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Process supply chains: Perspectives from academia and industry

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ABSTRACT

Process systems engineering (PSE) has been an active research area for nearly seventy years and addresses multiple systems from the process industry. Among these are Process Supply Chains that can be described as interconnected sets of entities responsible for the sourcing, production and distribution of a large set of chemical and/or bio- based products. Due to the high diversity of materials, processes and information flows such networks result in highly complex systems that are very difficult to manage. The PSE community has a critical role to support the design and management of such systems through the development of tools that are able to address such complexity. Focusing initially on a real-world process supply chain, the industrial gas supply chain, this paper identifies and discusses current contributions, challenges and perspectives in process supply chains that can guide research professionals to address such challenges. In general, such challenges encompass supply chain scope representations, modeling approaches, data management and implementation. Examples include supply chain risk and uncertainty, multiscale decisions, sustainability and resiliency.

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1. Introduction

Supply chains (SC) play a crucial role in organizations as they are responsible to guarantee product and service availability to the final consumer and accordingly the financial success of the involved entities. Nevertheless, the management of such systems is quite complex due to the multiplicity of material and information flows, diversified characteristics of entities, and often-present contradicting objectives. Moreover, the high level of uncertainty inherent to supply chain operations further augments its complexity.

Additionally, process supply chains face challenging market and societal demands that are characterized by shorter product life-cycles, mass customization, the drive for more sustainable processes and products and the rapid and effective supply of products (Barbosa-Povoa, 2014). To cope with such challenges, process supply chains must be flexible, resilient and efficient, while guaranteeing customers' specific demands at minimum cost, under an uncertain environment.

The Process Systems Engineering (PSE) community can make an important contribution to address the challenges above through the development of tools that support the required process supply chain flexibility (Barbosa-Povoa, 2014). Such contributions already exist and span from strategic (e.g. Network Design in Cardoso et al., 2013 and Mitra et al., 2014a) to tactical (e.g. Planning in You and Grossmann, 2013 and Malinowski et al., 2018) and operational problems (e.g. scheduling, routing and inventory management in Amaro and Barbosa-Povoa, 2008; Dong et al., 2014; and Zhang et al., 2016a).

Several works provide a detailed analysis of such contributions and challenges. Sargent (2005), in his paper "Process Systems Engineering: a retrospective view with questions to the future", stated that the process systems techniques can play an important role when addressing supply chains by helping to identify the real problems and to address them. In the same year, (Shah 2005) identified the main requirements of process supply chains, focusing on the pharmaceutical case. (Papageorgiou 2009) provided a comprehensive review of the design and planning of process supply chains. (Stephanopoulos and Reklaitis 2012) highlighted the contributions and future of the PSE community in several areas, from which supply chain was identified as essential. (Grossmann 2012) presented the enterprise–wide optimization concept and highlighted the need of developing optimization tools that explore the integration of decisions across the different operations along the supply chain, considering different levels of detail. (Lainez-Aguirre et al., 2012) reviewed developments for the pharmaceutical supply chain and (Barbosa-Povoa 2014) investigated the literature on process supply chain considering multiple decision levels. (Garcia and You 2015) reviewed the multi-scale,

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multi-objective and multi-player aspects of the process supply chain as major technical challenge areas, while looking at the integration of supply chain design with operation decisions. Recently, (Barbosa-Povoa et al., 2018a) reviewed sustainable supply chains and concluded that particularly (bio) process supply chains have been actively addressing sustainability issues. However, there are still many research opportunities to address.

All the above reviews converge to a common set of critical problems, some under investigation by the research community, whereas many others require further attention. Additionally, it is important to mention that different types of process supply chains are emerging, and additional opportunities will appear in the near future. Examples are the new energy supply chains such as hydrogen, solar, waste-to-value and biomass.

This paper focuses on the past, present and future of Process Supply Chains from an industrial and academic perspectives. Rather than providing a comprehensive review of the numerous scientific achievements in the field, its objective is to assess the challenges that exist in the area from an industrial and academic perspectives on process supply chains by focusing on the industrial gas supply chain, as well as to point to current and future research challenges that are important to be undertaken based on industrial needs.

The paper is organized as follows. In the next section, we illustrate some of the existing opportunities in the context of a real-world, complex process supply chain – the industrial gas supply chain. While some challenges have been addressed, the implementation of PSE is still far from effective. Thus, significant progress is still required in addressing critical issues, both from an industrial and an academic perspective, as discussed in Section 3. Finally, in the last section we conclude that process supply chain research has a major potential financial impact on the process industry and brings scientific challenges where the PSE community has an unquestionable role to play.

2. Process supply chains

According to the process industry chain framework as presented by (Marquardt et al., 2000), process supply chains are at the macro scale level (see Fig. 1). Such systems deal mainly with chemical, bio-based networks and involve a diverse and large set of entities, materials and information that have the common goal of transforming raw materials into final products, using different types of transforming processes, so as to satisfy market demand in terms of quality, quantity and time.

Process supply chains are diverse and range from the utilities and oil and gas sectors to environmental and food chains. Due to their diversity and complexity, several challenges exist when managing such systems and subsequently both industrial and the academic communities should be dedicated to address such challenges in close collaboration.

Although every supply chain has its own features, we use the industrial gas supply chain as an example of process supply chains where its different characteristics are described, and corresponding challenges identified.

2.1. Industrial gas supply chain

The manufacturing of Oxygen, Nitrogen and Argon is considered, as well as the retail business (hardgoods). The supply chain comprises upstream, production, distribution and consumer entities (Fig. 2). Other process gas supply chains such as carbon dioxide, helium and hydrogen are not discussed in this paper.

Electricity can be purchased from utility companies through various power contracts that differ in price, availability, and penalty for under- or overconsumption (Zhang et al., 2016a). Discount prices and penalties can also be defined with respect to the amount of electricity purchased over a certain period, which could be hours, days, or even weeks. In practice, this means that the cumulative electricity purchase must be recorded, and there are pre-defined meter reading times at which the amount of electricity purchased since the last meter reading is computed. Based on this cumulative electricity purchase between consecutive readings, discounts and penalties are issued (Zhang et al., 2016b).

Cryogenic air separation plants produce liquid oxygen (LO2), nitrogen (LN2) and argon (LAr) as well as gaseous oxygen (GO2) and nitrogen (GN2), all at high purities. Cryogenic processes achieve separation through liquefaction followed by low-temperature distillation. All liquid products can be stored on-site in storage tanks. In contrast, gaseous products cannot be stored and must be delivered immediately to customers.

Regarding distribution, industrial gas companies serve customers through three primary distribution modes: large process plants, cryogenic liquid and packaged gases (PAG) (Megan and Bruton, 2017).

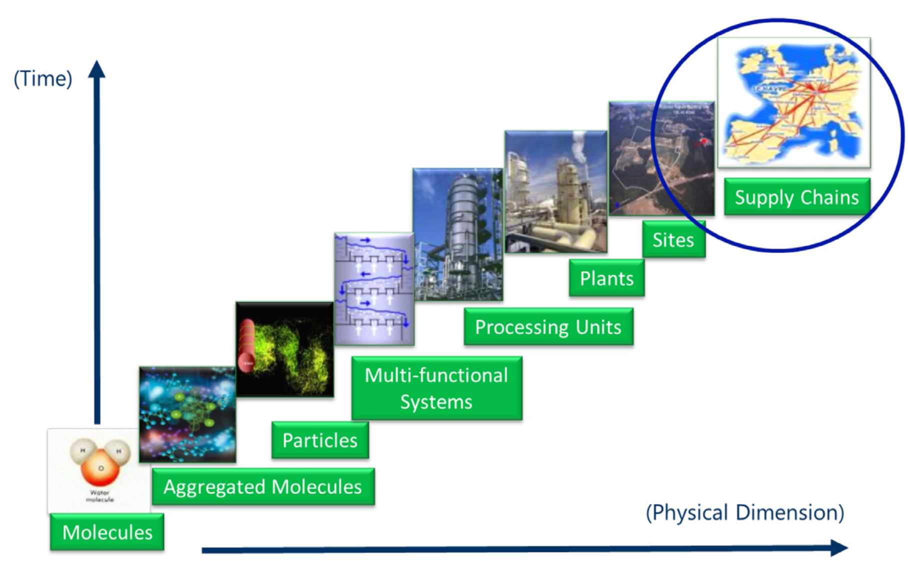

Fig. 1. Process Industry Chain (adapted from Marquardt et al., 2000).

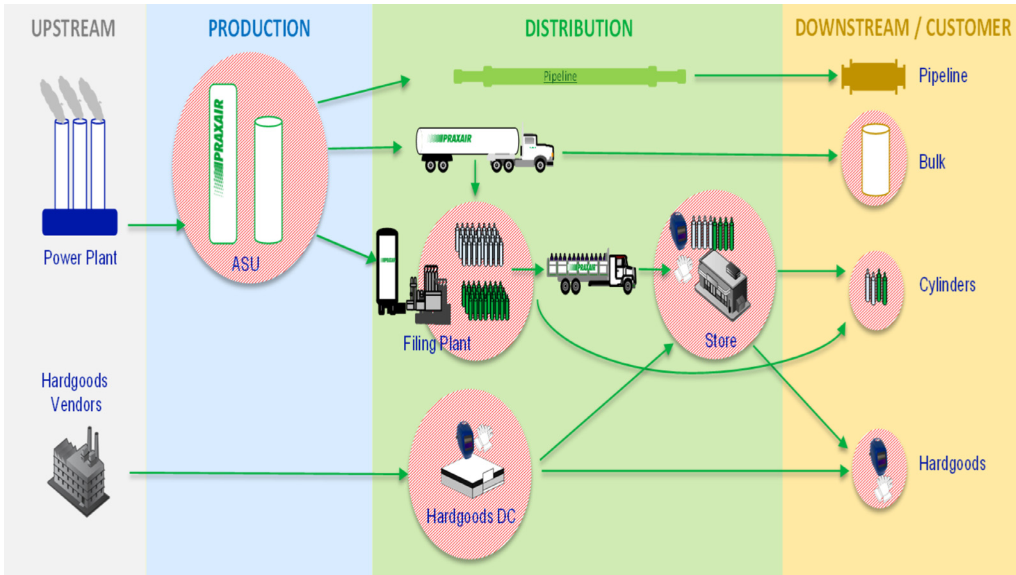

Fig. 2. Industrial Gas Supply Chain (Praxair, Inc.).

For the largest customers, such as refineries and steel mills, industrial gas plants operate adjacent to their facilities and distribute products via pipelines. Air separation units are built on or adjacent to customers' sites to continuously supply atmospheric gases at required pressure levels, which act as feedstocks or reactants. Their role is typically similar to that of utility and water companies. In case of disruption in plant production, liquid products are vaporized and sent to pipelines, In the extreme case that liquid storage is depleted, liquid is brought in from neighboring plants.

