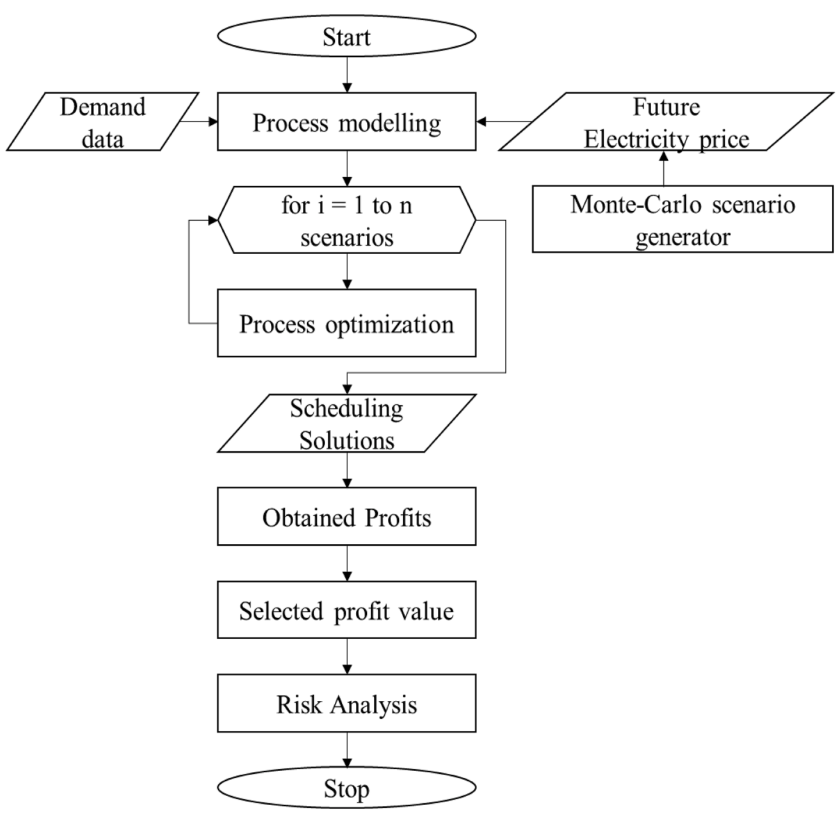

Fig. 3. Overview of the proposed methodology.

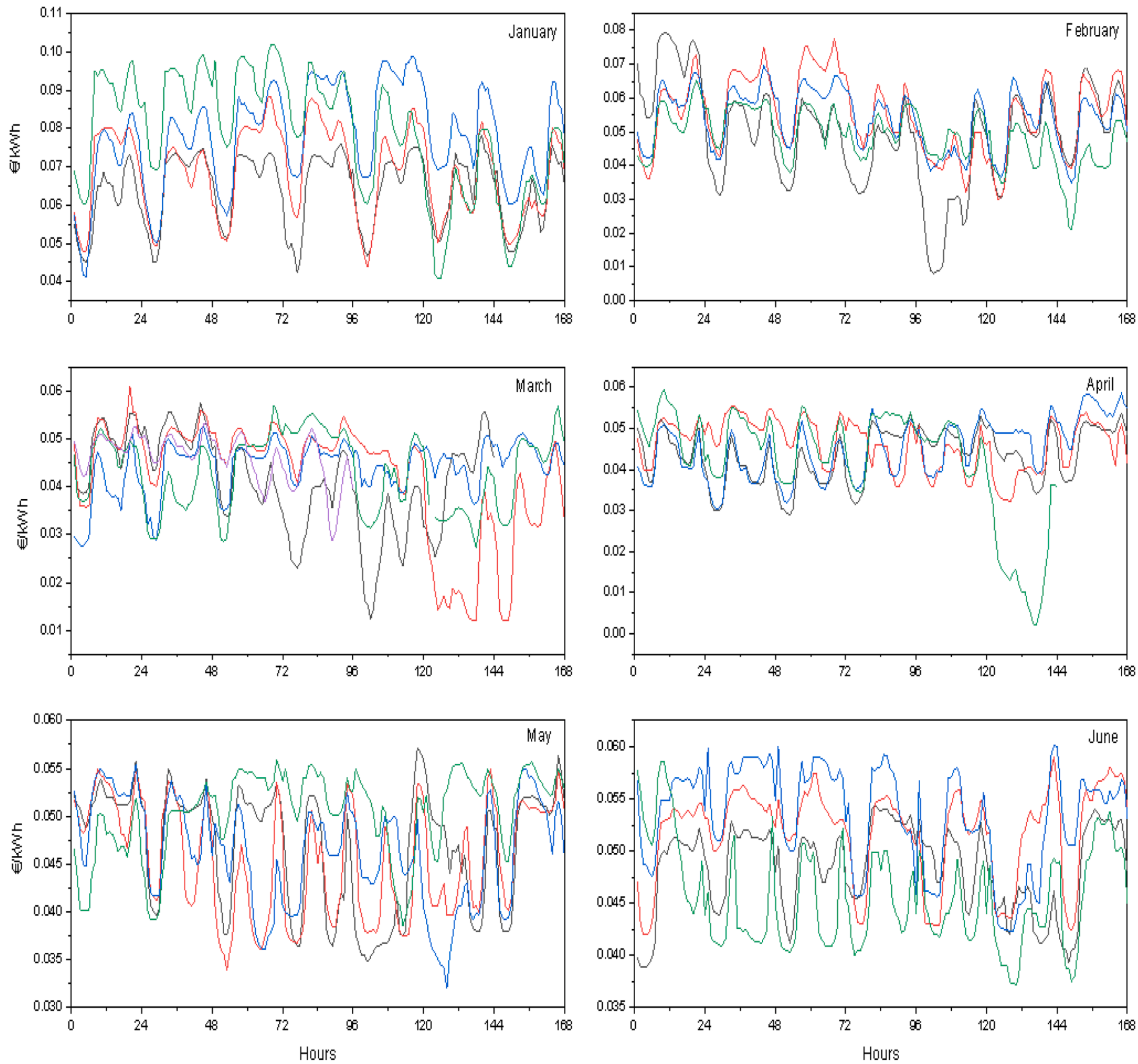

Fig. 4. Hourly electricity price data for weeks one to four from January to June (week 1, week 2, week 3, week 4).

electricity price data. These data is first forecasted deterministically using a statistical model, and then, probable scenarios are generated using Monte-Carlo sampling based on the average error of the forecasting model. The scenarios generated are discrete in nature and each generated scenario is an independent time series data set for the planning horizon.

The nature of energy market is very complex. It is complexly correlated and intertwined with the movement of fossil fuel market and renewable energy market. The nature of USA's energy market was studied by Dowling et al. (2017), who presented the revenue opportunities available in real time energy market and concluded that there is always tradeoff between risk and revenue while trading the energy markets. Gao et al. (2022) also studied the impact of multi-source integrated energy system on the electricity market. In a similar study Sorourifar et al. (2020) studied the impact of battery energy storage system on the energy market and cost of operation for the energy producer. In extension of the energy market study, Elmore et al. (2021) analysed economic opportunities available for large industrial facilities by frequency regulation market, demonstrating that frequency regulation participation in industry has major limitations from the aspect of implementation. Dowling et al. (2018) developed an augmented dynamic mode decomposition method for the forecasting of electricity prices in the day ahead market in the state of California, USA.

Forecasting electricity prices is a particular instance of the more general problem of forecasting time series data (Conejo et al., 2005). Weron (2014) categorized the electricity price forecasting methods according to their modelling approach: multiagent, fundamental, reduced form, statistical and computational intelligence. Weron(2014) found that statistical models were preferred due to readiness for physical interpretation. In the context of the electricity market, a plethora of statistical models have been developed. Mazengia et al.(2008) compared Auto-regressive Moving Average, ARIMA (Auto-Regressive Integrated Moving Average), Transfer Function and Regression Analysis for time series of hourly electricity price forecast, finding that, for weekly predictions of the Spanish electricity market ARIMA provided acceptable errors (4.78%−11.27%). Conejo et al., al.(2005) and Jakaša et al. (2011) also used ARIMA to predict the Spanish and the European energy markets, respectively.

ARIMA is a forecasting model for time-series data prediction based on historical data, that incorporates seasonality. It has been widely used by Jakaša et al. (2011), Conejo et al. (2005), and Ierapetritou et al. (2002) to name a few. In our case, where time-series consist of hourly electricity prices, the forecasted electricity price for a future hour $t+1$ is given by Eq (1):

$$\text{price}(t') = f(price(t), p) + \varepsilon(t')\ t' > t \tag{1}$$

where $f(price(t), p)$ is the ARIMA function framework used to forecast prices in future periods t'. Price(t') is based on electricity prices in past periods *t*, i.e., price(t) and a set of framework parameters *p* cumulatively representing autoregressive terms, moving average order, differencing and seasonality. Then $\varepsilon(t')$ provides the stochastic term sampled from the distribution of model residuals (i.e., error). Due to its autoregressive nature, ARIMA can incorporate the unprecedented increase in electricity prices very early in its future forecast, thus, making it a robust time series forecasting model. In this work, ARIMA has been implemented to generate hourly electricity forecast using the historical electricity price data obtained from the Spanish electricity market operator OMIE for a week ahead using software EViews10 SV("EViews.com," n.d.).

For scenario generation approach, we have preferred discrete scenarios approach over the scenario tree approach. The reason is that the latter is used for moving/rolling horizon method, which would cause multiple forecasting instances with frequent scheduling changes during the production period, which would be difficult to implement for a 24 × 7 operation for a short time horizon.

To obtain discreet electricity price scenarios, we developed a Monte-Carlo scenario generator (MCSG) following the flowchart shown in Fig. 5. MCSG is an appropriate technique to generate scenarios that has been successfully applied for time-series forecasting (Breeden and Ingram, 2010). To generate scenarios, first, prices are (deterministically) forecasted for a period whose prices we know historically (i.e., week 1). Then, the forecasted price is compared with the actual price and the mean average percentage error (MAPE) is calculated. If MAPE is more than the accepted value (15% in this case), the forecasting process is repeated until the MAPE value falls under the accepted limit. Then, we generate a normal distribution of the MAPE with σ = 5% (i.e. MAPE $\sim N(\mu = 0,\ \sigma = 0.05 \cdot$forecasted price$)$). Then, the electricity price scenarios are generated by multiplying the obtained MAPE values with the forecasted electricity price scenario and then adding the forecasted electricity price scenario to this multiplication result, e.g. if 'x' is the MAPE error and P is the forecasted electricity price then probable electricity price is obtained as $P + P \times x$. The method follows the Monte Carlo simulation approach and thus, we call this tool Monte Carlo Scenario Generator. At that point, we forecast the electricity price for the future (unknown) time horizon (i.e., week 2 onwards) using the Monte-Carlo scenario generator.

