Mario R. Eden, Marianthi Ierapetritou and Gavin P. Towler (Editors) Proceedings of the 13th International Symposium on Process Systems Engineering – PSE 2018
July 1-5, 2018, San Diego, California, USA
https://doi.org/10.1016/B978-0-444-64241-7.50009-4

Challenges and Perspectives of Process Systems Engineering in Supply Chain Management

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Abstract

Supply chain management is concerned with the efficient integration of interconnected entities so that products are sourced, manufactured and distributed in the right quantities, to the right locations and at the right time, thus satisfying customer requirements at minimal total system cost. Such systems face complexity due to the multiple material and information flows. In this context, the Process System Engineering (PSE) community has an important role to play in addressing such complexity. Departing from a real-world process supply chain, the industrial gas supply chain, while considering existing PSE contributions, this paper discusses challenges in terms or modeling and implementation. This work also presents perspectives in supply chain management from the industrial and academic standpoints that ought to be explored by the PSE community.

Keywords: Supply Chains, Industrial Gases, Uncertainty, Multiscale, Challenges, Perspectives.

1. Introduction

Supply chains (SC) are systems that comprise several entities placed in different geographical locations. These interconnected systems play a crucial role in organizations as they dictate product availability to the final consumer and consequently the financial success of the involved companies. The management of SC is complex due to the involvement of a large multiplicity of material and information flows, diversified characteristics of the associated entities and often-present conflicting objectives.

Within the process industry, this is not an exception and process supply chains must be flexible, resilient and efficient while guaranteeing customers' demands at minimum costs. Moreover, as the process industry is often associated with a high level of resource consumption and often deal with non-friendly environment processes and products, special attention to supply chain sustainability is required when managing such systems (Barbosa-Póvoa, 2014; Mota et al., 2018).

To deal with such complexity and underlying challenges, both industrial and academic communities identify the application of Process Systems Engineering (PSE) tools as a path to follow (Grossmann, 2012). Such tools support the integration of supply chain decisions under uncertainty while minimizing risk, maximizing service levels, sustainability levels and simultaneously guaranteeing the main SC goals – profitable and reliable operation.

The PSE community can contribute highly in the answer to such challenges (Barbosa-Póvoa, 2014) by studying real-world supply chain problems. These 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 decisions (e.g. scheduling, routing and inventory management in Amaro and Barbosa-Póvoa, 2008; Dong et al., 2014; and Zhang et al., 2015).

Several reviews provide a detailed analysis of such challenges. 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 and Stephanopoulos and Reklaitis (2012) highlighted the past and future contributions of the PSE community in several areas, from which the supply chain study 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 et al. (2012) reviewed the pharmaceutical supply chain and Barbosa-Póvoa (2014) analyzed the published papers on process supply chain considering the multiple decision levels. Recently, Barbosa-Póvoa et al. (2018) reviewed sustainable supply chains and conclude that particularly (bio) process supply chains have been actively addressing sustainability issues, which nevertheless present a large set of research opportunities.

All the above reviews tend to converge to a common set of critical problems, some already under study by the academic community, whereas many others call for further research. In the next section, we illustrate some of the problems in the context of an industrial gas supply chain. Additionally, while some challenges have been addressed, the implementation of PSE in industry is still far from effective. Significant progress must be achieved in critical issues that are discussed in this paper, both from an industrial and an academic perspective. We conclude that supply chain research has a major financial impact to the process industry and brings scientific challenges where the PSE community has an unquestionable role to play.

2. Process Supply Chain

Process Supply Chains deal with chemical and/or bio-based networks that involve a set of entities, materials and information that transform raw materials into final products using different types of transforming processes. Among these supply chains, several examples exist as is the case of the oil, pharmaceutical, biomass, and gas supply chains. Several challenges exist with respect to the management of such systems and consequently both industrial and the academic communities should be committed to address such problems in close collaboration.

We use an industrial gas supply chain as an example of process supply chains where its different characteristics are described and corresponding challenges identified. This is represented in Figure 1. The manufacturing of Oxygen, Nitrogen and Argon is considered, as well as the retail business (hardgoods) and the supply chain comprises upstream, production, distribution and consumer entities.

Electricity can be purchased from utility companies through various power contracts that may differ in price, availability, and penalty for under- or overconsumption (Zhang et al., 2015). Discount prices and penalties can also be defined with respect to the amount of electricity purchased over a certain period of time, 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., 2016a).

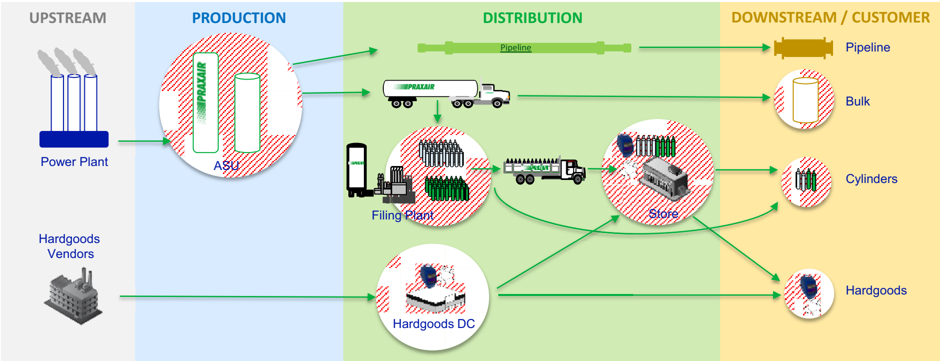

Figure 1- Industrial Gas Supply Chain (Praxair, Inc.)