Liquified products from air separation units serve medium-volume customers (2500 to 250,000 m^3/month) at multiple pressure levels in multiple industries, such as electronics, chemicals, healthcare, pharmaceuticals, among others. Customer facilities have liquid storage tanks with remote telemetry. The liquid product is vaporized to serve the companies' needs. Tank inventory is monitored in real-time and product is delivered by a tanker-truck fleet. The industrial gas supplier determines the most cost-effective time and date to replenish the tank inventory, making sure the customer does not run out of product. This is also referred to as a vendor-managed inventory model.

The delivery of packaged gases constitutes the third mode and involves the largest number of customers. These range from small retail to large manufacturing sites. These customers require industrial, medical and specialty gas mixtures; the latter are needed for high value applications such as semiconductor manufacturing, calibration, and laser cutting. As seen in Fig. 2, cylinders are either distributed directly to customers or shipped to depots or stores, from which additional deliveries are made or customers pickup their products. The industrial gas company typically owns the cylinder assets and leases them to customers. Cylinders have regulators that provide flow control as well as pressure and time-to-empty readings; for some high-value products, telemetry is also provided. Effective management of cylinder inventory across the supply chain is critical for maintaining holding costs and service levels. Differently from the liquid customers, most packaged gas customers place orders rather than rely on vendor-managed inventory policies.

In addition to cylinders, stores also retail hardgoods that are purchased from vendors and shipped through multiple distribution centers. These in turn either ship products directly to customers or to stores for pickup or further delivery. Deliveries of hardgoods are made with third party companies and range from small packages to multiple pallets. Major costs involve product handling, shipping and inventory.

The above industrial gas supply chain clearly illustrates the complexity of the design and management of real-world supply chains and the need for a systems approach that is able to define and solve its underlying challenges, thus providing the necessary tools and processes to support decision-makers. Being the focus of PSE the systematic and model-based solution of process systems problems, where systems thinking and systems problem solving are prioritized rather than the mere application of computational problem-solving methods (Karsten-Ulrich and Marquardt, 2009), the PSE community must play an active role in providing the right solutions to present and future process supply chain challenges.

2.2. Literature review of industrial gas supply chains

The goal of this section is to review the contributions made in the PSE area, regarding industrial gas supply chains. Contributions from the authors are addressed in detail in the next sections and therefore are not presented here.

Within the industrial gas supply chain, there are a few contributions that focus on its individual elements or subsections. Ierapetritou et al. (2002) focused on the scheduling of air separation plants based on a two-stage stochastic programming approach for uncertain power prices. (Zhu et al., 2011) focused on the operation of air separation units to capture uncertain electricity prices and product demands; the authors developed a multiperiod nonlinear programming formulation that includes a nonlinear, dynamic first-principle model. (Cao et al., 2016) provided a dynamic strategy of product liquefaction and vaporization for air separation units based on electricity prices and demand profiles. (Pattison et al., 2016) proposed a methodology to integrate control and scheduling decisions based on empirical models generated from operating data and applied to an air separation unit.

Manenti and Rovaglio (2013) expanded the scope to industrial gas supply chains by considering a network of air separation plants with power agreement contracts that contain multiple penalties and take-or-pay clauses, as well as liquid storage. (Puranik et al., 2016) addressed a similar problem by fitting a data-driven regression model for each equipment as a function of various input variables. These functions were then a part of an MINLP optimization problem to solve a network of plants and pipeline customers. However, this approach did not consider any liquid demand at the plants and assumed fixed energy prices at the plants.

In the context of liquid distribution, Campbell et al. (1998) presented the basic IRP (Inventory Routing Problem), reviewed existing solution methods and developed two new approaches based on integer programming and dynamic programming to solve the deterministic and stochastic versions, respectively. Campbell et al. (2002) presented a two-phase approach for solving the IRP that defines firstly the customers that receive a delivery on each day of the planning horizon and their delivery volumes, and secondly an insertion heuristic that determines vehicle routes and schedules. Campbell and Savelsbergh (2004a) addressed the IRP from a delivery volume perspective and described a linear time algorithm for optimizing delivery volume. Various extensions that occur in practice were introduced and modifications of the solution method were described. Savelsbergh and Song (2008) developed a variation of the IRP, namely the IRP with continuous moves (IRP-CM). In this case, the customers are served using sleeper teams that distribute product over multiple days, picking product at multiple facilities and moving continuously. In (Campbell and Savelsbergh 2004b), the authors developed a two-phase approach to solve large scale instances; phase 1 consists of an integer program to determine a high-level plan for a longer time horizon that consists of which customers to serve on each day and an estimate of volume to be delivered to them. Phase 2 then converts Phase 1 output into routes by using an insertion heuristic with a scoring function.

One of the few contributions that focused on the integrated industrial gas supply chain is Marchetti et al. (2014), who proposed a multi-period mixed-integer linear programming model including production plants, distribution depots, gas customers and liquid customers. It assessed the benefit of optimal coordination by testing different strategies ranging from fixed sourcing to dynamic sourcing of multi-plant/depot system. The production model included multiple sites capable of operating at various modes with focus on the cost of electricity. Distribution was modeled as an IRP, with a general framework for generating a list of feasible routes and entering a subset of proposed routes as an input to the fully coordinated network optimization model. Misra et al. (2018) focused on formulating the same problem to curtail the number of binary variables to make the network computationally efficient, by dividing the distribution network into regions to guide the optimizer to select the vehicles closest to the plants. Zamarripa et al. (2016) proposed a rolling horizon approach on the full-space optimization problem. It decomposes the problem by dividing the time horizon into detailed and aggregated blocks.

3. Challenges

This section describes the main research and implementation challenges from an industrial perspective and how they have been addressed by the PSE community, including joint academia-industry collaborations Within the industrial perspective four main challenges are addressed: supply chain modeling; different modelling approaches; data and implementation. The academic perspective focuses on how previous industrial needs have been addressed, as well as on novel academic challenges. These are multiscale modeling; uncertainty, risk and resilience modeling; sustainability modeling; efficient solution methods; and data management. It is important to note that the topics covered in this section represent the background and experience of the authors and should not be considered a comprehensive review.

3.1. Industry perspective

Given the wide variety of features encountered in process supply chains and in particular in industrial gases supply chains, it is not surprising that a large number of planning and scheduling models can be found in the literature. Modeling challenges within the supply chain involve the accurate representation of the key decisions regarding sourcing, production and distribution at the scheduling and planning levels. On the other hand, it is critical to develop models which are also computationally tractable. Consequently, approaches that address uncertainty and multiscale problems must be carefully incorporated to have a real-world impact. As supply chain models are data intensive, these must integrate with modern techniques that involve advanced analytics and big data. Finally, multiple implementation challenges are discussed, such as the "build vs. buy" dilemma and the computational performance of software tools, as well as the management of change regarding the work process and the end-users of these tools.

3.1.1. Supply chain scope challenges

Supply Chain Planning – Planning the merchant liquid supply chain is a very challenging problem (Marchetti et al., 2014; Zamarripa et al., 2016; Zhang et al., 2017; Misra et al., 2018). Liquid plants, while all making the same basic set of products, often vary in capacity and efficiency. As merchant liquid customers may receive shipped product from multiple locations, continuously optimizing this supply chain can be challenging. Uncertainties, such as varying customer demand and time-of-day electricity prices, make the system quite dynamic. There is a need for sophisticated forecasting tools (Weron, 2018) and large mixed integer linear programming models in order to determine optimum production and distribution plans on a continuous basis (Marchetti et al., 2014; Zamarripa et al., 2016; Zhang et al., 2017; Misra et al., 2018). These planning tools, which should plan over a multi-week time horizon, then must guide the operational tools designed for minute-to-minute optimization of the plants and logistics.

Fig. 3 illustrates the hierarchical decision-making process. At the tactical level, a planning optimization tool minimizes the overall sourcing, production and distribution costs within a cluster of plants and customers, as well as defines the plant production schedule and allocates production and customers to plants. Production decisions are enforced through real-time optimizers and model predictive controllers. Once customers are allocated to plants at the planning level, routing decisions are made, either manually or with inventory routing solvers.

Many supply chain problems are traditionally solved in a sequential fashion due to work processes and technological limitations. Nevertheless, benefits may be obtained if they are integrated in a single optimization model. For instance, in the PAG business the shuttle distribution optimization suggests how frequently products are delivered to stores. Ideally, this problem should be solved in tandem with a multi-echelon cylinder inventory optimization by trading-off distribution costs and the capital cost associated with the required cylinders. The resulting model is a large-scale MINLP which calls for customized solution/decomposition strategies.

Demand Side Management (DSM) – DSM refers to electric energy management on the consumers' side and encompasses energy efficiency and Demand Response (DR). DR presents challenges and opportunities, primarily the optimization of operational flexibility through the integration of production and energy management. On the strategic level, large industrial electricity consumers often enter into long-term contracts with favorable rates. However, such power contracts require the consumers to commit themselves to the amount that they are going to purchase years in advance when future demand is not yet known with certainty. Hence, there is the need to simultaneously optimize long-term electricity procurement and production planning while considering uncertainty in product demand (Zhang et al., 2018). Regarding mid-term (tactical) decisions, the main challenge is to integrate energy management, production, sourcing and customer-plant allocation (Zhang et al.,

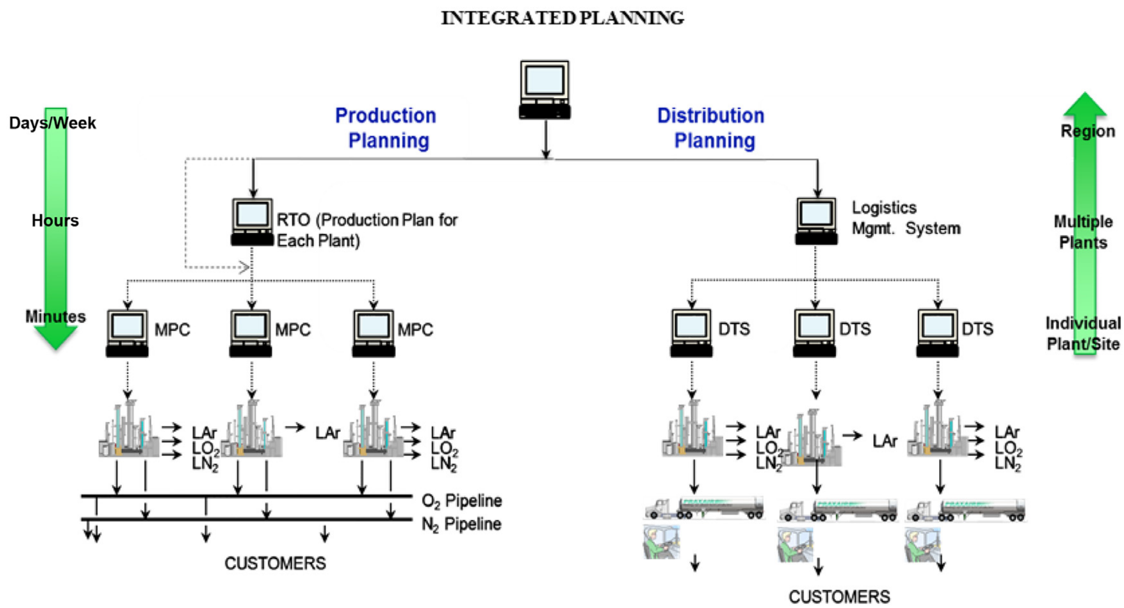

Fig. 3. Hierarchical decision-making process.