We assume that the realization probability is same for all the scenarios generates. Note, however, that, since scenarios are sampled from a normal distribution, central scenarios are more likely to be sampled than extreme scenarios. As an example, if an infinite number of scenarios were sampled, 95.45% of these scenarios would be expected to fall within μ±2σ. This assumption would later allow us to follow the worst-case approach for risk analysis which in real time would provide us with extra cushion against the uncertainty of electricity market making the solution reliable.

3.3. Multi-period stochastic model

The operation of the air separation unit is optimized for maximum profit using model M-ASUOPT, explained in detail in this section. This model is a modification of the ASUOPT model presented by Fernández et al. (2017), which is enhanced here to consider, not only a single deterministic scenario, but every generated scenario for electricity prices.

3.3.1. Mass balance constraints

Mass balances are demarcated for every process units and time interval. A sketch of generic units and the sets defined around it is shown in Fig. 2. Here, SIi and SOi are the input and output streams of unit 'i', respectively. For processes having more than one input and output streams, another set MSi (MOi) have been defined for these units. Knowing that most units do not accumulate material, Eq. (8) applies,

$$\sum_{s\in SO_i} F_{s,t,sn} = \sum_{s'\in SI_i} F_{s',t,sn}\ \forall\ t, sn \quad i \in VU,\ ECU1,\ ECU2,\ CBU,\ PTU,\ CU1-CU5,\ SP1-SP14,\ MX1-MX8,\ PU1-PU9 \tag{2}$$

Here $F_{s,t,sn}$ denotes volumetric flow rate of stream *s* in time period *t* for scenario *sn*. Note that these are expressed in [Nm³], therefore, the constraint of mass balance holds even.

For the DCU, the output flows are determined by

$$F_{s,t,sn} = \sum_{s'\in MS_i} F_{s',t,sn}\ YIELDVOL_{i,s,sn} + \sum_{s''\in SI_i\backslash MS_i} F_{s'',t}\ YVC_{i,s,sn}\ \forall\ t, s, sn \in SO_i, i = DCU \tag{3}$$

where $YIELDVOL_{i,s,sn}$ is a parameter denoting volumetric yield of stream *s* in unit *i* for scenario *sn* and $YVC_{i,s}$ is a correction coefficient for the volumetric yield if there is a recycle (i.e., stream from T4) into the DCU.

For CBU unit, mass balance is computed separately for oxygen and nitrogen stream as they flow separately inside the unit. CF parameter provides the appropriate ratio between nitrogen and oxygen for the unit.

$$\sum_{s\in MO_i} F_{s,t,sn} = \sum_{s'\in MS_i} F_{s',t,sn}\ \forall\ t, i, sn = CBU \tag{4}$$

$$\sum_{s\in SO_i\backslash MO_i} F_{s,t,sn} = \sum_{s'\in SI_i\backslash MI_i} F_{s',t,sn}\ \forall t, i, sn = CBU \tag{5}$$

$$CF \sum_{s\in MS_i} F_{s,t,sn} = \sum_{s'\in SI_i\backslash MS_i} F_{s',t,sn}\ \forall t, i, sn = CBU \tag{6}$$

To consider the accumulation in the storage tanks (T1 – T5) we include Eqs. (7) and 8:

$$INVini_i + TIME\left(\sum_{s\in SI_i} F_{s,t,sn} - \sum_{s'\in SO_i} F_{s',t,sn}\right) = INV_{i,t,sn}\quad \forall\ i \in ST, t, sn = 1 \tag{7}$$

$$INV_{i,t-1,sn} + TIME\left(\sum_{s\in SI_i} F_{s,t,sn} - \sum_{s'\in SO_i} F_{s',t,sn} = INV_{i,t,sn}\right)\quad \forall\ i, sn \in ST, t > 1 \tag{8}$$

Here, $INV_{i,t,sn}$ represents the inventory of storage tank *i* in time period t for scenario *sn, TIME* is the duration of time period, and ST is the set of storage tank units (T1 – T5). Parameter *INVini* provides the initial inventory of tank *i*.

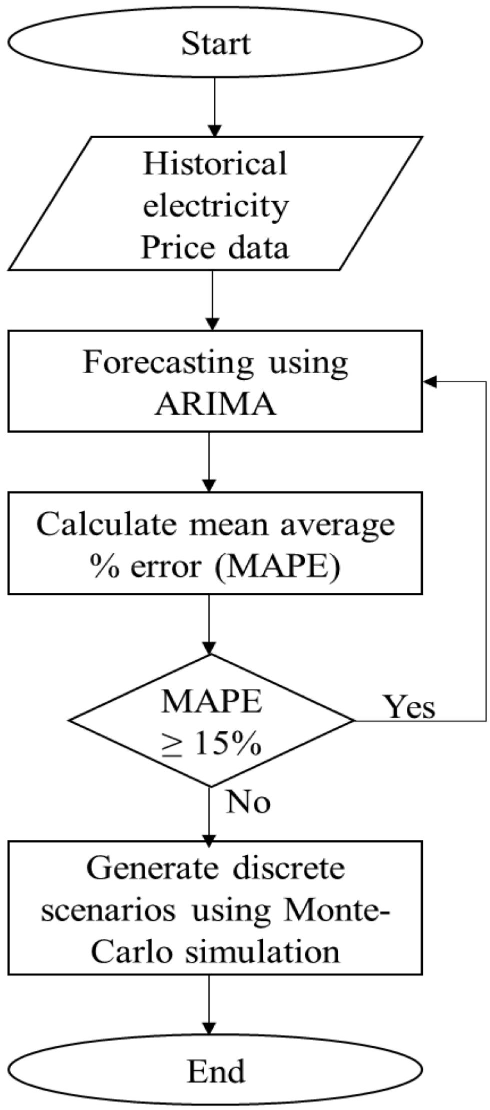

Fig. 5. Flowchart for the Monte-Carlo scenario generator using ARIMA. MAPE: mean average percentage error.

To model the real operation, the system has the possibility of purchasing two external streams OGOX and OGAN. The price is equal to the price of electricity consumed in the EDCU, ECU1 and ECU2 to produce them. It is then linked to the demand flow network through contractual arrangements. Again, EDCU has limitation of producing OGAN, which is related to the amount of OGOX, due to the air composition and the process itself. To model this, the *CF2* parameter is used.

$$\sum_{s' \in SO_i \setminus MO_i} F_{s',t} \leq CF2 \sum_{s \in MO_i} F_{s,t} \ \forall \ t, i \in EDCU \tag{9}$$

3.3.2. Capacity constraints

Due to unit's size limitations, we have capacity constraints in the model. For instance, the storage tanks' level must lie between a lower and upper level bound. Parameters $MININV_i$ and $MAXINV_i$ indicate the minimum and maximum inventory level for unit i of set ST (storage tanks), whereas, $INVCAP_i$ represents the 100% capacity of the tank. These bounds are imposed as:

$$MININV_i INVCAP_i \leq INV_{i,t,sn} \leq MAXINV_i INVCAP_i \tag{10}$$

$$yi_{i,t,sn} \ MINCAPVOL_i \leq \sum_{s \in MS_i} F_{s,t,sn} \ \forall \ t, i, sn \in MINCAP \tag{11}$$

$$\sum_{s \in MS_i} F_{s,t,sn} \leq yi_{i,t,sn} \ CAPVOL_i \ \forall \ t, i, sn \tag{12}$$

where $yi_{i,t,sn}$ is a binary variable which corresponds to on and off condition of the operating unit at a particular time. *MINCAP* is a set that contains the minimum input flow rates of all the units (PTU, PU1, PU3, LQU1, LQU2, CBU, ECU1 and ECU2). Limits on EDCU output streams are applied through the input streams of compressors ECU1 and ECU2.

Process units LQU1 and LQU2, have a characteristic delay between the start and the moment they start producing. This idle period of starting is modelled via:

$$\begin{bmatrix} YON_{i,t,sn} \\ \sum_{z \in MS_i} F_{s,t,sn} \leq DT.CAPVOL_i \end{bmatrix} \vee \begin{bmatrix} -YON_{i,t,sn} \\ \sum_{z \in MS_i} F_{s,t,sn} \leq DT.CAPVOL_i \\ YON_{i,t} \in \{True, False\} \end{bmatrix} \quad \forall t, i = LQU1, LQU2 \tag{13}$$

Here, *DT* is a parameter which computes the effect of idle time (limiting the amount of product produced from the moment it is on; $DT \leq 1$). The model uses parameter $YON_{i,t}$ (true if the unit is on; false otherwise) to model this time-delay. Convex hull reformulation has been used to transform this disjunction in a mathematical equation. The simplified equations imposing lower bound on the capacities of input flows:

$$T.MINCAPVOL_i YON_{i,t,sn} \leq FD^1_{s,t,sn} \leq DT.CAPVOL_i YON_{i,t,sn} \quad \forall i, t, sn = LQU1, LQU2, s \in MS_i \tag{14}$$

$$MINCAPVOL_i \left(YI_{i,t,sn} - YON_{i,t,sn}\right) \leq FD^2_{s,t} \leq CAPVOL_i \left(YI_{i,t,sn} - YON_{i,t,sn}\right) \quad \forall \ t, i, sn = LQU1, LQU2, s \in MS_i \tag{15}$$

$$FD^1_{s,t,sn} + FD^2_{s,t,sn} = F_{s,t,sn} \quad \forall t, i, sn \in LQU1, LQU2, s \in MS_i \tag{16}$$

Here $FD^1_{s,t,sn}$ and $FD^2_{s,t,sn}$ are disaggregated variables. Eqs. (14) and (15) will force both $FD^1_{s,t,sn}$ and $FD^2_{s,t,sn}$ variables to be 0 if the unit *i* is inactive. On the other hand, an active unit *i* (i.e. $YI_{i,t,sn} = YON_{i,t,sn} = 1$) will let $FD^1_{s,t,sn}$ to take any value from $DT.MINCAPVOL_i$to $DT.CAPVOL_i YON_{i,t,sn}$.