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 process 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.

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

For the largest customers, such as refineries and steel mills, industrial gas plants operate adjacent to their facilities and distribute products via pipeline. These plants act as a vital utility to those customers, similar to electricity and water, and provide an uninterrupted supply of industrial gases to support their operation.

Medium-volume customers, such as hospitals and universities, typically have liquid storage located at their facility, which is then used to provide product throughout their operations. Their inventory is monitored in real time with telemetry and the delivery of product is performed, using a tanker truck fleet, without the customer needing to place an order. This proactive, vendor-managed inventory model provides high reliability for customers while enabling the supplier to manage effectively their costs.

The third mode involves packaged gases. Here a wide variety of smaller packaged gases to laboratories, hospitals and other customers is at stake. These products can range from a cylinder of nitrogen to specialty gas mixtures needed for emissions testing, advanced manufacturing and semiconductor fabrication. As seen in Figure 1, cylinders are either distributed directly to customers or shipped to stores, from which additional deliveries are made or customers pickup their products. A variety of services is also offered, such as embedded regulators and telemetry. The cylinder assets, which helps ensure continuous supply to our customers are owned by the gas company.

In addition to cylinders, stores also retail hard goods that are purchased from vendors and shipped through multiple distribution centers. These in turn either ship products directly to customers or to the stores for pickup or further delivery.

3. Challenges

This section describes the main research and implementation challenges from an industrial perspective as well as these are addressed from the PSE community, including joint collaborations academia-industry.

3.1. Industry perspective

3.1.1. Supply Chain Modeling Challenges

Supply Chain Planning – Planning the merchant liquid supply chain is a very challenging problem. 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 and large mixed integer linear programming models in order to determine optimum production and distribution plans on a continuous basis. 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.

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., 2017). This coordination problem gives rise to a multi-scale optimization problem because while a detailed production scheduling model must capture all critical operational constraints on a fine time grid, vehicle routing has to 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., 2014a; Zhang et al., 2015).

Inventory Route Planning – Executing a 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. 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. One of the main objectives in solving the IRP is to reduce the overall distance driven per volume delivered to customers, which has a sustainability impact by reducing fuel emissions.

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. As part of the 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., 2016b).

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. 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). Figure 2 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.

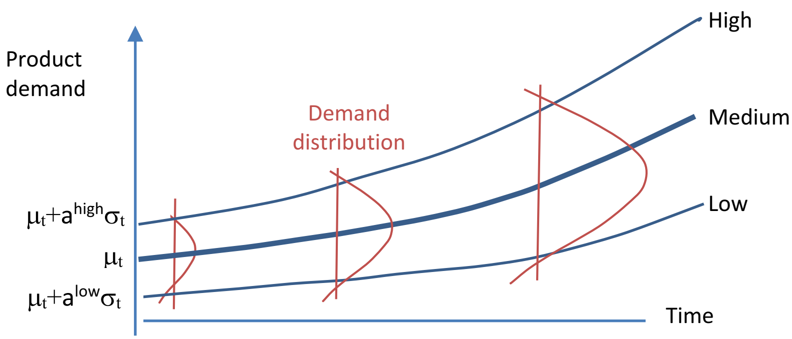

Figure 2. Product demand trajectories in short term and long term (Mitra et al., 2014a). Parameters μ_t and σ_t denote the expected demand and the standard deviation in time t.

Customer demand for packaged gases can also be received dynamically over the planning horizon. Routing plans should flexibly accommodate potential customers who have not yet called in to request service. Subramanyan et al. (2017) model future potential customers as binary random variables, and seek to determine a visit schedule that remains feasible for all anticipated realizations of service requests.

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 allows access to bulk tanks. These may affect delivery times or even prevent deliveries at end of routes.

Multiscale Modeling – One of the biggest challenges on 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 10-15 year horizon. Investigating the trade-off between capital or retrofits, and the operating costs, related to electricity prices, which can vary on an hourly basis, leads to a complex multiscale optimization problem (Mitra et al., 2014a; 2014b). On the mid-term level, there is also the need to coordinate multiple time scales for production (fine) and distribution (coarse), as in Zhang et al. (2017).

3.1.3. Data Challenges

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 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.

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. The 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 may increase by one order of magnitude. Data provided may 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.

3.1.4. Implementation Challenges

Computational Performance – The complexity of real-world industrial problems translates into large scale models, in terms of constraints and variables. Most SC 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 multiscale 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 is proposed (Dong et al., 2017), and for the production scheduling of air separation units under uncertainty, an integrated stochastic mixed-integer linear programming model is developed; Conditional value-at-risk is incorporated into the model as a measure of risk, and scenario reduction with multi-cut Benders decomposition are implemented to solve large-scale real-world instances (Zhang et al., 2016b).