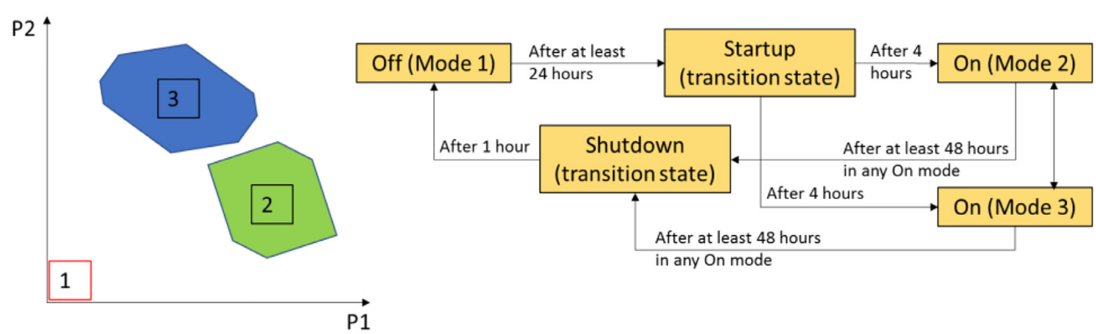

Fig. 4. (a) Surrogate model in product space and (b) transition modes.

2017). This coordination problem gives rise to a multiscale optimization model because while a detailed production scheduling representation must capture all critical operational constraints on a fine time grid, vehicle routing can be considered in each time period of a coarser time grid.

Process Modeling – The traditional way of modeling a process involves heat and mass balances, which requires the detailed description of the system's performance (e.g. thermodynamics, kinetics). The disadvantage of this approach is that the model can become prohibitively hard to solve in the context of supply chain optimization due to its nonlinearities and its size. An alternative approach is to build surrogate models in reduced space, e.g. the product space. To determine the feasible region of the plant in the product space, production data can be obtained from extreme operating points or from a sequence of steady-state simulations. Moreover, production modes may represent state of equipment, e.g. "off", "production mode" or "ramp-up transition." Only one mode can be active, in other words the modes are disjoint. The data for each mode is represented as a collection of operating points (slates) that are the extreme points in terms of the products (Mitra et al., 2014 a; Zhang et al., 2016 a).

Fig. 4 shows an example of the feasible operating region of a process in two- dimensional product space, in terms of flow rates. In this case, there are two products (P1 and P2) and three operating modes. The feasible space of mode 1 is a single point (zero production). Modes 2 and 3 are described by two polytopes; these represent approximations of the true feasible region, which is in general nonconvex and nonlinear. Transitions between different modes can be represented via a transition graph, also shown in Fig. 4, with four different modes (off, on, startup and shutdown). The arcs indicate the directions and the corresponding time constraints (Zhang et al., 2016 a). With respect to Fig. 4a, mode "on" could encompass

As discussed in (Harjunkoski et al., 2014) in the context of production scheduling but generalizable to supply chains, modeling of time can be classified into (i) precedence vs time-grid based, (ii) global vs. local or unit-specific and (iii) continuous vs. discrete time domain. Industrial gas supply chain models fall into a network, rather than a sequential structure and are naturally represented as time grid models (Harjunkoski et al., 2014). Existing supply chain models are represented as global grids in discrete time but there are opportunities in achieving higher solution efficiency by addressing unit specific and continuous time representations, particularly in route scheduling.

In terms of modeling elements, models can be classified into batches and material amounts (Harjunkoski et al., 2014). Interestingly, in the context of industrial gas supply chains, bulk processes are logically represented in terms of material amounts, whereas packaged gases are represented as batches. Finally, there are significant opportunities in capturing transient operations and complex plant behavior (Cao et al., 2016; Pattison et al., 2016; Zhu et al., 2011) as well as key process variables that impact

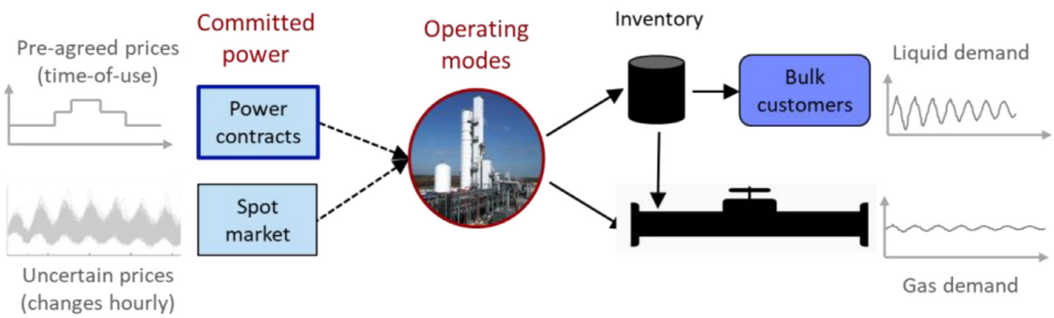

Fig. 5. Uncertainties in the industrial gas supply chain.

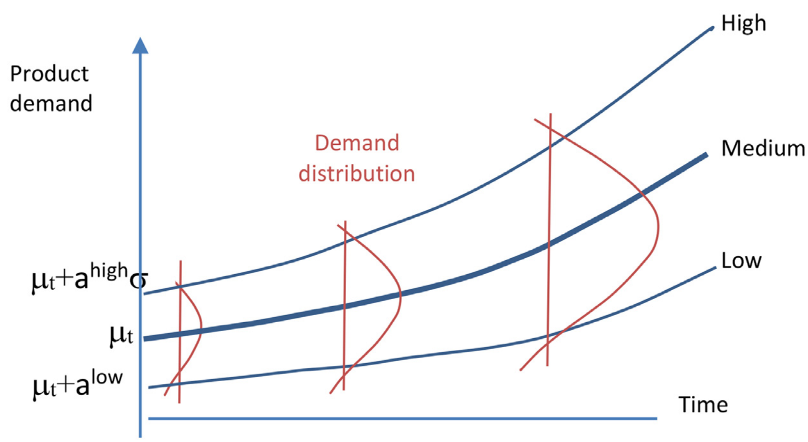

Fig. 6. Product demand trajectories in short term and long term (Mitra et al., 2014a). Parameters μ_t and σ_t denote the expected demand and the standard deviation in time t.

optimal conditions. Main challenges are that the resulting models would become dynamic and nonlinear, as opposed to the existing (mixed integer) linear planning and scheduling models.

Ye et al. (2019) investigated the tradeoff between design and operations based on a superstructure with equipment redundancy. Using a Markov-chain based MILP framework, the authors introduced stochastic failures and repair schedules in order to calculate the optimal number of units in order to maintain plant availability.

Inventory Route Planning – Executing a Vendor Management Inventory (VMI) policy in an effective way is nontrivial, because it requires the integration of two components of SC management, inventory control and distribution routing (Dong et al., 2014). In inventory control, the goal is the determination of orders (time and amount) of customers, while in distribution routing the goal is the generation of schedules to meet these deliveries. Delivery frequency to customers should be such that they are visited when their tank levels are close to safety stock levels. The integration of the two problems, which can have a dramatic impact on overall system performance, leads to the inventory routing problem (IRP) which is at the heart of all VMI policies. The main objectives in solving the IRP are to reduce the overall distance driven per volume delivered to customers while ensuring that there are no product outages, which have a sustainability impact by reducing fuel emissions and managing supply risk.

3.1.2. Challenges in modeling approaches

Uncertainty – Uncertainty plays a crucial role in the management of the supply chain. Electricity prices may fluctuate on an hourly basis in certain markets; moreover, to ensure the stability of the power grid, backup capacities are called upon when electricity supply does not meet demand due to unexpected changes in the grid (Fig. 5). As part of demand response efforts in recent years, industrial gas companies are encouraged by financial incentives to provide such operating reserve in the form of load reduction capacities (interruptible load). However, a major challenge lies in the uncertainty that one does not know in advance when load reduction will be requested (Zhang et al., 2016c).

Although industrial gas sites operate at a very high level of availability, there are circumstances in which there are unplanned shutdowns that are caused by electricity supply and/or equipment failure. As mentioned in the previous section, typically plants are directly connected to customer by pipelines to supply gaseous products. Liquid storage tanks are usually installed onsite to be used as a backup when the plant is in outage. Assuming there are data for historical reliability data of individual assets, the main question is how to make design and operations decisions to maximize plant availability. Supply chain management plays an important role in supplying liquid products during plant downtime to guarantee uninterrupted supply to pipeline customers (Fig. 5). Hence, the study of supply chain resiliency could bring benefits to the industry.

Besides electricity and plant availability, demand uncertainty plays a pivotal role in production planning & scheduling, inventory routing as well as in long-term capital investments (Mitra et al., 2014b). Fig. 6 illustrates product demand uncertainty in short term and long-term decisions, which ultimately affect all operational (production, routing), tactical (safety stock) and strategic (tank sizing, plant capacity) decisions.

Fig. 6. Product demand trajectories in short term and long term (Mitra et al., 2014a). Parameters μ_t and σ_t denote the expected demand and the standard deviation in time t.