The value of $YON_{i,t,sn}$ corresponds to the value of $YI_{i,t,sn}$ given by the Eqs. (17)-(19).

$$YON_{i,t,sn} \geq YI_{i,t,sn} - YI_{i,t-1,sn} \ \forall i, t, sn > 1 \tag{17}$$

$$YON_{i,t,sn} \leq YI_{i,t,sn} \ \forall i, t, sn > 1 \tag{18}$$

$$YON_{i,t,sn} \leq 1 - YI_{i,t-1,sn} \ \forall i, t, sn > 1 \tag{19}$$

Further, compressor CU3 is modelled as two separate units CU3a and CU3b as it can operate with two different products (i.e., N_2 and O_2). However, maintenance work is required before it can handle the other product. This is shown via Eqs. (20)-(22).

$$Y_{i,d,t,sn} + Y_{i',d,t,sn} \geq 1 \ \forall t, i, sn = CU3a, i' = CU3b, d = 1 \tag{20}$$

$$YI_{i,t,sn} \leq 1 - YI_{i',t',sn} \ i = CU3a, i' = CU3b, \forall t, t' |t\rangle t' > (t - PCHT) \tag{21}$$

$$YI_{i,t,sn} \leq 1 - YI_{i',t',sn} \ i = CU3b, i' = CU3a, \forall t, t' |t\rangle t' > (t - PCHT) \tag{22}$$

Here, parameter *PCHT* indicates the time required to change the product in the compressor. Eq. (26) checks that unit CU3 cannot be used simultaneously to process both products.

To avoid failure, due to big step changes in flow rate, the operation is kept smooth by imposing a limit MFC_s on the changes in flow rates over consecutive time periods Eqs. (23)-(25).

$$F_{s,t,sn} - F_{s,t-1,sn} \leq AV_{s,t,sn} \ \forall \ t > 1, s \in FCL \tag{23}$$

$$F_{s,t-1,sn} - F_{s,t,sn} \leq AV_{s,t,sn} \ \forall \ t > 1, s \in FCL \tag{24}$$

$$AV_{s,t,sn} \leq YFC_{s,t,sn}MFC_{s,t,sn} \ \forall \ t > 1, s \in FCL \tag{25}$$

Here $AV_{s,t,sn}$ represent the absolute value of the increment or decrement in the flow rate of stream in consecutive time periods. Whereas, *FCL* comprises the set of streams on which the limitation is put on. $YFC_{s,t,sn}$ is a binary variable that equals 1 if there is a change in the flow rate of stream *s* in time interval *t*; 0 otherwise.

If a storage tank has reached its upper limit during the production, there is an option to partially empty the tank by filling the road tankers and sending them to nearby additional storage plant that belongs to the same company. This is done by using splitters (SP10-SP13) which also act as a switch for these situations. Sometimes these road tankers are also used to sell the product. To differentiate between these two operations, a set MO_i, is used containing the streams of the product to be sold. Therefore, a lower bound is imposed on the streams not contained in MO_i, which allows other flows to be constrained by demand. This is modelled as:

$$\begin{gathered} YW_{i,t,sn}SMINCAP_s \leq F_{s,t,sn} \leq YW_{i,t,sn}SMAXCAP_s \\ \forall \ t, i, sn \in SPW, s \in SO_i \backslash MO_i \end{gathered} \tag{26}$$

$$F_{s,t,sn} \leq \left(1 - YW_{i,t,sn}\right)GSCAP \ \forall \ t, i, sn \in SPW, s \in MO_i \tag{27}$$

where, the binary variable $YW_{i,t,sn}$ is '1' if splitter i is sending the product to the outside storage, otherwise '0'. $SMINCAP_s$ and $SMAXCAP_s$ are lower and upper limits on the flow requirements of stream *s*. *SPW* and *GSCAP* represent a set containing the splitters (responsible for sending the tankers to storage plants) and a generic limit on the stream's flowrate respectively.

Tanks are used for this purpose only if the level in the tank (represented by $INV_{i,t-1,sn}$) of (t-1) time interval is higher than the threshold value ($VSINV_i$). To model this:

$$\left[\begin{gathered} YINV_{i,t}, sn \\ VSINV_iINVCAP_i \leq INV_{i,t,sn} \leq MAXINV_iINVCAP_i \end{gathered}\right] \vee \left[\begin{gathered} -YINV_{i,t}, sn \\ MININV_iINVCAP_i \leq INV_{i,t,sn} \leq VSINV_iINVCAP_i \end{gathered}\right] \tag{28}$$
$$\forall \ t, i \in TVS \ \& \ YINV_{i,t} \in \{True, \ False\}$$

Here, set *TVS* consists of units of tanks which are sending the product to the storage plant. In eq (28) $YINV_{i,t,sn}$ is the binary variable with value '1' if the tank level is between the maximum and the threshold value; '0' otherwise. The above disjunction leads to:

$$\begin{gathered} VSINV_iINVCAP_iYINV_{i,t} \leq INVD^1_{i,t} \leq MAXINV_iINVCAP_iYINV_{i,t} \\ \forall \ t, i, sn \in TVS \end{gathered} \tag{29}$$

$$\begin{gathered} MININV_iINVCAP_i\left(1 - YINV_{i,snt}\right) \leq INVD^2_{i,t,sn} \\ \leq VSINV_iINVCAp_i\left(1 - YINV_{i,t,sn}\right) \\ \forall \ t, i \in TVS \end{gathered} \tag{30}$$

$$INV_{i,t,sn} = INVD^1_{i,t,sn} + INVD^2_{i,t,sn} \ \forall \ t, i.sn \in TVS \tag{31}$$

In Eqs. (29)-(31) $INVD^1_{i,t}$ & $INVD^2_{i,t}$ are disaggregated variables from the convex hull reformulation. Further, Eq. (32) prevents the tank discharge when the level is below the threshold value.

$$YW_{i',t,sn} \leq YINV_{i,t-1,sn} \ \forall \ t > 1, i \in TVS, \ i' \in SPTI_i \tag{32}$$

Here, the set $SPTI_i$ contains the splitters associated with tank i. In the case of period 1, the value of $YW_{i',t}$ is '0'. Splitter SP8 has only one pump and therefore can only handle one output stream. So, to distinguish the output streams going to unit CBU or to tank T5, we use binary variable $YI_{i,t}$ in following equations.

$$\sum_{s \in SI_i \backslash MS_i} F_{s,t} \leq YI_{i,t}GSCAP \ \forall \ t, i = CBU \tag{33}$$

$$\sum_{s \in SO_{i'} \backslash SI_i} F_{s,t} \leq \left(1 - YI_{i,t}\right)GSCAP \ \forall \ t, i = CBU, \ i' = SP8 \tag{34}$$

where GSCAP is the generic limit on the stream flow rates.

The production unit is set to satisfy the demand which varies from one time interval to another and is denoted by $DEM_{s,t}$ (demand has to be satisfied with all products and time periods).

$$F_{s,t,sn} = DEM_{s,t,sn} \ \forall \ t, s, sn \ \in FP \tag{35}$$

where *FP* is a set of streams containing final products.

A final inventory level is defined and enforced for the last time interval of the production using parameter $INVfin_i$:

$$INV_{i,t,sn} + \partial^+_{i,t,sn} + \partial^-_{i,t,sn} = INVfin_i \ \forall \ t = tfin, i \in ST \tag{36}$$

$$0 \leq \partial^+_{i,t,sn} \leq UB_i \ \forall \ t = tfin, i \in ST \tag{37}$$

$$-UB_i \leq \partial^+_{i,t,sn} \leq \ 0 \ \forall \ t = tfin, i \in ST \tag{38}$$

where $\partial^+_{i,t,sn}$ and $\partial^-_{i,t,sn}$ are slack variables to accommodate the deficit or excess of final product compared to $INVfin_i$, and UB_i is imposed as an upper bound on both slack variables.

3.3.3. Utility consumption

Only two utilities, electricity and gasoil, are considered here.

There are two types of electricity consuming units:

1) Consumption does not depend upon the stream flow rate, contained by set *EC* {LQU1, LQU2, P1-P9}.
2) Consumption depends upon the stream flow rate, contained by set *EV* {CU1-CU5, ECU1, ECU2, PTU}.

For (1)

$$UTCONS_{i,u,t,sn} = YI_{i,t,sn}UTRATE_{i,u} \ \forall \ t, i, sn \in EC, \ u = UE \tag{39}$$

where $UTCONS_{i,u,t,sn}$ is a variable accounting the consumption of utility *u* in unit *i* in time period *t* for scenario *sn*. $UTRATE_{i,u}$ denotes the rate of consumption of utility *u* by unit *i* during operation.

For units which consumption depends upon the stream flow rate, a piecewise linear function is defined as depicted in Fig. 6. Sector 'd1' indicates when there is no operation, sector 'd2' presents a region where electricity consumption is constant, while sector 'd3' shows the part where electricity consumption is proportional to the flow rate. Also, the

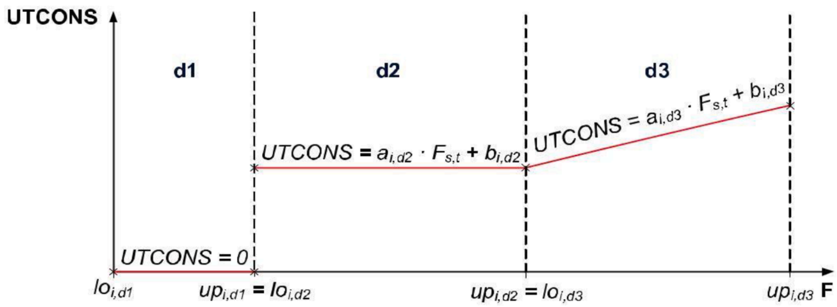

Fig. 6. Linear approximation of electricity consumption as a function of flow rate processed. d1 is oversized for visualization. Gathered from (Fernández et al., 2017).

upper limit ($up_{i,d1}$) of 'd1' is very small (≈0).

$$\bigvee_d \begin{bmatrix} Y_{i,d,t,sn} \\ a_{i,d}F_{s,t,sn} + b_{i,d} = UTCONS_{i,u,t,sn} \\ lo_{i,d} \le F_{s,t,sn} \le up_{i,d} \end{bmatrix} \tag{40}$$

$\forall\ t, i, sn \in EV,\ u = EC,\ Y_{i,d,t,sn} \in \{True,\ False\}$

Here, $a_{i,d}$ and $b_{i,d}$ are parameters of linear function denoting the consumption of electricity of unit *i* sector d. This disjunction gives rise to the equations:

$$\sum_d \left(\left(a_{i,d} Z_{i,d,t,sn} + b_{i,d} Y_{i,d,t,sn} \right) \right) = UTCONS_{i,u,t,sn} \quad \forall\ t, i, sn \in EV,\ u = UE \tag{41}$$

$$\sum_d Z_{i,d,t,sn} = \sum_{s \in SI_i} F_{s,t,sn}\ \forall\ t, i, sn \in EV \tag{42}$$

$$lo_{i,d} y_{i,d,t,sn} \le Z_{i,d,t,sn} \le up_{i,d} y_{i,d,t,sn}\ \forall\ d, t, i, sn \in EV \tag{43}$$

$$\sum_d y_{i,d,t,sn} = 1\ \forall\ t, i, sn \in EV \tag{44}$$

where $Z_{i,d,t,sn}$ is a disaggregated variable for the convex hull reformulation. The value of the binary variable $Y_{i,d,t}$ is enforced, for the internal units with variable electricity consumption, by:

$$1 - Y_{i,d,t} \le YI_{i,t} \le 1 - Y_{i,d,t}\ \forall\ t, i \in EV,\ d = d1 \tag{45}$$

Please, note that the external compressors are embedded in the set EV, while the external distillation column EDCU is not included, as it needs a different treatment and has been modelled as:

$$\sum_d Z_{i,d,t,sn} = \sum_{s \in MO_i} F_{s,t,sn}\ \forall\ t, i, sn = EDCU \tag{46}$$

$$lo_{i,d} y_{i,d,t,sn} \le Z_{i,d,t,sn} \le up_{i,d} y_{i,d,t}, sn\ \forall\ d, t, i, sn \in EDCU \tag{47}$$

$$MINCAPVOL_{i'} \left(1 - Y_{i,d,t,sn}\right) \le \sum_{s \in SO_i \setminus MO_i} F_{s,t,sn} \le CAPVOL_{i'} \left(1 - Y_{i,d,t,sn}\right) \quad \forall\ t, i, sn = EDCU,\ i' = ECU1 \tag{48}$$

$$\sum_d Y_{i,d,t,sn} = 1\ \forall\ t, i, sn = EDCU \tag{49}$$

$$1 - Y_{i,d,t} \le YI_{i,t} \le 1 - Y_{i,d,t}\ \forall\ t, i \in EO, d = d1 \tag{50}$$

where, *EO* contains the external units (e.g., {EDCU}).

