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Smart Process Manufacturing—Perspective

A Perspective on Smart Process Manufacturing Research Challenges for Process Systems Engineers

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ABSTRACT

The challenges posed by smart manufacturing for the process industries and for process systems engineering (PSE) researchers are discussed in this article. Much progress has been made in achieving plant- and site-wide optimization, but benchmarking would give greater confidence. Technical challenges confronting process systems engineers in developing enabling tools and techniques are discussed regarding flexibility and uncertainty, responsiveness and agility, robustness and security, the prediction of mixture properties and function, and new modeling and mathematics paradigms. Exploiting intelligence from big data to drive agility will require tackling new challenges, such as how to ensure the consistency and confidentiality of data through long and complex supply chains. Modeling challenges also exist, and involve ensuring that all key aspects are properly modeled, particularly where health, safety, and environmental concerns require accurate predictions of small but critical amounts at specific locations. Environmental concerns will require us to keep a closer track on all molecular species so that they are optimally used to create sustainable solutions. Disruptive business models may result, particularly from new personalized products, but that is difficult to predict.

1. Introduction

Smart manufacturing is a stated priority of most major economies, including those of the United States, China, and the European Union. It is mostly framed in terms of better use of big data—that is, measurements and market data—and intra-machine connectivity, particularly using the Internet of things. While comprehensive and timely data and massive connectivity are necessary conditions for this revolution, they are not sufficient. It is also important to have smart algorithms for intelligent and timely use of the data. This is the domain of process systems engineering (PSE). Process manufacturing, in which products are mostly continuous fluids or solid streams with fluid-like properties and molecular differentiation, presents different challenges than those of mechanical manufacturing. This paper reviews perspectives on smart process manufacturing and the potential contribution of and challenges for PSE, its research, and its practice community, in making the most of this revolution. This is a short perspective, so references are very selective and are not meant to be comprehensive.

The smart manufacturing revolution is said to have three phases:

- Factory and enterprise integration and plant-wide optimization,
- Exploiting manufacturing intelligence, and
- Creating disruptive business models.

All three phases have resonance in the process industries. The first phase is already underway, and the PSE community has been in the vanguard of providing tools and techniques for facilitating integrated design and operation. Ideas and research results for the second phase suggest that whole supply chains can be integrated more seamlessly in order to provide products more quickly, efficiently, and sustainably; however, such integration certainly remains a major challenge for the industry. Although we have seen little change in business models in the process industry over the past decades, smart manufacturing promises to enable us to develop new business models—for example, to deliver personalized medicine—in an

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efficient and sustainable way in the future. The current model of long-term contracts for the supply of large amounts between each part of the supply chain, which is common in chemicals, would not be appropriate. We need a model that allows the supply of bespoke products in small amounts, which will likely be of much higher added value and which will require the direct influence of the cost of product development, cost of manufacture, and strength of demand. This remains a major challenge.

A set of challenges for smart process manufacturing in the United States was discussed at a workshop in April 2008, resulting in a comprehensive report [1]. A specific test bed was proposed—the steam reforming of methane—in order to demonstrate and benchmark progress [2]. More recently, Li [3] addressed the challenges for the petrochemical industry from an industrial perspective. These challenges are common internationally for countries with a well-developed process industry base. It is clear from both these contributions that PSE lies at the heart of the smart process manufacturing challenge.

Over the past 50 years, PSE researchers have been developing methodologies—mostly computational, but not all—to be able to optimize whole systems, whether at the unit, plant, or enterprise level. A recent issue of the *American Institute of Chemical Engineers* (*AIChE*) *Journal* [4] celebrated the work of a pioneer in this field, Professor Roger Sargent, who has been working since the 1950s. Sargent has taught many people around the world and has inspired many more, as reflected in the 38 papers in this issue, most of which are relevant to this topic.

This paper considers each of the three phases in turn, and then examines some of the key technical challenges that arise. I will particularly consider research progress and challenges that confront the PSE research community in enabling smart process manufacturing to progress more rapidly. I will reflect not only on petrochemical and commodity chemical manufacturing, but also on specialties and medicines, as well as on contributions that consider wider environmental impacts that are part of the system of systems that we influence. While some challenges and opportunities are similar to those in other manufacturing sectors, there are distinctive differences.

2. Factory and enterprise integration and plant-wide optimization

A key tenet of smart manufacturing is plant-wide optimization, which is not new in process engineering. Process engineers have been considering systems of connected unit operations and looking for better—or even optimized—solutions for a long time, with these activities driving their education.

Plant-wide optimization is at the heart of PSE thinking. The routine use of simulation tools with embedded optimization capability has resulted in plants being optimized for profitability and, increasingly, for minimizing environmental impact while seeking sustainable production. Many tools for process integration have been developed (using a heuristic [5,6], optimization-based [7], or properties-based [8] approach), all of which are based on steady-state models. Process integration approaches have been used to design heat-integrated plants and, to some extent, whole sites [9]. Real-time optimization and model-based control have enabled solutions for optimizing the dynamic behavior of operations in short to medium timescales (see e.g., Ref. [10]). Their implementation is not universal, but it is common, particularly in petrochemical plants [3]. Enterprise integration has also been a goal through the use of whole supply chain models and business software systems.

Many tools are available, and some experience of deploying these tools is discussed in Section 5. Plant-wide optimization is an area that would benefit from more benchmarking and testing to give more confidence. Coordination of multiple enterprises and their customers, most of whom are other businesses within an extended supply chain, remains a challenge. Although this is a technical problem, it is also about relationships: ensuring that the valuable commercial and strategic relationships that have been developed are not disrupted by any proposed technical solutions.