Supply chain management is a dynamic process with new information continuously available and with multiple sources of uncertainty. Rescheduling is performed regularly to address uncer-

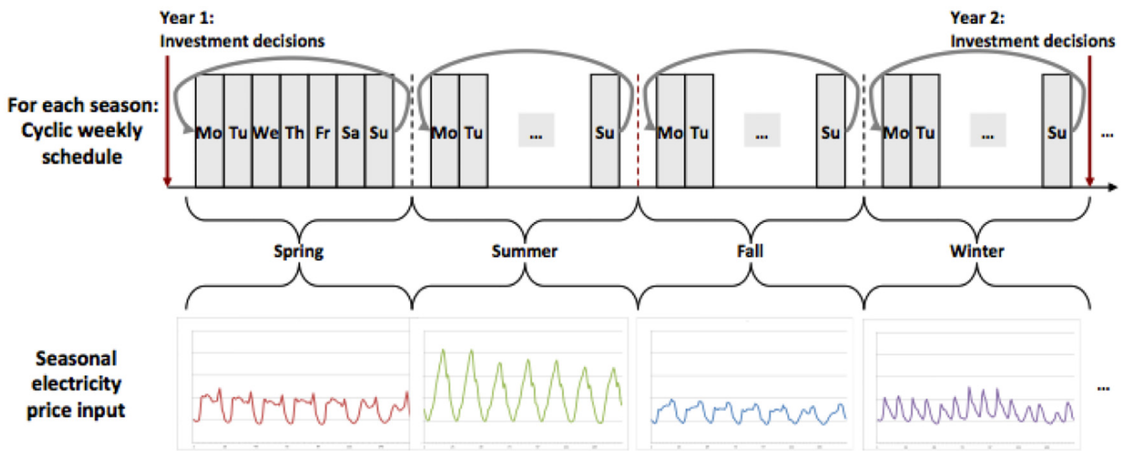

Fig. 7. Multiscale decisions in the industrial gas supply chain (Mitra et al., 2014 a).

tainty and the arrival of new information, e.g. resource availability (Harjunkoski et al., 2014). Rescheduling is typically done over a moving (rolling or receding) horizon framework by fixing part of the current solution. Alternatively, stochastic or robust optimization approaches can be used to explicitly account for uncertainty. As an example, it is important to characterize call-in orders uncertainty in the PAG route optimization to develop robust multi-period distribution models. The work of (Subramanyam et al., 2017) is a step towards this direction. Opportunities to evaluate customer delivery window flexibility and its impact in the distribution cost can be further explored with this type of models. To the best of the authors' knowledge there is no known implementation of approaches that account for uncertainty in process supply chains and particularly in industrial gas applications, given the challenges in representing scenarios or uncertainty sets and the computationally expensive approaches that address real-world problems.

Finally, in the context of inventory routing for the bulk business, in addition to customer demand, there are uncertainties with respect to travel times, service times at customers and delivery time windows, i.e., when customers allow access to bulk tanks. Such uncertainties depend on the time of the day, traffic accidents, weather conditions and other external factors. These may affect delivery times or even prevent deliveries at end of routes.

Multiscale Modeling – One of the biggest challenges for the design and long-term capacity planning of industrial gas plants is the incorporation of short-term operational decisions. Typically, capacity planning is performed over a 10 to 15-year horizon. Investigating the trade-off between capital or retrofit, and operating costs, related to electricity prices, which can vary on an hourly basis, leads to a complex multiscale optimization problem (Mitra et al., 2014a,b). Fig. 7 illustrates the multistage, multiscale nature of the problem, in which investments are reviewed annually, and operational decisions are made based on short term demand. In order to simplify operational decisions, four periods are defined for each year that correspond to the seasonal behavior of electricity prices. Furthermore, each season is considered with a representative week that is repeated cyclically and in which electricity prices are specified in an hourly basis. With the proposed approach, a one-year model is represented with 672 time slots (4 seasons with 168 h per week) in contrast to 8760 h in one-year.

At the tactical, mid-term level, there is also the need to coordinate multiple time scales. In this case, monthly plans must be defined to coordinate sourcing, production and distribution decisions, as in (Zhang et al., 2017). Production decisions are optimized at the hourly level to leverage energy price changes, whereas distribution decision require a coarser time grid to manage inventory levels in plant and customer sites, as well as fleet and driver utilization.

3.1.3. Data challenges

Data Availability and Management – Data must be available for the successful implementation of any decision-support solution. In many instances, data availability is a bottleneck. The most common internal data sources for supply chain applications are the business ERP system, spreadsheets, production historians and logistics systems. Unfortunately, data is in many cases inaccurate, incomplete or inconsistent. In this regard, effective master data management (MDM) becomes vital for the successful implementation of any supply chain management initiative. Increasingly, analytics can be used to cleanse, integrate and orchestrate data across multiple processes, systems, departments, lines of business and geographic regions. For instance, MDM can enforce business rules around data quality, prevent duplicate, inaccurate or incomplete data. ETL (Extract, Transform and Load) and machine learning tools help businesses in this regard by effectively curating the data, cleaning it up and writing it into MDM for use in decision-support solutions. Moreover, with the growing number of sensors available in the supply chain, real-time data has emerged as an MDM priority. Hence, high availability master data becomes a key requirement, as volume, velocity and variety of data increase. Inbound and outbound data processing is often a batch procedure in conventional MDM systems. Multidomain and multivector are emerging technologies that allow data systems to integrate several data domains and move towards an event driven or continuous process (Walker and Moran, 2017).

Data Analytics – Industrial gas plants require a high degree of automation and data analytics to ensure that they continuously operate safely, reliably and efficiently (Megan and Bruton, 2017). Examples include condition and predictive monitoring of equipment such as motors and compressors to reduce failures and therefore unplanned downtime. As with large process plants, the vendor managed inventory model for bulk customers requires a variety of analytics, from optimizing assets to scheduling daily deliveries. Packaged gases are a very transaction-intensive business with many distinct products, which leads to many opportunities to use analytics to manage the supply chain, understand margins and better target the sales force. Every supply chain planning activity requires forecasting tools to predict inputs such as customer demand and energy costs. Forecast accuracy is a common challenge within companies. Forecasts are used for different purposes, ranging from short term replenishment and capacity planning to long term investment and procurement contracts. It is important to note that demand at the customer level is important for the short term that is required by manufacturing, distribution center replenishment and customer shipment; whereas aggregate forecasting tends to be more accurate in the long term in cases such

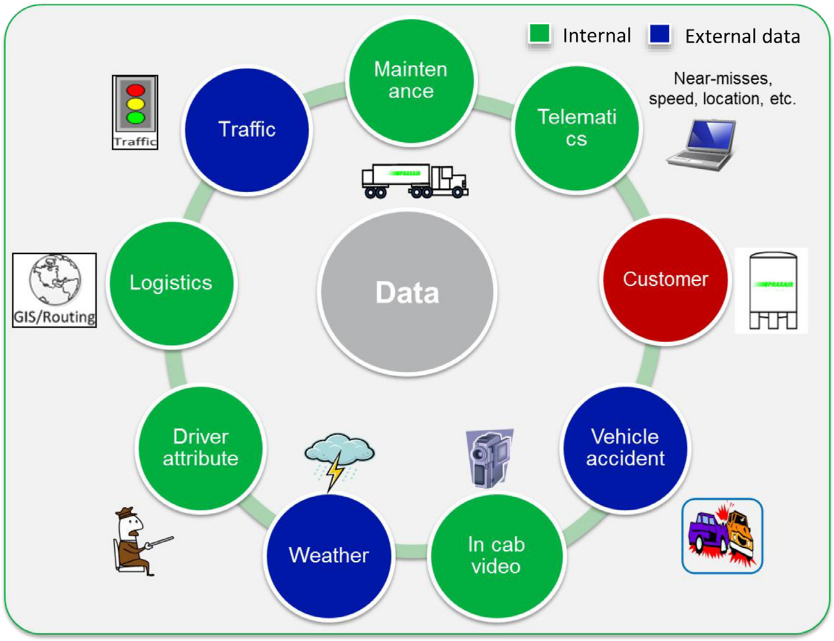

Fig. 8. Data sources for route optimization systems.

as strategic decisions on supply chain network design. Extending quantitative forecasting from the traditional statistical methods and time series analysis to more complex machine learning algorithms is an area that also requires further exploration in the industrial gas supply chain. Nevertheless, there are still some issues to address in this arena such as generation of confidence intervals and uncertainty estimation, minimization/avoidance of overfitting and model interpretation (Makridakis et al., 2018).

Big Data Analytics – There has been a paradigm shift in leveraging data for supply chain, particularly external data, which has been experiencing tremendous growth in the past few years. The traditional approach has been to utilize internal data, from few core applications that track the activity of the company and automate various processes. Internal data is mostly structured and stored in data warehouse(s). Moreover, data is relatively clean and models activity related to customers and processes. With the arrival of external big data, the number of systems and applications will multiply. External data will not be clean or structured; neither will be stored in data warehouses. Models will be a lot more complex as they will relate to both internal and external processes. In addition, a big data strategy must be defined and implemented.

Activities that can be directly impacted are customer service, inventory replenishment, dynamic pricing, credit checks, among others. In the context of the industrial gas supply chain the availability of external data presents new opportunities. A real-world application that would benefit from external data is route optimization (Fig. 8). In this context, plans that either result from Inventory Routing (IRP) or Vehicle Routing (VRP) policies typically rely on internal data sources, such as transactional logistics systems, fleet maintenance & telematics, and customer demand forecasting systems. Under this scenario, a plan is generated over a short-term horizon (one day to one week) and the goal is to execute the trips as closely as possible. Notwithstanding, external data such as traffic and weather, as well as accident data, can be used for real time dynamic routing. This business model would allow for added same-day new orders and existing plans could be continuously reoptimized. It is important to note that there are significant challenges in implementing such model because systems need to adapt much faster to last minute changes. Moreover, in this scenario real-time information must be passed back to logistics planning systems from either mobile apps or telematics solutions.

3.1.4. Implementation challenges

Enterprise Organization – Supply chain management provides an opportunity to integrate multiple functions within an organization, which are often siloed in their decision-making. However, the process of implementation of optimal supply chain decisions can be very challenging due to conflicting objectives. For instance, a decision-support tool that optimizes operational decisions in a plant would minimize the total power costs under varying hourly power prices; such a tool might recommend frequently switching equipment on and off to avoid consuming power during a peak time of the day. However, such frequent swings of an equipment will have adverse effects on its life, resulting in significant reduction in the availability of the overall plant. Similarly, from the distribution perspective, optimal inventory routing decision under a cost minimization objective would try to reduce product tank levels at customer locations as low as possible in order to save trips to the customer sites. However, under uncertainty, if the customers' usage increases, the tanks will run out of product sooner than predicted.

Software Tools – One of the main challenges in the development and implementation of decision-support software tools concerns the "build versus buy" decision. Off-the-shelf software presents itself as a faster and cheaper solution. However, off-the shelf software cannot satisfy every requirement or would demand significant effort to modify built-in features. This limitation leads to lack of customization, which can result in low software usage and in some cases even incorrect business decisions. Nevertheless, it is important to note that off-the-shelf solutions are preferred for companies with limited budget and technical proficiency or for companies for which technology resulting from the software would not result in competitive advantage. Proprietary software requires investment in people and resources and a comprehensive plan to develop and maintain. For instance, it may be advantageous to develop an integrated software platform rather than a set of multiple point-to-point solutions. Also, a comprehensive maintenance, support and update plan must be established for the long term; this involves a resourcing and funding model, which are equivalent to the annual fees paid to third-party software companies.