The total energy consumed by the process is restricted in a given time interval due to contract requirements with energy suppliers. The breach of these contracts gives rise to penalties.

$$\sum_{i \in UPRI} UTCONS_{i,u,t,sn} + PHTR_{t,sn} + PLQ3_{t,sn} \le MAXPR1_{t,sn} + MAXPR2_{t,sn}\ \forall\ t, u, sn = UE \tag{51}$$

Here, the limits on the power consumed by the process networks are given by $MAXPR1_{t,sn}$ and $MAXPR2_{t,sn}$ including the units of the main process (*UPR1*) and the units of external supplier (*UPR2*). Parameters $PHTR_{t,sn}$ and $PLQ3_{t,sn}$ consider the power consumed by the machines working in discontinuous mode. Thus, to calculate the total electricity over the simulated time (*ECONS)*:

$$ECONS = TIME \sum_t \sum_i UTCONS_{i,u,t}\ u = UE \tag{52}$$

where *TIME* is a parameter representing the simulated time consisting of every time period of operation of every length of every time interval.

Only unit VU consumes gasoil. The fuel used during time interval *t*, is modelled by the continuous variable $UTCONS_{i,u,t,sn}$ which is proportionally related by the parameter $UTRATE_{i,u}$ to the flow rate $F_{s,t,sn}$ processed in that time interval in unit *i*.

$$UTCONS_{i,u,t,sn} = \sum_{s \in MS_i} F_{s,t,sn} UTRATE_{i,u}\ \forall\ t, i, sn = VU, u = UGO \tag{53}$$

The value of $UTRATE_{VU}$, *UGO*, is calculated using the lower heating value of the gasoil assuming a thermal efficiency (η) of 0.75. Hence, total utility *UGO* consumed over the complete simulated time (*GOCONS)* is calculated from $UTCONS_{I,u,t,sn}$ for the time length of the time interval (*TIME*):

$$GOCONS = TIME \sum_t \sum_i UTCONS_{i,u,t,sn}\ u = UGO \tag{54}$$

Also, VU and the corresponding tank T5 are only used if EDCU is not operated. This is modelled as:

$$YI_{i,t,sn} \le Y_{i',t,sn}\ \forall\ t, i, sn = VU, i' = EDCU \tag{55}$$

3.3.4. Objective function

We seek to maximize the profit of the plant denoted by the continuous variable *PROFIT*, which is computed as in Eq. (56)

$$PROFIT = SALES + DISC - EEC - GOC - MAINTENANCE\ COST \tag{56}$$

Here, *SALES* is the revenue generated from the product produced and is computed as in Eq. (57), *DISC* is the discount obtained from the external supplier when products are purchased from EDCU and is calculated as shown in Eq. (58), *EEC*, computed in Eq. (59), and *GOC*, computed in Eq. (60), are electricity and gas utility costs, respectively, and *MAINTENANCECOST* is the cost involved in the maintenance of compressors.

$$SALES = TIME \sum_t \sum_{s \in FP} F_{s,t} PRICE_s \tag{57}$$

$$DISC = TIME.DRATE\sum_t \sum_{s \in MO_i} F_{s,t} \; i = EDCU \tag{58}$$

$$EEC = TIME\sum_t \left(PCON_t ECONCOST_t + \left(\sum_t UTCONS_{i,u,t} - PCON_t\right).ECOST_t\right., u = UE \tag{59}$$

$$GOC = GOCONS.GOCOST \tag{60}$$

Where, DRATE is parameter relating the amount of product obtained through EDCU.

In the objective function (OF), several types of PENALTIES are deducted from the profit to prevent the model from incurring in abnormal schedules from a practical point of view (e.g., penalty associated with number of startup and shutoff of equipment, penalties associated with not meeting the required inventory for a particular storage tank at a particular instance of time etc.). Penalties help to make the operation more realistic. Thus, the value of *OF* provides the expected net profit.

$$OF = PROFIT - PENALTIES \tag{61}$$

Thus, M-ASUOPT is formulated from Eqs. (2)-(61). The adopted methodology allows solving M-ASUOPT for all the uncertain but plausible scenarios in a decoupled manner which enables the model flexibility for making changes in the first and second stage variables if required under any scenario. First stage variables correspond to input variables while second stage variables correspond to on/off decisions, operational settings etc. In this case we are considering uncertainty only in electricity price which is a first stage variable for this model. The second stage variables are unaffected with respect to electricity price scenarios with this methodology.

3.4. Risk analysis metrics

Model M-ASUOPT is solved for every plausible scenario, as described in Section 3.3, thus providing multiple solutions. Since scenarios are uncertain, there is a risk that the estimated profit is not achieved, which can affect the financial planning of decision makers. Therefore, we compute some risk metrics to deal with the risk associated with equally probable scenarios. All the risk metrics are described in detail by Knopf et al. (2015) and Medina-gonzález et al. (2017), yet a brief mathematical explanation follows. If the estimated profit value is denoted by 'Ω', then the risk metrics associated to this 'Ω' are calculated as follows:

a) $Risk_\Omega$: It calculates the probability of not achieving an estimated value (Ω) of the profit, and it is calculated by using Eq. (68):

$$Risk_\Omega = \sum_{sn} prob_{sn} Z_{\Omega sn} \tag{68}$$

where,

$$Z_{\Omega sn} = \begin{cases} 1, & Profit_{sn} \le \Omega \\ 0, & otherwise \end{cases} \tag{69}$$

a) Downside Risk (DR_Ω) represents the positive deviation of the expected profit from an estimated profit value, Ω, for different scenarios (represented by index *sn*). It is mathematically expressed as:

$$DR_\Omega = E\{\delta_{\Omega sn}\} = \sum_{sn} prob_{sn} \delta_{\Omega sn} \tag{70}$$

where,

$$\delta_{\Omega sn} = \begin{cases} \Omega - Profit_{sn}, & Profit_{sn} < \Omega \\ 0, & otherwise \end{cases} \tag{71}$$

Further, it is also important to gauge the performance of a solution (i.e., profit realization of the optimized scheduling plan) for any plausible scenario in terms of the statistical confidence level of achieving a defined target value. In this context, two risk management metrices are widely used by portfolio management institutions to reduce the expected losses and optimize the profit: VaR (Value at Risk) and CVaR (conditional value at Risk) (Sarykalin et al., 2008). Calculation of these risk metrices for our estimated profit provides us with a quantitative value of shortfall in the estimated profit, where a higher CVaR and VaR values indicate greater shortfall and vice versa. A detailed explanation and comparison of these metrices has been given by Rockafellar and Uryasev (2002). Use of these metrices, for similar case study, has also been performed by Li et al. (2021b). Therefore, these metrics can help the management team to choose for a low or high-risk scheduling strategy based on the risk-taking capacities.

4. Results

Model capabilities were tested using real-time data from an existing industrial facility located in Tarragona (Spain). Also, comparison of the forecasting techniques revealed that even though the Spanish electricity market has tariff periods and empirical relations to compute electricity prices for those periods, forecasting techniques for time-series data are better suited to compute the electricity prices. A detailed analysis of the findings is provided in ensuing subsections.

To achieve this, we used modified ASUOPT (Fernández et al., 2017) (M-ASUOPT) model and optimized in GAMS 25.0.1 (General Algebraic Modelling System)("GAMS software," n.d.) using the solver XPRESS v33.01 ("XPRESS Solver," n.d.) on a 64 bit/MS Windows 10 computer with Intel® Core™ i5–7500 CPU @ 3.4 GHz processor and 16 GB RAM. The model used 6.24 CPU-hours to solve for 100 scenarios in series. Note that this amount of time is already long enough considering that electricity prices change on a daily basis. If a traditional stochastic programming model, considering the 100 scenarios simultaneously, were to be solved, there is a significant risk that its solution will not arrive on time to provide a proper reaction to updated prices. In addition, the proposed methodology could be further expedited by parallelizing calculations, since scenarios are independent from each other.

4.1. Tariff periods and electricity price scenarios

To schedule the air separation plant, we need hourly electricity price values in advance for the selected time horizon. In the Spanish system, there are six different electricity tariff periods depending on the hour and on the typology of the day (i.e., working, weekend, vacation and not-working), which dictate the cost of the spot electricity prices. Specifically, electricity prices are calculated daily using the following relation:

$$P_i = A_i \times B_i + C_i \tag{72}$$

where P represents the electricity price, '*i*' represents the index for the tariff period, *A* is the base electricity price; *B* is a cofactor corresponding to tariff period and *C* represents additional costs. Hence, even for the same type of day and tariff period in a given month, hourly variations on the values of parameters A, B and C result in different electricity prices in the spot market (see Fig. 7a).