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 oversees 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.

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-Póvoa, 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. Uncertainty; sustainability concerns; risk and resilience management should be targeted. Additionally, the availability of large amounts of data is nowadays a reality, which should be explored to lead to more accurate industrial representations and allow further decision-sharing (Ning and You, 2017). The integration of tactical-operational decisions is also an open issue and it 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. Multi-scale supply chain models will help to answer to these challenges where an Enterprise Wide Optimization approach (Grossmann, 2012) should be explored. In this context, not only centralized supply chain decisions, as commonly treated by the academic community, should be considered but rather trade-offs between different supply chain entities need to be accounted for, where decentralized decisions may be at stake (Sahay and Ierapetritou, 2014).

Uncertainty, Risk, Resilience Modeling – uncertainty has been explored mainly using stochastic and robust approaches. The first one focuses on the establishment of representative scenarios to model uncertainty, as the use of a large number of scenarios leads to intractable models. One possible way to tackle this problem is by exploring the use analytics on uncertain parameters data, e.g. in demand and supply (see Figure 2). Statistical, data mining or machine learning techniques, amongst others should be explored to help the definition of more realistic possible scenarios. This has been studied by some authors (Yue and You, 2016; Lima et al., 2018) and constitutes an emerging research area. On the robust approach, 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. Linked to uncertainty arises risk modeling. Different measures have been explored and the authors identify the CVar as the most adequate one (Zhang et al., 2016a). But few works have explored risk when modeling supply chain decisions. With risk comes the need of guaranteeing supply chain resilience (Cardoso et al., 2015), a characteristics critical to supply chains due to the uncertain environment under which they operate. Nevertheless, resilience modeling is not yet well understood and there still exist a long way to trail on this topic.

Sustainability Modeling – increased concern for the management of sustainability in supply chain decisions has been observed in the last decade, often pressed by governmental regulations and societal pressures (Barbosa-Póvoa et al., 2018). This calls for decisions that consider trade-offs between the three sustainability pillars: economic; environmental and social. However, the academic community, when addressing supply chain problems, has been mainly focused on the economic pillar where typically the minimization of costs or the maximization of profit have been considered. But often important aspects have been left out as few models addressed international supply chain characteristics such as international taxes; transfer prices, duties as well as multi-modes and outsourcing options. Regarding the environmental and social pillars, a limited number of works have addressed such concerns (Mota et al, 2018), which are very important when addressing process supply chains. Often process supply chains deal with pollutant and/or hazardous products and/or processes, and a well-defined treatment of such concerns within the supply chain is required. For example, and as mentioned above, the optimization of energy consumption is a constant industrial need, which should be explored not only with an economic objective but also with an environmental concern. Moreover, researchers have been trying to understand the best method to quantify environmental impacts and how this could be used to establish a trade-off with economic concerns leading to a solution of compromise. The LCA method has been one of the main methods studied and along with it different approaches have been explored namely, the Eco-indicator 99, Recipe, and PEF. But comprehensive models that address in a sound form the environmental aspects when designing, planning and operating supply chains are still required. More recently, the social concern has been also studied, but in this case very few works studied this issue. This area is then a great challenge to the PSE community (Barbosa-Póvoa et al., 2018).

Efficient Solution Methods – the treatment of the above identified concerns evidently requires the development of models with increasing complexity. This need calls for new solution methods, where efficient decomposition methods, meta-heuristics, amongst others methods should be explored by the PSE community. Also the solution of non-linear models still needs further treatment (Su et al., 2018).

Finally, the so-called **"Supply Chain 4.0"**is nowadays a reality and the wide availability of data from supply chain process, customer demand, consumption of resources, as well as other associated internal and external activities opens a new challenging research area.

4. Conclusions and Perspectives

Supply Chain optimization presents multiple opportunities for implementation 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 SC solutions.

In this paper, we describe a real-world, process supply chain through an industrial gas SC whose goal is to illustrate the complexity of the decisions and information involved. Several challenges are discussed that relate to the modeling of entities (energy, production, distribution), the different approaches that result from integrated decision support systems, such as multiscale and mainly uncertainty and its treatment. Finally, we also discuss implementation challenges that result from large scale models that require custom solution methods, as well as the impact of decision support tools that requires the need for the management of change.

The supply chain work available in the literature indicates the need of comprehensive decision support tools required to coordinate cross-functional models. Such tools should allow the treatment of real supply chain characteristics in which different aspects must be considered: the presence of uncertainty - modeling resilience and risk; sustainability goals - accounting simultaneously for economic; environmental and social concerns; international taxes; transfer prices, duties as well as multi-modes and outsourcing options, amongst others. Such challenges lead to further complex, often multiscale models that demand the investment in efficient solution methods.

To conclude we want to raise the need to combine the traditionally PSE models and methods with big data analytics, machine learning, and advanced statistical methods, amongst others, so as to be able to inform the supply chain decision process supporting better decisions. This calls for a close integration between academia and industry aiming to reduce the gap between research and implementation.

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