Supply chain planning tools will also need to be able to allow quick analysis through modern human machine interfaces and meet the ever-increasing expectation of improved solution time among supply chain decision-makers. Especially for short term operational decisions, this will lead to more frequent optimization and implementation of optimal decisions.

Computational Performance – The complexity of real-world industrial problems translates into large scale models, in terms of constraints and variables. Most supply chain problems result in mixed-integer linear programming models, which require the investigation of customized solution techniques to obtain good (not necessarily optimal) feasible solutions in reasonable time. Examples in strategic and tactical planning are: a hybrid bi-level decomposition scheme for a two-stage stochastic programming problem with mixed-integer recourse that results from a multi-scale capacity planning problem with investment and operational decisions (Mitra et al., 2014b), and Helium SC planning in which a rolling horizon strategy is developed (Malinowski et al., 2018). Short term examples are as follows: IRP for which a dynamic preprocessing algorithm followed by a two-level decomposition solution method (Dong et al., 2017), and production scheduling of air separation units under uncertainty, for which an integrated stochastic mixed-integer linear programming model is developed, Conditional Value-at-Risk (CVaR) is incorporated into the model as a measure of risk, and a strategy based on scenario reduction with multi-cut Benders decomposition is implemented to solve large-scale real-world instances (Zhang et al., 2016b). Increasing trend of on-demand high performance cloud computing will also aid in creating such tools allowing quicker analytics and optimization of complex supply chain networks.

Change Management – One of the main challenges in the implementation of decision support tools is the management of change with decision makers as well as with the business organization. Unfortunately, the PSE community does not have the training and often disregards the impact of change management in the successful implementation of optimization tools. The change management area has been primarily addressed by the business management community (Cameron and Green, 2015) and ranges from mergers & acquisitions to projects. Although not core to the PSE community, change management should be part of any implementation project. Indeed, there are opportunities to bring design thinking into the area to better understand the interrelationship between tools and decision makers.

Supply Chain Visibility – Companies are increasingly using methods such as “Supply Chain Digital Twin” to perform simulation and what-if analysis for linking low level operation level decision with total cost and high level strategic objectives (Schlager, 2018). Such tools aid supply chain decision-makers by providing full supply chain visibility (SCV) and effectively implement change management with all functions of the organization. Modern data visualization and BI (Business Intelligence) tools are also helping with SCV and making relevant supply chain data quickly available to the decision- makers to act upon. Such tools have the potential to transform how users interact with data and make decisions. The concept of supply chain control tower has emerged to provide supply chain visibility and deliver the information necessary to support collaboration and decision-making in real-time (Titze et al., 2018). Modeled like an airport control tower, a unified system, ideally at a single physical location, helps in implementing critical decisions with impact on the entire supply chain. As more data is available with digital enabled supply chains, the business case for this type of platforms is becoming more favorable.

3.2. Academic perspective

Process supply chains have been studied by the PSE community with increased focus in recent years. Different challenges have been addressed in line with some of the industrial needs mentioned in the previous section. These span from operational to strategic decision levels and have been covering different types of problems (Barbosa-Povoa, 2014), but further research is still required.

Multiscale Modeling – At the strategic level, optimal design and planning of supply chains is a well-known problem that, however, continuously faces new challenges. The integration of strategic and tactical decisions is still an area to explore where comprehensive models that account for different supply chain characteristics are required. For instance, uncertainty, sustainability, risk and resilience management should be targeted. Additionally, the availability of large amounts of data is nowadays a reality, which entails further study to lead to accurate industrial representations and allows further decision-sharing (Ning and You, 2017).

The integration of tactical-operational decisions is also an open issue that has been seldom studied. Supply chain planning and operations appear as a research opportunity, where production planning, inventory management and logistics decisions should be considered simultaneously. Multiscale supply chain models will help to answer to these challenges where Enterprise Wide Optimization approaches (Grossmann, 2012) ought to be explored. In this context, not only centralized supply chain decisions, as commonly treated by the academic community, should be analyzed but rather trade-offs between different supply chain entities need to be accounted for, where decentralized decisions are at stake (Sahay and Ierapetritou, 2014).

Game theoretic approaches may be used to address problems where conflicting objectives are often present. Some have been explored within the PSE community, including the effect of market competition. For instance, Nash-based approaches have been applied by (Gjerdrum et al., 2001;Gjerdrum et al., 2002) for the fair optimization of transfer prices among multi-enterprise supply chains. (Zamarripa et al., 2012) proposed the construction of Pareto-optimal fair solutions for supply chains under cooperative and competitive scenarios, whose pay-off matrix was computed through a series of multi-objective MILPs. The case of capacity planning in a competitive environment has recently been addressed by Garcia-Herreros et al. (2016) and Florensa et al. (2017) from a bilevel and a trilevel perspective, respectively. The strategic planning of petroleum refineries was recently studied through a game theoretic perspective by Tominac and Mahalec (2017), who formulated the problem as a game where several refineries are engaged in a Cournot oligopoly and solved the resulting non-convex (MI-)NLP. Hjaila et al. (2017) explored a Stackelberg-game-based approach for the coordination of multi-enterprise supply chains in a competitive uncertain environment. Yue and You (2017) used the Stackelberg-game-based approach for supply chain design and planning optimization, while recently (Gao and You 2018) studied the influence of multiple stakeholders' uncertain performance in non-cooperative supply chains.

Uncertainty, Risk, Resilience Modeling – uncertainty is inherent to supply chains. Different approaches exist to model it, such as constraint programming; multi parametric; fuzzy systems; among others – see the comprehensive review by Sahinidis (2004). However, with supply chains the main approaches explored have been stochastic and robust. The first one focuses on the establishment of representative scenarios to model uncertainty but the use of a large number of scenarios leads to intractable models. One possible way to tackle this problem is to explore the use analytics on uncertain parameters, e.g. in demand and supply so as to establish the most representative scenarios. Moreover, statistical, data mining or machine learning techniques, amongst others may also be explored. This has been studied by some authors (Yue and You, 2016; Lima et al., 2018) and constitutes an emerging research area. An example is shown in Fig. 9, based

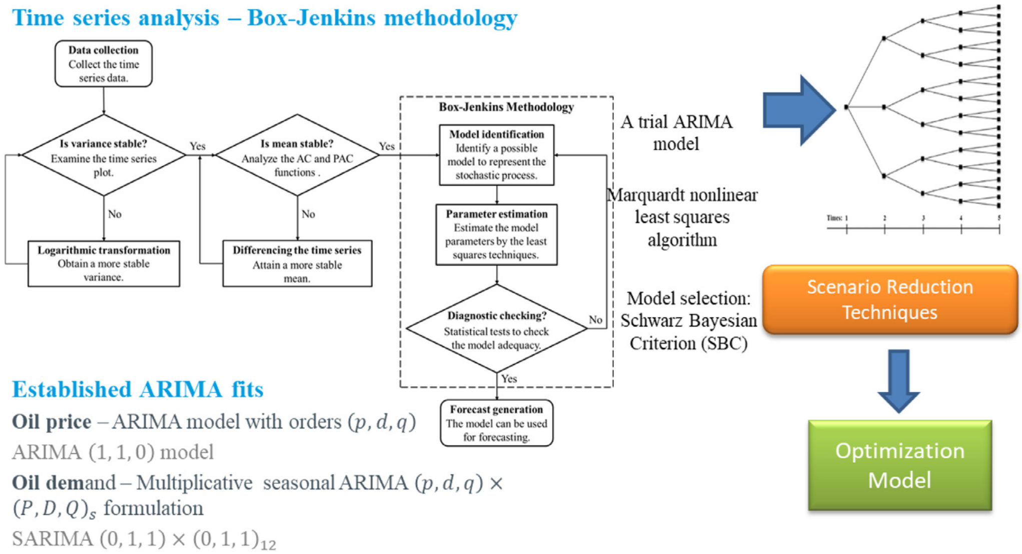

Fig. 9. Stochastic approach to the treatment of uncertainty in the planning of oil supply chains (Lima et al., 2018).

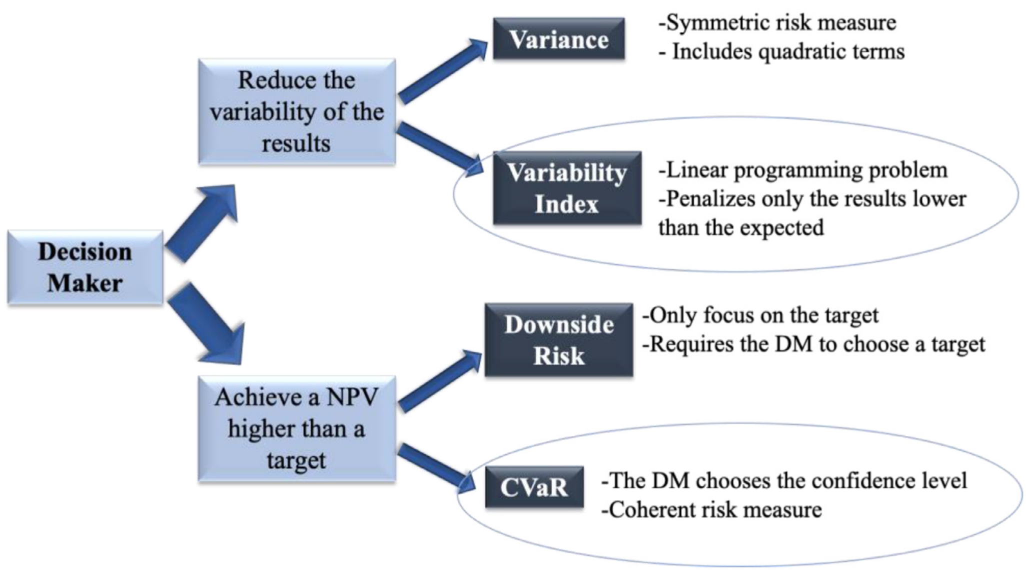

Fig. 10. Risk measures analysis (Cardoso et al., 2016).

on the work of Lima et al. (2018), where a multistage stochastic programming approach to optimally solve the distribution problem of refined products was developed. The stochastic model uses historical data and relies on a time series analysis, as well as on a scenario tree analysis, in order to effectively deal and represent uncertainty in oil price and demand. The Autoregressive Integrated Moving Average (ARIMA) methodology is used to study the time series of the random parameters, aiming to provide their future outcomes, which are then used in the scenario-based approach. As the designed methodology leads to a large-scale optimization problem, a scenario reduction approach is employed to reduce model size and improve its computational performance.

Regarding robust optimization-based approaches, research has been focused on how to minimize the conservativeness of the models, but a clear understanding of the problem is still needed. The modeling of different exogenous and endogenous uncertainties is also a problem to be tackled.