Historical electricity prices can be fed to the ARIMA method to forecast electricity prices for the different tariff periods in the future (Fig. 7b). However, there is always the possibility that the hourly electricity prices differ from the average price of their respective tariff periods. Indeed, a close comparison of Fig. 7a and b reveals that the

Hours

Days	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	47.3	45.5	44.5	44.5	44.7	44.2	45.1	46.2	47.9	49.6	48.7	47.2	46.5	46.5	51.6	59.1	62.1	64.2	60.7	59.1	52.0	55.0	50.2	47.1
2	45.8	45.0	46.9	50.2	59.1	65.0	65.0	68.5	66.0	65.8	65.0	61.2	59.7	61.0	69.2	72.2	73.2	70.1	65.0	60.1	58.8	54.7	52.7	49.3
3	45.0	45.2	49.3	57.7	70.5	71.6	72.7	73.3	73.3	72.7	71.7	70.5	69.9	71.1	72.8	73.7	74.3	74.9	71.6	68.7	67.4	62.7	56.0	54.1
4	52.0	51.4	53.0	62.4	72.3	73.0	73.0	72.9	72.5	71.7	71.6	69.0	67.1	68.3	72.2	73.3	73.7	72.5	69.3	65.0	62.0	51.2	48.4	50.0
5	47.5	42.3	45.2	54.1	66.2	69.7	72.6	73.0	72.6	72.5	71.5	71.1	70.5	69.7	73.9	75.2	76.1	73.7	71.7	66.8	69.2	59.6	54.0	52.1
6	48.1	46.7	48.4	53.3	60.2	63.2	66.2	70.6	71.0	71.5	71.0	68.5	65.6	66.2	70.6	73.9	74.7	75.1	75.1	73.9	71.7	66.0	60.0	56.0
7	52.0	50.8	50.7	54.1	56.3	61.3	67.2	73.5	70.7	70.7	70.1	70.0	64.9	60.2	70.0	76.5	78.3	73.9	73.5	70.1	66.1	69.2	61.1	55.5

a

Days	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	65.0	65.0	65.0	65.0	65.0	65.0	65.0	65.0	78.0	78.0	78.0	78.0	78.0	78.0	65.0	65.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
2	65.0	65.0	65.0	65.0	65.0	65.0	65.0	65.0	78.0	78.0	78.0	78.0	78.0	78.0	65.0	65.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
3	65.0	65.0	65.0	65.0	65.0	65.0	65.0	65.0	78.0	78.0	78.0	78.0	78.0	78.0	65.0	65.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
4	65.0	65.0	65.0	65.0	65.0	65.0	65.0	65.0	78.0	78.0	78.0	78.0	78.0	78.0	65.0	65.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
5	65.0	65.0	65.0	65.0	65.0	65.0	65.0	65.0	78.0	78.0	78.0	78.0	78.0	78.0	65.0	65.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
6	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0
7	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0	50.0

b

Days	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	59.4	52.9	48.3	46.6	47.7	51.7	57.5	63.7	68.7	71.1	70.4	66.8	61.4	55.5	50.8	48.6	49.5	53.3	58.9	65.0	69.8	72.1	71.3	67.6
2	62.1	56.1	51.4	49.1	50.0	53.7	59.3	65.3	70.0	72.3	71.5	67.9	62.3	56.4	51.6	49.4	50.2	53.9	59.5	65.4	70.2	72.5	71.7	68.1
3	62.5	56.6	51.8	49.5	50.3	54.0	59.6	65.5	70.3	72.6	71.8	68.2	62.7	56.7	52.0	49.7	50.5	54.2	59.7	65.7	70.4	72.8	72.0	68.4
4	62.8	56.9	52.2	49.9	50.6	54.3	59.8	65.8	70.5	72.8	72.1	68.5	63.0	57.0	52.3	50.0	50.8	54.4	60.0	65.9	70.7	73.0	72.2	68.6
5	63.1	57.2	52.5	50.2	50.9	54.5	60.1	66.0	70.7	73.1	72.3	68.7	63.3	57.4	52.6	50.3	51.1	54.7	60.2	66.2	70.9	73.3	72.5	69.0
6	63.5	57.6	52.9	50.6	51.3	54.9	60.4	66.3	71.1	73.4	72.7	69.1	63.7	57.8	53.1	50.8	51.5	55.1	60.6	66.5	71.2	73.6	72.9	69.3
7	63.9	58.0	53.3	51.0	51.7	55.3	60.7	66.6	71.4	73.7	73.0	69.5	64.1	58.2	53.5	51.2	51.9	55.4	60.9	66.8	71.5	73.8	73.2	69.6

c

Fig. 7. (a) Heat map for actual electricity prices during the first week of the year 2017, (b) Heat map for the electricity prices forecasted in the deterministic case, (c) Heat map for the electricity prices forecasted incorporating uncertainty in ARIMA.

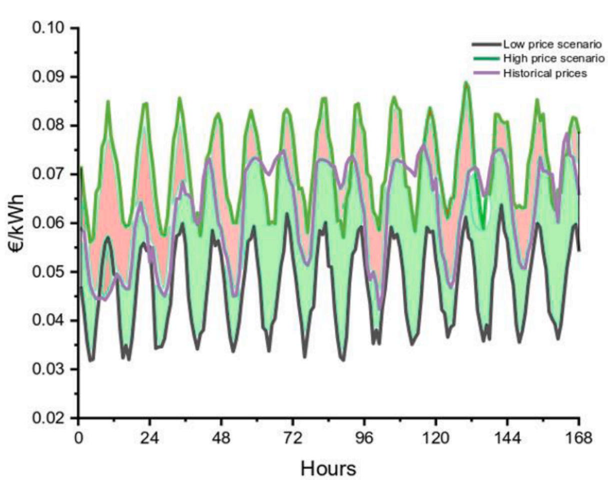

Fig. 8. Forecasted scenarios for the electricity cost during the first week of January using ARIMA and Monte Carlo scenario generation.

electricity price forecasted using empirical relations in low tariff periods is higher than in some higher tariff periods (and vice versa) on multiple occasions (47% price predictions higher than the actual price and 23% price predictions lower than the actual price, with 30% price predictions matching the actual price). This translates in an average relative error of ~70% which means that the deterministic approach (Fernández et al., 2017) might lead to high error in profit calculation under uncertain scenarios.

To overcome this limitation, we incorporate uncertainty into the electricity prices forecasted by means of ARIMA. For ARIMA, the average forecasting error is 15% in our case, which demonstrates that ARIMA prediction considering uncertainty can reduce the error in forecasting electricity prices if compared with the method previously used in Fernández et al., al.(2017) (15% vs 70%). This proves that scheduling of an energy-intensive plant based on ARIMA, which includes seasonality and weekly variation, leads to more realistic assumptions than those based only in tariff periods.

Therefore, MCSG is used to generate 100 discrete plausible scenarios for electricity prices of the subsequent week. The historical data for electricity prices was provided by the OMIE (Spanish electricity market regulator) for the years 2015,2016 and 2017. We used 3 months (12 weeks) of historical data to generate the scenarios for the upcoming week using our MCSG tool. A wide distribution of the generated scenario is shown in Fig. 8.

To validate the forecasting model and its output, a validation test for the similarity of historical and forecasted scenarios is first performed (Breeden and Ingram, 2010). Fig. 8 represents the forecasted 100 scenarios generated using MCSG for the second week of January 2017, where pattern similarity can be identified. Also, Kandell τ test for coefficient correlation is used to assess the degree of similarity between the two datasets ("Artificial Intelligence and Expert Systems," 2012). The range of Kandell τ test for similarity varies from $[-1, 1]$ where '-1' indicates a complete dissimilarity while '$+1$' denotes a complete similarity (Brossart et al., 2018). The average value for Kandell τ test for the predicted electricity price scenarios is 0.68. This means that the pattern of predicted electricity price scenarios has a strong resemblance to the pattern of historical electricity prices.

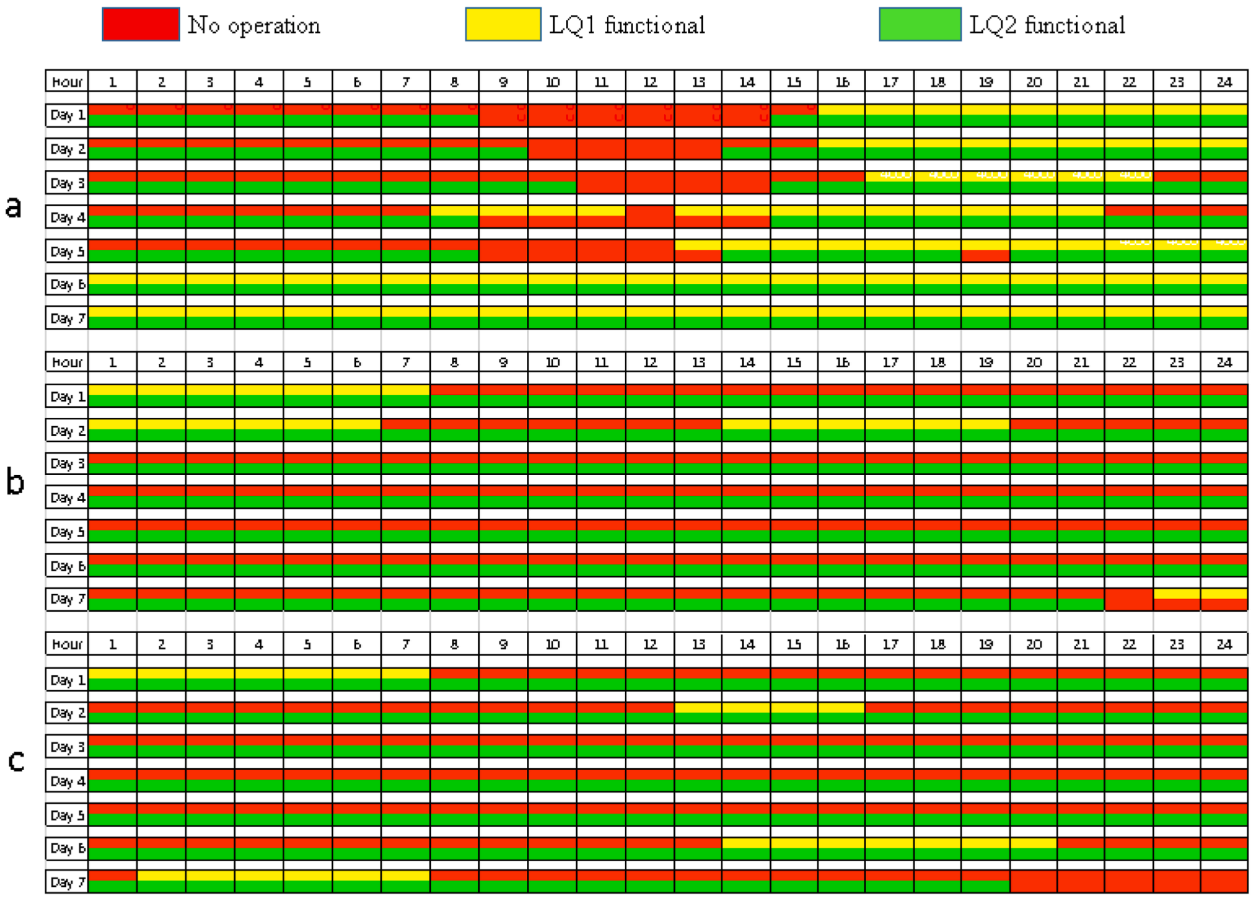

Fig. 9. Optimal scheduling schemes for (a) deterministic forecast of electricity prices (b) scenario corresponding to the lower quartile the profit distribution (c) scenario corresponding to the upper quartile of the profit distribution.