Highly interconnected to uncertainty rises the challenge of risk modelling, where the search for adequate measures is very important. Different metrics have been explored and many authors have identified CVaR (Conditional Value at Risk) as the most adequate one (Zhang et al., 2016b; You et al., 2009). This is summarized in Fig. 10 where four main risk measures are analyzed within the design and planning of supply chains (Cardoso et al., 2016). On the one hand, the variability index appears the most adequate when decision-makers are risk averse and when the main objective is to reduce the variability of the results (blue circle in Fig. 10). On the other hand, when decision makers are risk takers CVaR is the most appropriate and allows the understanding of any long tail that can appear in the objective function –NPV (Net Present Value) in the application considered – as identified with the blue circle in Fig. 10. Note that the latter also appears as a coherent risk measure, which is an important feature of risk metrics (Artzner et al., 1999).

With risk comes the need of guaranteeing supply chain resilience, a critical feature to supply chain management due to the uncertain environment under which they operate. Adhitya et al. (2009) explored a HAZard and OPerability (HAZOP) analysis method so as to systematically generate deviations in

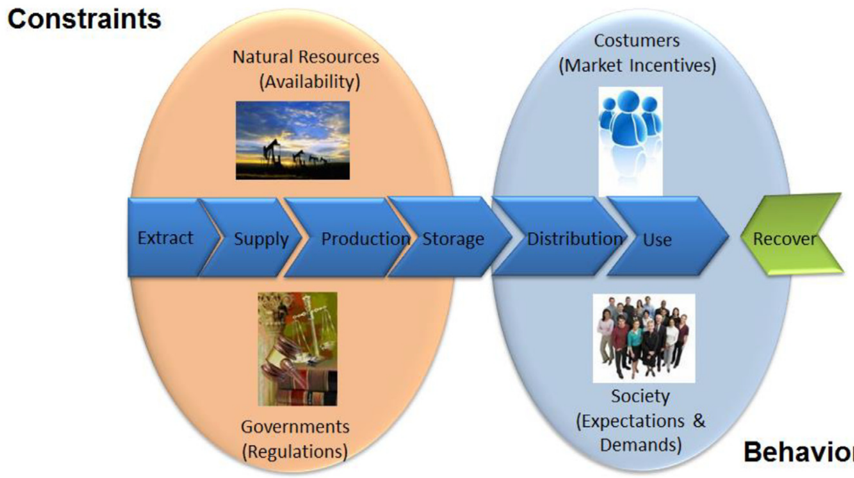

Fig. 11. Extended Supply Chain – towards sustainable a supply chain.

several supply chain parameters and identify their possible causes, consequences, safeguards, as well as mitigating actions.

More recently, Cardoso et al. (2015) also addressed risk and modeled disruptions in a probabilistic manner, resulting in the incorporation diverse sources of uncertainty. Eleven indicators are considered to assess supply chain resilience, which comprise network design, centralization and operational indicators. The authors conclude that when resiliency is considered from the initial design of the network, fewer mitigation strategies are required to cope with disruptions. Nevertheless, added redundancy does not necessarily result in the most resilient supply chain. Cardoso et al. (2015) is one of the few works that address explicitly resilience in supply chains. Thus, resilience modeling is not yet well understood and there still exists a long way to trail on this topic (Ribeiro and Barbosa-Povoa, 2018).

Sustainability Modeling – increased concern for the management of sustainability in supply chain decisions has been witnessed in the last decade, often pressed by governmental regulations and societal pressures (Barbosa-Povoa et al., 2018a). This calls for decisions that seek for a solution of compromise between the three sustainability pillars: economic; environmental and social. An extended supply chain view must then be adopted (Fig. 11), where supply chain activities must be linked not only through forward flows, to satisfy costumers needs, but also incorporate reverse flows, where waste generated along the chain is recovered and transformed into supply chain added value (e.g. end of life products; non-conform materials other activities waste generation). In this way supply chains become more sustainable systems where environmental concerns (e.g. sustainable natural resource availability; sustainable operations) as well as societal expectations (e.g. creation of jobs in less developed regions) are incorporated.

In this context, a set of challenges can be thus identified. starting with the economical pillar. Although this has been widely addressed by the academic community the developed studies have mainly focused on the minimization of costs or on the maximization of profit. Important aspects have been left out, which are part of supply chains as these operate in a wide geography. These are related to international characteristics as taxes, transfer prices, duties as well as multi-modes and outsourcing options (Barbosa-Povoa et al., 2018a). Regarding the environmental and social pillars, a limited number of works have addressed such concerns (Mota et al., 2018). Nonetheless, these concerns are of extreme importance in process supply chains as these often deal with pollutant and/or hazardous products and/or processes, and thus their adequate treatment must be in place (Bojarski et al., 2009). As an example, and as discussed above, the optimization of energy consumption is a great industrial need, which should target not only economic objectives but also environmental concerns. Hence, it is necessary to understand what the most adequate method should be to quantify environmental impacts so as to seek a solution of compromise between economic and environmental goals. The LCA method has been identified as one of the most comprehensive methods, and it has been studied using different current approaches as the Impact 2002+, Eco-indicator 99, ReCiPe, and PEF. But comprehensive models are still missing that should soundly address the environmental aspects in the design, planning and operation of supply chains. Finally, very few works have addressed the third sustainability pillar, the social concern, which is a challenging research issue to address due to the subjectivity involved (Mota et al., 2018).

The scope of sustainable process supply chains must be then further developed from a PSE standpoint. Firstly, it is important to clearly define the problem in study. Recently, Barbosa-Povoa et al. (2018b) proposed a framework – SusFrame, to guide practitioners and/or researchers in the development of optimization models for the design and planning of sustainable supply chains. This is represented in Fig. 12 where four main steps are identified as crucial, when addressing sustainable supply chains through optimization approaches.

The first important step is to set the boundaries of the problem, which allows the definition of the data set. Problem boundaries relate to the type of supply chain in study: forward, reverse, or both (closed-loop supply chains). The second step calls for a clear identification of the decisions to be made: strategic and tactical (e.g. suppliers' selection, location of entities, transportation options, product recovery strategies, or inventory levels). The third and fourth steps define the constraints and objectives. The former describes the problem restrictions and may be of economic, environmental or social focus; the same applies to the latter – and here the question on which the best indicator is remains open. Finally, the fifth step investigates the outputs and solution approaches. The model could target a single objective where environmental and social concerns may be transformed into a common monetary unit, using for instance the EPS method (Silva et al., 2018), or follow a multi-objective approach, where methods as the augmented ε-constraint method proposed by Mavrotas (2009), in which the range of the objective functions over the efficient set is calculated through the use of a lexicographic optimization for every objective function (Mota et al., 2018). In the latter, environmental concerns can be treated through LCA methods, being

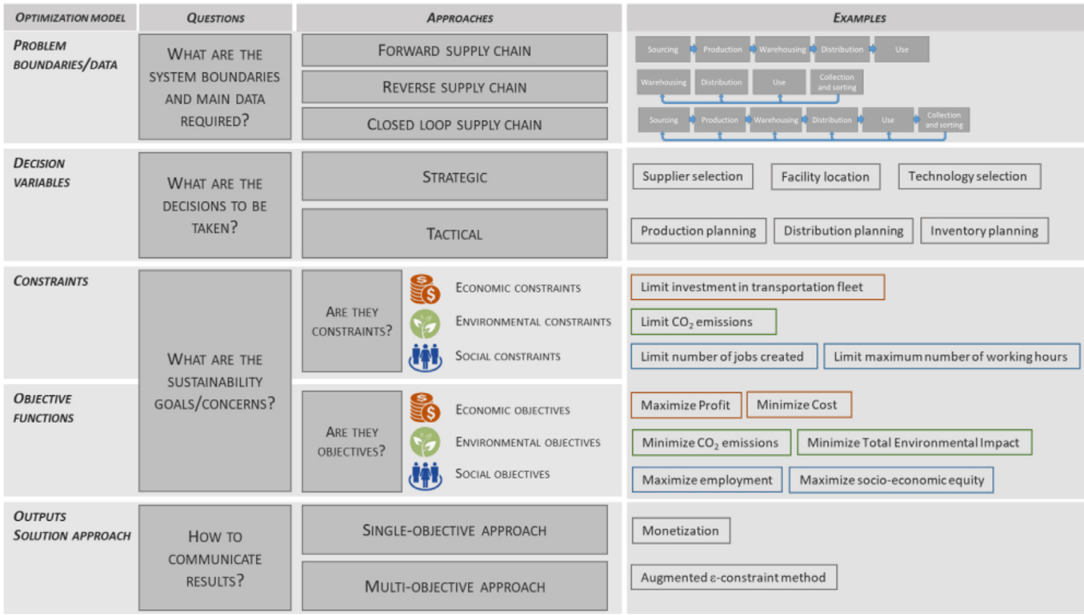

Fig. 12. SusFrame framework (from Barbosa-Povoa et al., 2018b).

ReCiPe and PEF the recommended ones, and social indicators may measure the creation of jobs in non-developed or less populated areas (Barbosa-Povoa et al., 2018a). In this topic, the PSE community has a lot to contribute towards developing methodological advances, which could be integrated into real-world problems.

Efficient Solution Methods – the treatment of the above identified concerns evidently requires the development of models with increasing complexity. This requires new solution methods, where efficient decomposition methods should be explored by the PSE community. One possible example is the use of math-heuristics, where evolutionary methods coupled with mathematical programming are explored, amongst other methods (Lima et al., 2016). Also, the mathematical representation of such challenges may lead to non-linear models, which the PSE research community should address (Misener and Floudas, 2014; Su et al., 2018). For instance, Lara et al. (2018) developed a global optimization algorithm for capacitated multi-facility continuous location-allocation.

Data Management – Finally, the so-called "Supply Chain 4.0" is nowadays a reality and the wide availability of data from the supply chain, customer demand, resource consumption, as well as other associated internal and external activities opens new challenging research areas. As identified in the industrial challenges, Big Data availability ought to increase the number of systems and applications, which implies that the use of analytics, coupled with PSE models, will support the improvement of model accuracy, applicability and solution, and therefore enhance solution quality. Analytics has the potential to transform data into decision-making insights for process supply chains (Fig. 13). Prescriptive analytics can improve decision making in different supply chain areas as planning, sourcing, logistics and transportation, and can be deployed to improve end-to-end supply chain performance. Some of the paths to explore are the incorporation of dimension-reduction techniques to transform big data series into valuable inputs, and the development of new data architectures combining data mining with machine learning algorithms. Moreover, improved data management will allow continuous inventory review that supports the optimization of safety stock levels across the supply chain, thus achieving a reduction of costs with no detriment to targeted service levels. Data access will also support a proactive supply-demand balance that allows the construction and analysis of scenarios that will impact supply chain profitability. Finally, supply chain digitalization coupled with PSE tools will create the conditions to monitor and proactively manage supply chain risks, improve supply chain resilience and so increase its ability to cope with unexpected, disruptive events. Some of the above aspects have been discussed by some authors within the PSE community as is the recent case of Lee et al. (2018), where the applicability of reinforcement learning to multi-stage decision problems was discussed and potential applications and research directions of machine learning techniques to handle data management were presented. Recently, Ning and You (2019) review advances in the field of optimization under uncertainty exploring data-driven optimization approaches.