4.2. Scheduling

The modified ASUOPT model was executed for all the generated scenarios separately for the upcoming week (i.e., the model optimized the plant scheduling for each scenario for week 2). We observed that the scheduling plan changes in every scenario and is exclusive to its corresponding scenario, which also translates into the discreet profit value in each scenario. Thus, at the end, when all scenarios have been optimized, we get a profit distribution. For the ease of understanding the scheduling change, we plotted the operational and shut down hours of liquefiers of the plant during the whole scheduling horizon. As liquefiers are the units with the highest energy consumption, their operation has the largest impact on the optimal scheduling, with a tendency to determine the scheduling of other lesser energy-consuming units. The optimal schedule for the liquefiers' operation is illustrated in Fig. 9, with Fig. 9a providing the optimal scheduling scheme for the deterministic case using nominal forecasted electricity prices, while Figs. 9b and 9c correspond to the optimal schedules for the scenarios achieving the lower and upper quartile of the profit distribution, respectively. As expected, both liquefiers are not fully utilized despite the demand is satisfied in all periods (Fig. 9b and c). Hence, the model selects the most economical units based on power consumption, start-up time and production rate collectively. The reason for this is that startup of any energy consuming device causes a power surge on the system in turn consuming even more energy. Therefore, in our model we introduced penalties for frequent startup/shutdown of the plant units and, thus, the model tries to reduce the penalties incurred due to the number of start-ups and shut down of each unit. Hence, some units are over-utilized under economically optimized scheduling. From Fig. 9b and c, it can be observed that, despite their similarities, the optimal scheduling schemes tend to reduce the implementation of alternative units as we move towards higher price scenarios (i.e., low-profit values). This reduces the penalties incurred for multiple start-ups and shutdowns. For example, in this case, the lower quartile scheduling scheme (in Fig. 9b) uses LQ1 for fewer hours compared to upper quartile scheduling scheme (in Fig. 9c).

4.3. Risk analysis

The deterministic optimization by Fernández et al. (2017) obtained a profit of 547,323 €, but as mentioned in Section 3.3, electricity prices vary on an hourly basis for spot market and cannot be forecasted with utmost certainty. Thus, a deterministic plant scheduling based on a single scenario will not capture the essence of the problem. To deal with the uncertainty, the methodology explained in Section 3.1 has been used to generate multiple scenarios for one week. For scenario-based approaches, a common practice is to compare base, best and worst case, although depending upon the level of uncertainty the number of

Table 1
Statistics summary of the different risk metrics evaluated with a 95% confidence. Lq: lower quartile profit; Uq: upper quartile profit.

Targeted profit	Ω (€)	$Risk_{\Omega}$	VAR (95)	CvaR (95)	DR_{Ω}	% deviation from $\Omega_{Average}$
$\Omega_{Worst\ case}$	440,644	–	–	–	–	6.305
$\Omega_{Average}$	477,312	0.566	−0.040	−0.052	0.560	0
Ω_{Median}	476,849	0.500	−0.039	−0.051	0.500	0.097
Ω_{Lq}	470,301	0.253	−0.025	−0.038	0.750	1.469
Ω_{Uq}	480,479	0.750	−0.046	−0.058	0.220	−0.664
$\Omega_{Best\ case}$	509,922	0.990	−0.101	−0.113	0.100	−6.940
$\Omega_{Deterministic}$	547,323	–	–	–	–	−14.079

scenarios required to achieve a certain confidence level in the predictions may be as high as 50, or even higher (Mohamed and Bouhania, 2014). In our case, we generated 100 scenarios for analysis to incorporate a wide spectrum of different possible realization within the feasible range. The result of this optimization of scenarios provides with multiple scheduling plans and a distribution of profit values which allows us to evaluate risk metrices corresponding to the scenario. Risk metrics provide the decision-makers with insight on the associated risk with the expected profit target in a particular scenario. For example, CVaR allows to evaluate the likelihood that a specific loss will exceed a certain value at risk (VaR) for a given confidence level (Vieira et al., 2018). Therefore, if a decision-maker chose the best case scenario for profit, they would be open to approximately 32,000 (= Ω x% deviation from $\Omega_{Average}$) € of value loss (over a one week period) with a 95% confidence level of achieving the calculated profit in this case.

Table 1shows the results for four representative cases: average, median, lower quartile and upper quartile profit values. Table 1indicates that all scenarios obtain profit (from +6.9% in the best scenario to –6.3% in the worst-case when compared to the average profit value of 477,312 €). The last column of Table 1shows the deviation from the expected profit in the different scenarios while the RISK value in the second column gives a fair idea about the selection of the scenario (the higher the target value, the higher the potential shortfall). The negative sign '- 'in CVaR/VaR indicates shortfalls. Table 1indicates that the deterministic profit has a positive deviation from the $\Omega_{Average}$ by a fair margin (~14.1%) but is more exposed to any variation in the electricity cost due to its different prediction model as depicted in Fig. 7 using heatmap. A conservative decision-maker choosing the scheduling corresponding to the optimal solution with the lower quartile or worst case profit, has the possibility of deviating from attainable average profit value by positive ~1.5% and ~7% respectively, while a risk-taking decision-maker (i.e. preferring upper quartile or best case scenario) would have a possibility of overshooting the average profit target value by negative ~0.6% and ~6.9%, respectively, and would also be exposed to the risk of falling short of the calculated profit (Ω_{Uq}) by 5.8% of Ω_{Uq}. For the worst-case scenario (where the profit is virtually uninfluenced by uncertainty) we are undershooting by 6.3% the expected average profit. This can also be seen in Fig. 10a and b, which depict the distribution of simulated expected profits. The spread of calculated profits distribution fits the normal curve which is expected as the MCSG uses normal distribution for generating the electricity price scenarios. Fig. 10b shows the expected shortfall in the case of choosing the scheduling from the lower quartile scenario, where CVaR(95) is 0.025 and the expected shortfall corresponds to 11,758 € from the targeted profit value.

4.4. Correlation amongst operational variables

In the cryogenic air separation plant, variation in profit is also correlated with the electricity sold back to the grid after having been bought from the futures market in the past. The Spanish electricity market maker has a derivative product called 'SWAP' (OMIE, n.d.) which allows the electricity consumer to sell back the unused contracted power in the futures market or in real time market. The market maker applies a penalty for breach of power contract and takes a commission for enabling the 'SWAP' to sell back the unused contracted power. In Fig. 11 we have presented a scenario in which how the contracted power can be surplus. For low spot market prices, the model schedule the plant for maximum production in those hours thus it becomes possible by the end of scheduling period some contracted power is unused and swapping back of this power presents with a better economic solution then letting the contract expire without use.

Energy blocks from futures market are purchased in two categories: weekday blocks and weekend block. Thus, we calculate the credits received from the electricity company for electricity sold back to the grid (Eliq) using:

$$Eliq = (TCP - TCC)_{Weekday} + (TCP - TCC)_{Weekend} \tag{73}$$

where TCP is total cost of energy block purchased and TCC is total cost of energy consumed.

Fig. 12 shows the values of output variables (i.e. profit, cost of electricity consumed, and revenues from electricity sold back to the grid) corresponding to the different targeted profit values.

Analysis of Fig. 13 suggests that expected profit has a reverse behaviour with the electricity sold back to the grid: the lower the 'Eliq', the higher the expected profit, which clearly indicates the importance of a good match of the ratio for the energy blocks to be purchased and the amount energy to be consumed from Spot market. Fig. 12 shows this behaviour for all the 100 scenarios.

5. Conclusions

We have developed a methodology to address the scheduling problem of energy intensive industries under the uncertainty of energy market operating 24 × 7 and applied it to optimally operate a cryogenic air separation plant under electricity price uncertainty for short term scheduling. The case study presented in this contribution corresponds to an installed ASU facility located in Tarragona, Spain. All the model parameters and the ARIMA method for forecasting electricity prices have been tuned to accurately represent the reality of this specific unit. We have used a discrete scenario approach due to the weekly pattern in the spot electricity prices and in the purchase orders. Further, we hybridized deterministic simulation optimization approach with the discrete scenarios, which resulted in the simplicity of deterministic optimization while incorporating the effectiveness of stochastic considerations by covering a wide range of electricity price scenarios while keeping calculations to a minimum. To develop this approach, we have used a MILP formulation, time series forecasting with ARIMA, and

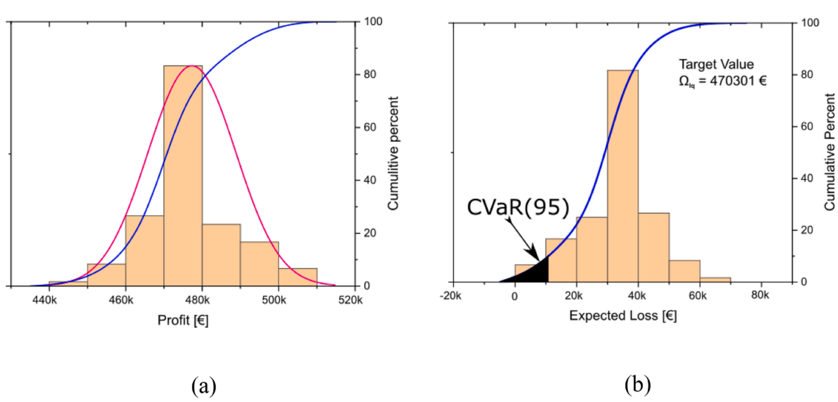

Fig. 10. (a) profit and (b) shortfall of the calculated profit value for lower quartile scenario.

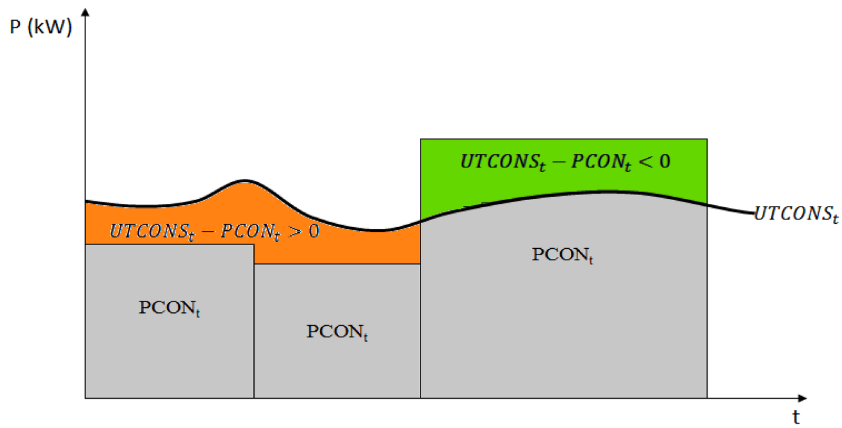

Fig. 11. An example of electricity consumed depending upon power contracted.

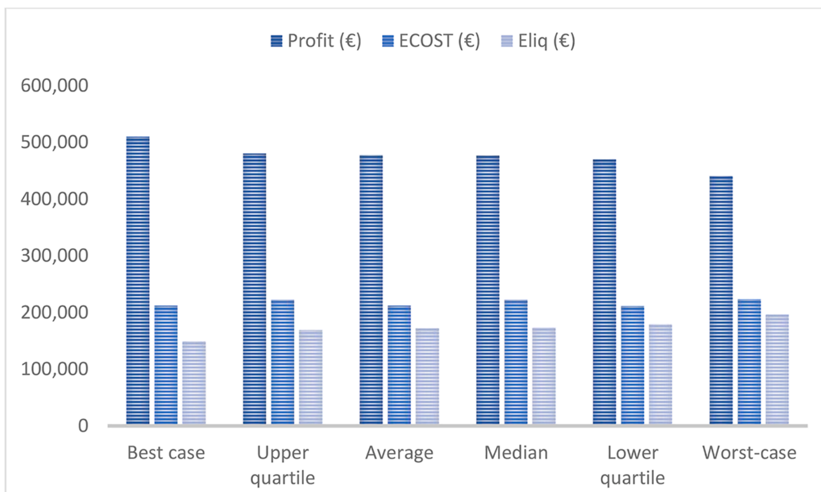

Fig 12. Output variable values for scenarios considered for risk analysis.

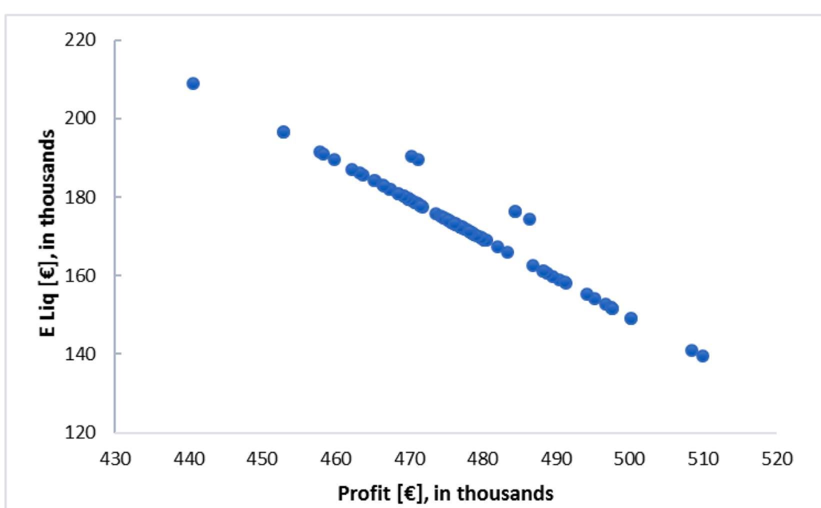

Fig. 13. Expected profit vs electricity liquidation correlation. 'Eliq' is the credit received for the electricity sold back to the grid. This process is implied under the assumption that the consumer is selling all the surplus contracted power at the spot price in real time market.

Monte-Carlo scenario generator. The MILP effectively copes with changing electricity prices while maximizing the plant performance. To this end, decisions on flow rates, starts-up and shutdowns of unit operations, and purchase orders are optimized according to the market needs of the existing industrial facility (i.e., demand of liquid N_2, O_2 and Ar and gaseous N_2 and O_2). To forecast hourly electricity prices (*e.g.*, spot market electricity prices) ARIMA model is used with a forecasting accuracy of 85%. The demonstrated approach is computationally affordable and easy to implement. Realistic process scenarios were analysed to exhibit and establish the usefulness of this methodology. The computational time for this scenario-based analysis was 6.24 CPU-hours for 100 scenarios (in series computation) with a 7-day (168 h) horizon period. The methodology uses a discrete scenarios approach, and thus can easily be used under the paradigm of parallel computing to significantly reduce the computational time by a factor of number of processors used. The optimization using 100 scenarios entailing different electricity prices shows how these prices affect the plant profit. In the situation of power limitations, the model adjusts the operation to fulfil contractual and demand liabilities, hence avoiding economic penalties. Expected profit values obtained (440,644€ - 509,922€) provides decision-makers with a wide range of probable values of the profit. Risk analysis facilitates the decision making of stakeholders in choosing a probable scenario for optimizing the scheduling of the plant with the risk involved for respective scenario by providing values of risk metrices associated (i.e. 0.566 for Ω_{average}) and expected shortfall (i.e. 0.052 for Ω_{average}) for each scheduling. Overall, the model identifies the most profitable ways to operate the plant under the uncertainty of electricity prices in near future. It assists managers to select one probable scenario (based on risk taking capacities) and help them plan their daily activities by effectively optimizing production planning, energy rules, sales and product stocks, at the same time considering external constraints and dynamic market conditions. The output of the methodology also helps financial planning of the organization in a subsequent manner from the insights of risk analysis. Thus, our method provides an encouraging alternative that can be extended to other energy-intensive industrial processes.

In general, the developed methodology is generic and can be easily implemented for the scheduling of any energy intensive industry operating 24 × 7 under the uncertainty of electricity price market. Also, the computational time can further be reduced by considering a fewer number of scenarios pertaining to statistically significant values while sampling the scenarios for simulation and optimization and using parallel computing.

The scope of this work can be extended in future by implementing the optimization of contracted power based on the prediction of spot electricity market and planning the scheduling under the scenarios of different power contracts and spot electricity price scenarios to reduce the losses incurring because of the breach of the power contract.

CRediT authorship contribution statement

Sachin Gangwar: Conceptualization, Methodology, Software, Formal analysis, Investigation, Data curation, Writing – original draft, Writing – review & editing, Visualization. **David Fernández:** Software, Investigation. **Carlos Pozo:** Conceptualization, Software, Writing – review & editing, Supervision. **Rubén Folgado:** Resources. **Laureano Jiménez:** Conceptualization, Resources, Writing – review & editing, Supervision, Project administration. **Dieter Boer:** Conceptualization, Resources, Writing – review & editing, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The data that has been used is confidential.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2023.108234.

References

Acevedot, J., Pistikopoulos, E.N., 1998. Stochastic optimization based algorithms for process synthesis under uncertainty. Comput. Chem. Eng.
Artificial Intelligence and Expert Systems, 2012. Lees' Loss Prevention in the Process Industries. Elsevier, pp. 2201–2312. https://doi.org/10.1016/b978-0-12-397189-0.00030-6.
Associates, C.R., 2005. Prime on Demand Side Management 2017-Janua, 71.
Breeden, J.L., Ingram, D., 2010. Monte Carlo scenario generation for retail loan portfolios Monte Carlo simulation 399–410. https://doi.org/10.1057/jors.2009.105.
Brossart, D.F., Laird, V.C., Armstrong, T.W., 2018. Interpreting Kendall's Tau and Tau-U for single-case experimental designs. Cogent Psychol 5, 1–26. https://doi.org/10.1080/23311908.2018.1518687.
Cao, Y., Huang, L., Li, Y., Jermsittiparsert, K., Ahmadi-Nezamabad, H., Nojavan, S., 2020. Optimal scheduling of electric vehicles aggregator under market price uncertainty using robust optimization technique. Int. J. Electr. Power Energy Syst. 117, 105628 https://doi.org/10.1016/j.ijepes.2019.105628.
Cao, Y., Swartz, C.L.E., Baldea, M., Blouin, S., 2015. Optimization-based assessment of design limitations to air separation plant agility in demand response scenarios. J. Process Control 33, 37–48. https://doi.org/10.1016/j.jprocont.2015.05.002.
Cao, Y., Swartz, C.L.E., Flores-cerrillo, J., 2016. Optimal Dynamic Operation of a High-Purity Air Separation Plant under Varying Market Conditions. https://doi.org/10.1021/acs.iecr.6b02090.
Castro, P.M., Grossmann, I.E., Zhang, Q., 2018. Expanding scope and computational challenges in process scheduling. Comput. Chem. Eng. https://doi.org/10.1016/j.compchemeng.2018.01.020.
Charitopoulos, V.M., Dua, V., 2017. A unified framework for model-based multi-objective linear process and energy optimisation under uncertainty. Appl. Energy 186, 539–548. https://doi.org/10.1016/j.apenergy.2016.05.082.
Chen, Y., Feng, X., Li, Z., Xu, Y., Miragha, A., 2020. Multi-stage coordinated operation of a multi-energy microgrid with residential demand response under diverse uncertainties. Energy Convers. Econ. 1, 20–33. https://doi.org/10.1049/enc2.12002.
Conejo, A.J., Plazas, M.A., Espinola, R., Molina, A.B., 2005. Day-Ahead Electricity Price Forecasting Using the Wavelet Transform and ARIMA Models. IEEE Trans. Power Syst. 20, 1035–1042. https://doi.org/10.1109/TPWRS.2005.846054.
Dias, L.S., Pattison, R.C., Tsay, C., Baldea, M., Ierapetritou, M.G., 2018. A simulation-based optimization framework for integrating scheduling and model predictive control, and its application to air separation units. Comput. Chem. Eng. 113, 139–151. https://doi.org/10.1016/j.compchemeng.2018.03.009.
Dowling, A.W., Kumar, R., Zavala, V.M., 2017. A multi-scale optimization framework for electricity market participation. Appl. Energy 190, 147–164. https://doi.org/10.1016/j.apenergy.2016.12.081.
Dowling, A.W., Zavala, V.M., 2018. Economic opportunities for industrial systems from frequency regulation markets. Comput. Chem. Eng. 114, 254–264. https://doi.org/10.1016/j.compchemeng.2017.09.018.
Elmore, C.T., Dowling, A.W., 2021. Learning spatiotemporal dynamics in wholesale energy markets with dynamic mode decomposition. Energy 232, 121013. https://doi.org/10.1016/j.energy.2021.121013.
Energy Use in Industry - Energy Explained, Your Guide To Understanding Energy - Energy Information Administration [WWW Document], n.d. URL https://www.eia.gov/energyexplained/index.php?page=us_energy_industry#tab1 (accessed 6.21.19).
EViews.com [WWW Document], n.d. URL http://www.eviews.com/home.html (accessed 7.29.20).
Fernández, D., Pozo, C., Folgado, R., Guillén-Gosálbez, G., Jiménez, L., 2017. Multiperiod model for the optimal production planning in the industrial gases sector. Appl. Energy 206, 667–682. https://doi.org/10.1016/j.apenergy.2017.08.064.
Finn, P., Fitzpatrick, C., 2014. Demand side management of industrial electricity consumption: promoting the use of renewable energy through real-time pricing. Appl. Energy 113. https://doi.org/10.1016/j.apenergy.2013.07.003.
GAMS software [WWW Document], n.d. URL https://www.gams.com/products/gams/gams-language/.
Gao, X., Knueven, B., Siirola, J.D., Miller, D.C., Dowling, A.W., 2022. Multiscale simulation of integrated energy system and electricity market interactions. Appl. Energy 316, 119017. https://doi.org/10.1016/j.apenergy.2022.119017.
Gebreslassie, B.H., Guillén-Gosálbez, G., Jiménez, L., Boer, D., 2009. Economic performance optimization of an absorption cooling system under uncertainty. Appl.