Fig. 13. Process supply chain 4.0 and analytics challenges.

Supply Chain Domains – process supply chains, as mentioned before, include a large range of sectors from utilities to pharmaceutical and food. Within this diverse set, new domains have been emerging and will gain higher importance in the near future. This is the case of energy supply chains where new energy sources as hydrogen (Moreno-Benito et al., 2017; Biqué and Zondervan, 2018), sun or biomass (Paulo et al., 2015; d'Amore and Bezzo, 2016), need to be further studied and integrated with more conservative energy sources, as oil. In such systems, apart from the challenges above identified, new ones exist as is the case of efficient storage for non-renewable energies or is the synchronization between supply and demand when facing high supply variability. When integration is at stake a critical factor that needs to be addressed is to identify the appropriate "insertion points" through which the supply chains should be connected. Another supply chain domain that is today facing a reorganization, is the agri-food supply chains. Higher market requirements for freshness and security imposes a move from global to local supply chains (Jonkman et al., 2019). In these new challenges emerge as is the case of moving to produce small where economies of scale cannot be anymore explored to optimize costs and how to restructure the existent system to answer to this new market demand. Finally, according to Laínez-Aguirre et al. (2012) and Gautam and Pan (2016) pharmaceutical supply chains are changing to more lean and focused companies, with the specialty products and emerging markets growing as key revenue streams. The new pharmaceutical supply chain is now expected to be highly focused on patient and value deliver. This brings new challenges where increased flexibility is the key.

Other supply chain domains are expected to emerge in the near future but above all the identified challenges with continue to apply adding to new challenges related to new technological contexts allied to new market needs.

4. Conclusions and perspectives

Supply Chain optimization presents multiple opportunities for value creation in the process industry and has been the focus of increasing research by the PSE community. However, there are many challenges that still prevent the successful implementation of decision-support technologies that are relevant to the design and management of supply chains.

This was demonstrated by addressing a real-world, process supply chain – the industrial gas SC and its components – whose goal was used to illustrate the complexity of the decisions and information involved. Based on the product and supply mode, we classified the main supply chains as bulk atmospheric gases (BAG) and process gases and packaged gases (PAG). In each part, we described the different SC activities such as upstream, sourcing, production, storage, and distribution, while underscoring the particularities of the industrial gas sector.

After outlining the main operations within each supply chain, we discussed contributions that address problems in the SC as well as ongoing challenges. Several challenges were discussed that relate to the modeling scope of supply chains, including planning and scheduling and the representation of entities (energy, production, distribution). Moreover, the paper addressed the different approaches that result from integrated decision support systems, such as multiscale and uncertainty, as well as their treatment. Data challenges were also discussed in terms of their management and the need for advanced analytics. Finally, implementation challenges were also discussed that result from the organization of the enterprise, large scale models that require custom solution methods, as well as the impact of decision support tools that requires the management of change and supply chain visibility. From this analysis it is possible to conclude that PSE tools have contributed to address real supply chain problems and are of critical importance when it comes to support the industrial decision-making process; however, further supply chain challenges are still to be dealt by the PSE community.

Such challenges align and converge from an industrial and an academic perspective. Namely, comprehensive decision support tools are required to coordinate cross-functional models. Such tools should consider the major supply chain challenges, such as: a multiscale decision-making – from strategic to tactical to operational decisions, the presence of uncertainty (variability, resilience and risk), sustainability targets – as new regulations are in place and society urges organizations to contribute to welfare. Moreover, these tools should manage data effectively, as data availability and complexity are increasing. Such challenges lead to further complex models that demand investment in efficient solution methods.

In addition to the challenges discussed in this paper, advances in sensors (Internet of Things), computing, AI and robotics will push automation of various supply chain decisions with the promise of increasing efficiency and performance. In industrial gases, this would mean improved and automated forecasting, automated predictive shipping, machines providing real-time information, automatic re-optimization of network (Alicke and Rachor, 2016), among other applications.

There will be an additional need to combine the traditional PSE models and methods with big data analytics, machine learning, and advanced statistical methods, amongst others, so as to be able to improve the decision-making process regarding supply chains. This will support the development of the Supply Chain Digital Twin" concept allowing the test of different integrated supply chain decisions linking low level operation decisions with high level strategic objectives. Process supply chains that will master the right mix of digital capabilities leveraging data management and will explore innovative decision supporting tools will be best positioned to innovate, compete and succeed in a digital business future. All the above aspects call for an increase in a close integration between academia and industry aiming to reduce the gap between research and development and the implementation of solutions that will make a significant impact on real-world process supply chains.

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.

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References

Adhitya, A., Srinivasan, R., Karimi, I.A., 2009. Supply chain risk identification using a HAZOP-based approach. AIChE J. 55, 1447–1463.
Alicke, K., Rachor, J., 2016. Supply chain 4.0 – the next-generation digital supply. McKinsey Q.. https://www.mckinsey.com/business-functions/operations/our-insights/supply-chain-40–the-next-generation-digital-supply-chain.
Amaro, A.C.S., Barbosa-Povoa, A.P., 2008. Planning and scheduling of industrial supply chains with reverse flows: a real pharmaceutical case study. Comput. Chem. Eng. 32, 2606–2625.
Artzner, P., Delbaen, F., Eber, J., Heath, D., 1999. Coherent measures of risk. Math. Finance 9, 203–228.
Barbosa-Povoa, A.P., 2014. Process supply chains management – Where are we? Where to go next? Front. Energy Res. 2 article 23.
Barbosa-Povoa, A.P., Silva, C., Carvalho, A., 2018a. Opportunities and challenges in sustainable supply chain: an operations research perspective. Eur. J. Oper. Res. 268, 399–431.
Barbosa-Povoa, A.P., Mota, B., Carvalho, A., 2018b. How to design and plan sustainable supply chains through optimization models? Pesq. Oper. 38, 363–388.
Biqué, A.O., Zondervan, E., 2018. An outlook towards hydrogen supply chain networks in 2050 – design of novel fuel infrastructures in Germany. Chem. Eng. Res. Des. 134, 90–103.
Bojarski, A.D., Laínez, J.M., Espuña, A., Puigjaner, L., 2009. Incorporating environmental impacts and regulations in a holistic supply chains modeling: an LCA approach. Comput. Chem. Eng. 33, 1747–1759.
Cameron, E., Green, M., 2015. Making Sense of Change Management, 4th Ed. Kogan Page Ltd., Great Britain.
Campbell, A., Clarke, L., Kleywegt, A., Savelsbergh, M., 1998. The inventory routing problem. In: Crainic, T.G., Laporte, G. (Eds.), Fleet Management and Logistics. Springer, Boston, MA, pp. 95–113.
Campbell, A.M., Clarke, L.W., Savelsbergh, M.W.P., 2002. Inventory routing in practice. In: Toth, P, Vigo, D (Eds.), The Vehicle Routing Problem. SIAM, Philadelphia, PA, pp. 309–330.
Campbell, A.M., Savelsbergh, M.W.P., 2004a. Delivery volume optimization. Transport. Sci. 38, 210–223.

Campbell, A.M., Savelsbergh, M.W.P., 2004b. A decomposition approach for the inventory-routing problem. Transp. Sci.. 38, 488–502.

Cao, Y., Swartz, C.L.E., Flores-Cerrillo, J., 2016. Optimal dynamic operation of a high--purity air separation plant under varying market conditions. Ind. Eng. Chem. Res. 55, 9956–9970.

Cardoso, S., Barbosa-Povoa, A.P., Relvas, S., 2013. Design and planning of supply chains with reverse logistics activities under demand uncertainty. Eur. J. Oper. Res. 226, 436–445.

Cardoso, S., Barbosa-Povoa, A.P., Relvas, S., 2015. Resilience metrics in the assessment of complex supply-chains performance under demand uncertainty. Omega 56, 53–73.

Cardoso, S., Barbosa-Povoa, A.P., Relvas, S., 2016. Integrating financial risk measures into the design and planning of closed-loop supply chains. Comput. Chem. Eng 85105–85123.

d'Amore, F., Bezzo, F., 2016. Strategic optimisation of biomass-based energy supply chains for sustainable mobility. Comput. Chem. Eng. 87, 68–71.

Dong, Y., Maravelias, C.T., Pinto, J.M., Sundaramoorthy, A., 2017. Solution methods for vehicle-based inventory routing problems. Comput. Chem. Eng. 101, 259–278.

Dong, Y., Pinto, J.M., Sundaramoorthy, A., Maravelias, C.T., 2014. MIP model for inventory routing in industrial gas supply chain. Ind. Eng. Chem. Res. 53, 17214–17225.

Florensa, C., Garcia-Herreros, P., Misra, P., Arslan, E., Mehta, S., Grossmann, I.E., 2017. Capacity planning with competitive decision-makers: trilevel MILP formulation, degeneracy, and solution approaches. Eur. J. Oper. Res. 262, 449–463.

Gao, J., You, F., 2018. A stochastic game theoretic framework for decentralized optimization of multi-stakeholder supply chains under uncertainty. Comput. Chem. Eng. 122, 31–46.

Garcia, D.J., You, F., 2015. Supply chain design and optimization: challenges and opportunities. Comput. Chem. Eng. 81, 153–170.

Garcia-Herreros, P., Zhang, L., Misra, P., Arslan, E., Mehta, S., Grossmann, I.E., 2016. Mixed-integer bilevel optimization for capacity planning with rational markets. Comput. Chem. Eng. 86, 33–47.

Gautam, A., Pan, X., 2016. The changing model of big pharma: impact of key trends. Drug Discov. Today 21, 379–384.

Gjerdrum, J., Shah, N., Papageorgiou, L.G., 2001. Transfer prices for multi-enterprise supply chain optimization. Ind. Eng. Chem. Res. 40, 1650–1660.

Gjerdrum, J., Shah, N., Papageorgiou, L.G., 2002. Fair transfer price and inventory holding policies in two-enterprise supply chains. Eur. J. Oper. Res. 143, 582–599.

Grossmann, I.E., 2012. Advances in mathematical programming models for enterprise-wide optimization. Comput. Chem. Eng. 47, 2–18.

Harjunkoski, I., Maravelias, C.T., Bongers, P., Castro, P.M., Engell, S., Grossmann, I.E., Hooker, J., Méndez, C., Sand, G., Wassick, J., 2014. Scope for industrial applications of production scheduling models and solution methods. Comput. Chem. Eng. 62, 161–193.