Therm. Eng. 29, 3491–3500. https://doi.org/10.1016/j.applthermaleng.2009.06.002.
Grossmann, I.E.I., Caballero, J.A.J., Yeomans, H., 1999. Mathematical programming approaches to the synthesis of chemical process systems. Korean J. Chem. Eng. 16, 407–426. https://doi.org/10.1007/BF02698263.
Ierapetritou, M.G., Wu, D., Vin, J., Sweeney, P., Chigirinskiy, M., 2002. Cost Minimization in an Energy-Intensive Plant Using Mathematical Programming Approaches. Ind. Eng. Chem. Res. 41, 5262–5277. https://doi.org/10.1021/ie011012b.
Jakaša, T., Andročec, I., Sprčić, P., 2011. Electricity price forecasting – ARIMA model approach. In: 2011 8th International Conference on the European Energy Market (EEM), Zagreb, Croatia, pp. 222–225. https://doi.org/10.1109/EEM.2011.5953012.
Kelley, M.T., Baldick, R., Baldea, M., 2020. Demand response scheduling under uncertainty: chance-constrained framework and application to an air separation unit. AIChE J. 66 https://doi.org/10.1002/aic.16273.
Kelley, M.T., Pattison, R.C., Baldick, R., Baldea, M., 2018. An MILP framework for optimizing demand response operation of air separation units. Appl. Energy 222, 951–966. https://doi.org/10.1016/j.apenergy.2017.12.127.
Kelley, M.T., Tsay, C., Cao, Y., Wang, Y., Flores-cerrillo, J., Baldea, M., 2022. A data-driven linear formulation of the optimal demand response scheduling problem for an industrial air separation unit. Chem. Eng. Sci. 252, 117468 https://doi.org/10.1016/j.ces.2022.117468.
Knopf, P.M., Teall, J.L., 2015. Risk Neutral Pricing and Financial mathematics: A primer, Risk Neutral Pricing and Financial Mathematics: A Primer. Elsevier Inc. https://doi.org/10.1016/C2014-0-00295-X.
Li, Z., Xu, Y., Feng, X., Wu, Q., 2021a. Optimal Stochastic Deployment of Heterogeneous Energy Storage in a Residential Multienergy Microgrid with Demand-Side Management. IEEE Trans. Ind. Informatics 17, 991–1004. https://doi.org/10.1109/TII.2020.2971227.
Li, Z., Xu, Y., Wu, L., Zheng, X., 2021b. A Risk-Averse Adaptively Stochastic Optimization Method for Multi-Energy Ship Operation under Diverse Uncertainties. IEEE Trans. Power Syst. 36, 2149–2161. https://doi.org/10.1109/TPWRS.2020.3039538.
Mazengia, D.H., 2008. Forecasting spot electricity market prices using time series models. In: 2008 IEEE Int. Conf. Sustain. Energy Technol, pp. 1256–1261. https://doi.org/10.1109/ICSET.2008.4747199.
Medina-gonzález, S., Pozo, C., Corsano, G., Guillén-gósalbez, G., Espu, A., 2017. Using Pareto filters to support risk management in optimization under uncertainty: application to the strategic planning of chemical supply chains 98, 236–255. https://doi.org/10.1016/j.compchemeng.2016.10.008.
Merkert, L., Harjunkoski, I., Isaksson, A., Säynevirta, S., Saarela, A., Sand, G., 2015. Scheduling and energy - Industrial challenges and opportunities. Comput. Chem. Eng. 72, 183–198. https://doi.org/10.1016/j.compchemeng.2014.05.024.
Misra, S., Kapadi, M., Gudi, R.D., Srihari, R., 2017. Energy-Efficient Production Scheduling of a Cryogenic Air Separation Plant. Ind. Eng. Chem. Res. 56, 4399–4414. https://doi.org/10.1021/acs.iecr.6b04585.
Mitra, S., Grossmann, I.E., Pinto, J.M., Arora, N., 2012. Optimal production planning under time-sensitive electricity prices for continuous power-intensive processes. Comput. Chem. Eng. 38, 171–184. https://doi.org/10.1016/j.compchemeng.2011.09.019.
Mohamed, K., Bouhania, G., 2014. Scenario-Based Methods and the Complexity of 04, 157–168.
Oberdieck, R., Diangelakis, N.A., Nascu, I., Papathanasiou, M.M., Sun, M., Avraamidou, S., Pistikopoulos, E.N., 2016. On multi-parametric programming and its applications in process systems engineering. Chem. Eng. Res. Des. 116, 61–82. https://doi.org/10.1016/j.cherd.2016.09.034.
OMIE, n.d. No Title [WWW Document]. URL https://www.omip.pt/en/electricity.
Pattison, R.C., Touretzky, C.R., Harjunkoski, I., Baldea, M., 2017. Moving horizon closed-loop production scheduling using dynamic process models. AIChE J 63, 639–651. https://doi.org/10.1002/aic.15408.
Rezaei, F., Najafi, A.A., Ramezanian, R., 2020. Mean-conditional value at risk model for the stochastic project scheduling problem. Comput. Ind. Eng. 142, 106356 https://doi.org/10.1016/j.cie.2020.106356.
Rockafellar, R.T., Uryasev, S., 2002. Conditional value-at-risk for general loss distributions. J. Bank. Financ. 26, 1443–1471. https://doi.org/10.1016/S0378-4266(02)00271-6.
Sahinidis, N.V., 2004. Optimization under uncertainty: state-of-the-art and opportunities. Comput. Chem. Eng. 28, 971–983. https://doi.org/10.1016/j.compchemeng.2003.09.017.
Sarykalin, S., Serraino, G., Uryasev, S., 2008. Value-at-Risk vs. Conditional Value-at-Risk in Risk Management and Optimization. State-of-the-Art Decis. Tools Information-Intensive Age 270–294. https://doi.org/10.1287/educ.1080.0052.
Scharfhausen, F.M., 2009. Electricity Tariff Structure: the Spanish case.
Smith, A.R., Klosek, J., 2001. A review of air separation technologies and their integration with energy conversion processes. Fuel Process. Technol. 70, 115–134. https://doi.org/10.1016/S0378-3820(01)00131-X.
Sorourifar, F., Zavala, V.M., Dowling, A.W., 2020. Integrated Multiscale Design, Market Participation, and Replacement Strategies for. Battery Energy Storage Syst. 11, 84–92.
Todd, D., Caufield, M., Helms, B., Starke, M., Kirby, B., Kueck, J., 2009. Providing Reliability Services through Demand Response: a Preliminary Evaluation of the Demand Response Capabilities of Alcoa Inc., Technical report ORNL/TM-2008/233.
Tsay, C., Kumar, A., Flores-cerrillo, J., Baldea, M., 2019. Optimal demand response scheduling of an industrial air separation unit using data-driven dynamic models R. Comput. Chem. Eng. 126, 22–34. https://doi.org/10.1016/j.compchemeng.2019.03.022.
U.S. Energy Information Administration, 2016. Chapter 7: industrial sector energy consumption [WWW Document]. Int. Energy Outlook. URL. https://www.eia.gov/outlooks/ieo/pdf/industrial.pdf. accessed 10.30.20.
Verderame, P.M., Elia, J.A., Li, J., Floudas, C.A., 2010. Planning and scheduling under uncertainty: a review across multiple sectors. Ind. Eng. Chem. Res. 49, 3993–4017. https://doi.org/10.1021/ie902009k.
Vieira, M., Paulo, H., Vilard, C., Pinto-Varela, T., Barbosa-Póvoa, A.P., 2018. Risk assessment for the design and scheduling optimization of periodic multipurpose batch plants under demand uncertainty. Computer Aided Chemical Engineering. https://doi.org/10.1016/B978-0-444-64235-6.50174-1.
Wang, Y.C., Chiu, M.C., Chen, T., 2020. A fuzzy nonlinear programming approach for planning energy-efficient wafer fabrication factories. Appl. Soft Comput. J. 95, 106506 https://doi.org/10.1016/j.asoc.2020.106506.
Weron, R., 2014. Electricity price forecasting: a review of the state-of-the-art with a look into the future. Int. J. Forecast. 30, 1030–1081. https://doi.org/10.1016/j.ijforecast.2014.08.008.
Weskamp, C., Koberstein, A., Schwartz, F., Suhl, L., Voß, S., 2019. A two-stage stochastic programming approach for identifying optimal postponement strategies in supply chains with uncertain demand. Omega (United Kingdom) 83, 123–138. https://doi.org/10.1016/j.omega.2018.02.008.
Wu, C.B., Huang, G.H., Li, W., Xie, Y.L., Xu, Y., 2015. Multistage stochastic inexact chance-constraint programming for an integrated biomass-municipal solid waste power supply management under uncertainty. Renew. Sustain. Energy Rev. https://doi.org/10.1016/j.rser.2014.09.019.
XPRESS Solver [WWW Document], n.d. URL https://gams.com/latest/docs/RN_26.html.
Zamarripa, M., Marchetti, P.A., Grossmann, I.E., Singh, T., Lotero, I., Gopalakrishnan, A., Besancon, B., André, J., 2016. Rolling Horizon Approach for Production-Distribution Coordination of Industrial Gases Supply Chains. Ind. Eng. Chem. Res. 55, 2646–2660. https://doi.org/10.1021/acs.iecr.6b00271.
Zhang, Q., Bremen, A.M., Grossmann, I.E., Pinto, J.M., 2018. Long-Term Electricity Procurement for Large Industrial Consumers under Uncertainty. Ind. Eng. Chem. Res. 57, 3333–3347. https://doi.org/10.1021/acs.iecr.7b04589.