Hjaila, K., Puigjaner, L., Laínez, J.M., Espuña, A., 2017. Integrated game-theory modelling for multi enterprise-wide coordination and collaboration under uncertain competitive environment. Comput. Chem. Eng. 122, 209–235.

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.

Karsten-Ulrich, K., Marquardt, W., 2009. Perspectives for process systems engineering – Personal views from academia and industry. Comput. Chem. Eng. 33, 536–550.

Lainez-Aguirre, J.M., Schaefer, E., Reklaitis, G.V., 2012. Challenges and opportunities in enterprise-wide optimization in the pharmaceutical industry. Comput. Chem. Eng. 47, 19–28.

Lara, C.L., Trespalacios, F., Grossmann, I.E., 2018. Global optimization algorithm for capacitated multi-facility continuous location-allocation problems. J. Glob. Optim. 71, 871–889.

Lee, J.H., Shin, J., Realff, M.J., 2018. Machine learning: overview of the recent progresses and implications for the process systems engineering field. Comput. Chem. Eng. 114, 111–121.

Lima, C., Relvas, S., Barbosa-Povoa, A.P., 2016. Downstream oil supply chain management: a critical review and future directions. Comp. Chem. Eng. 92, 78–92.

Lima, C., Relvas, S., Barbosa-Povoa, A.P., 2018. Stochastic programming approach for the optimal tactical planning of the downstream oil supply chain. Comp. Chem. Eng. 108, 314–336.

Jonkman, J., Barbosa-Póvoa, A.P., Bloemhof, J.M., 2019. Integrating harvesting decisions in the design of agri-food supply chains. Eur. J. Oper. Res. 276, 47–258.

Makridakis, S., Spiliotis, E., Assimakopoulos, V., 2018. Statistical and machine learning forecasting methods: concerns and ways forward. PLoS ONE 13.

Malinowski, E., Karwan, M., Pinto, J.M., Sun, L., 2018. A mixed-integer programming strategy for liquid helium global supply chain planning. Transport. Res. E-Log. 110, 168–188.

Manenti, F., Rovaglio, M., 2013. Market driven operational optimization of industrial gas supply chains. Comp. Chem. Eng. 56, 128–141.

Marchetti, P.A., Gupta, V., Grossmann, I.E., Cook, L., Valton, P.-M., Singh, T., Li, T., André, J., 2014. Simultaneous production and distribution of industrial gas supply-chains. Comp. Chem. Eng. 69, 39–58.

Marquardt, W., Wedel, L.von, Bayer, B., 2000. Perspectives on lifecycle process modeling. In: Malone, M.F., Trainham, J.A. (Eds.), Proceedings of the 5th FOCAPD 1999, AIChE Symp. Ser. 323, 26, pp. 192–214.

Mavrotas, G., 2009. Effective implementation of the ε-constraint method in multi-objective mathematical programming problems. Ap. Math. Comp. 213, 455–465.

Megan, L., Bruton, K.2017. Corporate profile: praxair, analytics.www.analitics-magazine.org, May/June, 56–62.

Misener, R., Floudas, C., 2014. ANTIGONE: algorithms for coNTinuous / integer global optimization of nonlinear equations. J. Glob. Optim. 59, 503–526.

Misra, S., Saxena, D., Kapadi, M., Gudi, R.D., Srihari, R., 2018. Short-Term planning framework for enterprise-wide production and distribution network of a cryogenic air separation industry. Ind. Eng. Chem. Res. 57, 16841–16861.

Mitra, S., Pinto, J.M., Grossmann, I.E., 2014a. Optimal multiscale capacity planning for power-intensive continuous processes under time-sensitive electricity prices and demand uncertainty. Part I: Modeling. Comp. Chem. Eng 84, 382–393.

Mitra, S., Pinto, J.M., Grossmann, I.E., 2014b. Optimal multiscale capacity planning for power- Part II: enhanced hybrid bi-level decomposition. Comp. Chem. Eng. 65, 101–112.

Moreno-Benito, M., Agnolucci, P., Papageorgiou, L.G., 2017. Towards a sustainable hydrogen economy: optimisation-based framework for hydrogen infrastructure development. Comp. Chem. Eng. 102, 110–127.

Mota, B., Gomes, I., Carvalho, A, Barbosa-Povoa, A.P., 2018. Sustainable supply chains: an integrated modelling approach under uncertainty. Omega 77, 32–57.

Ning, C., You, F., 2017. Data-driven adaptive nested robust optimization: general modeling framework and efficient computational algorithm for decision making under uncertainty. AIChE J. 63, 3790–3817.

Ning, C., You, F., 2019. Optimization under uncertainty in the era of big data and deep learning: when machine learning meets mathematical programming. Comp. Chem. Eng. 125, 434–448.

Papageorgiou, L.G., 2009. Supply chain optimisation for the process industries: advances and opportunities. Comp. Chem. Eng. 33, 1931–1938.

Pattison, R.C., Touretzky, C.R., Johansson, T., Harjunkoski, I., Baldea, M., 2016. Optimal process operations in fast-changing electricity markets: framework for scheduling with low-order dynamic models and an air separation application. Ind. Eng. Chem. Res. 55, 4562–4584.

Paulo, H., Azcue, X., Relvas, S., Barbosa-Póvoa, A.P., 2015. Supply chain optimization of residual forestry biomass for bioenergy production: the case study of Portugal. Biomass Bioenergy 83, 245–256.

Puranik, Y., Kilinç, M., Sahinidis, N.V., Li, T., Gopalakrishnan, A., Besancon, B., Roba, T., 2016. Global optimization of an industrial gas network operation. AIChE J. 62, 3215–3224.

Ribeiro, J., Barbosa-Povoa, A.P., 2018. Supply chain resilience: definitions and quantitative modelling approaches – a literature review. Comp. Ind. Eng. 115, 109–122.

Sahay, N., Ierapetritou, M.G., 2014. Hybrid simulation based optimization framework for centralized and decentralized supply chains. Ind. Eng. Chem. Res. 53, 3996–4007.

Sahinidis, N.V., 2004. Optimization under uncertainty: state-of-the-art and opportunities. Comp. Chem. Eng. 28, 971–983.

Sargent, R.W.H., 2005. Process systems engineering: a retrospective view with questions for the future. Comp. Chem. Eng. 29, 1237–1241.

Savelsbergh, M., Song, J.-.H., 2008. An optimization algorithm for the inventory routing problem with continuous moves. Comp. Oper. Res. 35, 2266–2282.

Shah, N., 2005. Process industry supply chains: advances and challenges. Comp. Chem. Eng. 29, 1225–1235.

Schlager, J., 2018. How SKF uses a supply chain twin to enable integrated planning. Supply Chain Q. 48–51. Q4 www.SupplyChainQuarterly.com .

Silva, C., Carvalho, A., Barbosa-Povoa, A.P., 2018. Sustainable supply chain: monetization of environmental and social impacts. Comp. Aided Chem. Eng. 43, 773–779.

Stephanopoulos, G., Reklaitis, G.V., 2012. Process systems engineering: from Solvay to modern bio- and nanotechnology.: a history of development, successes and prospects for the future. Chem. Eng. Sci. 66, 4272–4306.

Su, L., Tang, L., Bernal, D.E., Grossmann, I.E., 2018. Improved quadratic cuts for convex mixed-integer nonlinear programs. Comp. Chem. Eng. 109 (4), 77–95.

Subramanyam, A., Mufalli, F., Pinto, J.M., Gounaris, C.E., 2017. Robust multi-period vehicle routing under customer order uncertainty. E-print: http://www.optimization-online.org

Titze, C., Payne, T., Pradhan, A., 2018. Don't believe the control tower hype – Buyer Beware what you need to know. Gartner Report G00366213.

Tominac, P., Mahalec, V., 2017. A game theoretic framework for petroleum refinery strategic production planning. AIChE J. 63, 2751–2763.

Walker, S., Moran, M., 2017. Three top trends in master data management solutions through 2017. Gartner Research G00319938.

Weron, R., 2018. Electricity price forecasting: a review of the state-of-the-art with a look into the future. Int. J. Forecast. 30, 1030–1081.

Ye, Y., Grossmann, I.E., Pinto, J.M., Ramaswamy, S., 2019. Modeling for reliability optimization of system design and maintenance based on Markov chain theory. Comp. Chem. Eng. 124, 381–404.

You, F., Grossmann, I.E., 2013. Multicut benders decomposition algorithm for process supply chain planning under uncertainty. Ann. Oper. Res. 210, 191–211.

You, F., Wassick, J., Grossmann, I.E., 2009. Risk management for a global supply chain planning under uncertainty: models and algorithms. AIChE J. 55, 931–946.

Yue, D., You, F., 2016. Optimal supply chain design and operations under multiscale uncertainties: nested stochastic robust optimization modeling framework and solution algorithm. AIChE J. 62, 3041–3055.

Yue, D., You, F., 2017. Stackelberg-game-based modeling and optimization for supply chain design and operations: a mixed integer bilevel programming framework. Comp. Chem. Eng. 102, 81–95.

Zamarripa, M.A., Aguirre, A.M., Méndez, C.A., Espuña, A., 2012. Improving supply chain planning in a competitive environment. Comp. Chem. Eng. 42, 178–188.

Zamarripa, M.A., Marchetti, P.A., Grossmann, I.E., Singh, T., Lotero, I., Gopalakrishnan, A., Besançon, B., André, J., 2016. Rolling horizon approach for production–distribution coordination of industrial gases supply chains. Ind. Eng. Chem. Res. 55, 2646–2660.

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.

Zhang, Q., Cremer, J.L., Grossmann, I.E., Sundaramoorthy, A., Pinto, J.M., 2016b. Risk-based integrated production scheduling and electricity procurement for continuous power-intensive processes. Comp. Chem. Eng. 86, 90–105.

Zhang, Q., Morari, M.F., Grossmann, I.E., Sundaramoorthy, A., Pinto, J.M., 2016c. An adjustable robust optimization approach to scheduling of continuous industrial processes providing interruptible load. Comp. Chem. Eng. 86, 106–119.

Zhang, Q., Sundaramoorthy, A., Grossmann, I.E., Pinto, J.M., 2016a. A discrete-time scheduling model for continuous power-intensive process networks with various power contracts. Comp. Chem. Eng. 84, 382–393.

Zhang, Q., Sundaramoorthy, A., Grossmann, I.E., Pinto, J.M., 2017. Multiscale production routing in multicommodity supply chains with complex production facilities. Comp. Chem. Eng. 79, 207–222.

Zhu, Y., Legg, S., Laird, C.D., 2011. A multiperiod nonlinear programming approach for operation of air separation plants with variable power pricing. AIChE J. 57, 2421–2430.