3. Manufacturing intelligence

Smart manufacturing seeks to involve the customer more closely in order to have a more responsive and agile system. Many supply chains producing domestic products now produce on demand, with very short production and delivery timescales. The process industry typically produces intermediate products that are either processed further or used to produce specific products. For example, the plastics industry produces many polymers and many different grades for different end uses. The manufacture of a raw polymer is followed by various stages of treatment, forming, molding, and assembly before the polymer becomes a final product for the consumer. As a result, most process manufacturers have a remote relationship with the end users of the final products. Each stage has its own dynamics, inventory, uncertainty, and commercial drivers. In order to become more responsive and agile, the process industry will need to incorporate information technology (IT)-enabled manufacturing intelligence, with communication occurring between all parts of the supply chain.

Clearly, commercial and technical challenges are associated with this objective. It will require computational methods that can handle multiple stages within the supply chain that support different types of commercial relationships as well as different dynamics at each stage. It will need to be able to take into account technical constraints on flexible manufacturing at each stage, and incorporate the ability to handle uncertainty in demand and production.

The processes will be customer-driven and sensitive to markets, but will include various contractual constraints in dealings between different elements of the supply chain. End-user suppliers will have huge amounts of data on trends in customer demand in order to allow the prediction of expected demands, as they currently do for consumer-oriented product industries. This will shift to incorporating more immediate-demand data, which should rapidly influence manufacturing in all parts of the supply chain. Although immediate-demand data is now common for the fresh food industry and for the processed food industry [11], it would be quite a departure for the chemical, petrochemical, and pharmaceutical industries. Cao et al. [12] presented a data-driven refinery-scheduling model that can incorporate unexpected events from data over a one-day period; however, this approach is still a long way from the overall system responsiveness that is common in the food industry. The aim of smart process manufacturing is to support an agile, robust, and sustainable process industry that minimizes waste while maximizing profitability.

4. Disruptive business models

Perhaps the biggest change in chemical plants over the last few decades was the introduction of the coordinated control systems that are now in place. The basic structure of the set of connected unit operations has not changed much for a considerable period of time. Environmental performance has added significant pressure to the industry, resulting in more integrated design and operation, with less end-of-pipe treatment.

Smart manufacturing could provide more motivation for significant change through small-scale and microscale local production, for example, which would bring production closer to the consumer. This would be essential for the potential development of personalized medicine, and perhaps also for the manufacture of more individualized personal products and smart materials for specialized use. Changes of this nature would require new process synthesis and intensification methods. We may also see significant changes to the molecules and mixtures that we produce. Perhaps the most significant change could be a broadening of cross-disciplinary research, as engineering interacts more closely with the natural sciences, the social sciences, and medicine in order to provide frameworks and tools for businesses that seek to meet customer demands more quickly and accurately.

This phase is inevitably the least clear of the three phases of smart manufacturing.

5. Technical research challenges

In the discussion above, I considered the three phases of smart manufacturing, as seen from the process industries. I now consider a set of enabling topics and related research challenges. These topics are: flexibility and uncertainty, responsiveness and agility, robustness and security, the prediction of mixture properties and function, and new modeling and mathematics paradigms.

5.1. "Who knows?" Flexibility and uncertainty

A key issue in smart manufacturing is the ability to be flexible and respond to uncertainties in the marketplace and in raw material quality. Since the 1980s, a rich seam of research work has tackled this problem. Based on assumed bounds for uncertainty, optimization-based approaches have been proposed to account for uncertainties, beginning with stochastic programming [13] and using a superstructure as the basis of an optimization problem to minimize a quantifiable uncertainty index [14]. A good recent review can be found in Steimel et al. [15]. Most approaches find that a design based on a steady-state analysis will satisfy all expected uncertain conditions, inevitably leading to conservative designs. Steimel et al. [16] demonstrated their two-stage optimization framework on the hydroformylation of dodec-1-ene.

We need a way to balance the likelihood of large excursions using a probabilistic approach that can also use historical data and patterns within the data to inform the design. Of course, extreme events may occur, making it necessary to have elements designed in to take account of extreme events and use patterns in the data to provide indications of an approaching extreme event, thus enabling us to avoid taking extreme action that may be environmentally damaging or may even cause shutdown. Although some researchers have considered uncertainty in the dynamic response [17–19] either through control measures or enhanced design, much is needed to make these efforts comprehensive and useable, given the need for discrete decisions and tradeoffs between many alternatives. Rather than solve the complete dynamic optimization problem, which is intractable for realistic problems, Wang and Baldea [19] use pseudo-random signals to identify a data-driven input/output model. Using process intelligence through simplification, data analysis, or multi-level representations provides a possible way to efficiently solve large-scale problems while allowing the continuous refinement of predictions and actions.

Deterministic optimization approaches identify the parameters yielding the smallest operating space that will accommodate the full range of expected uncertainties. These approaches produce conservative results since the outer extremities of uncertainty ranges are very unlikely and may not be critical. The earliest paper listed above [17] uses a stochastic approach with great potential, as discussed in the review by Sahinidis [20]. Stochastic solutions allow a designer to determine what level of risk is acceptable, and then design accordingly; thus, they require some engineering judgment about final design robustness and whether extreme events must be handled or not.

All these methods are very expensive computationally, as they require the solutions for many optimization problems. Thus, there is much scope for improving their efficiency, as well as for testing and evaluating methods on substantially sized problems from industrial practice. We can then identify the limitations and weaknesses of these methods more fully. However, we have a fairly comprehensive toolset to use. It is challenging to find ways to make these methods both practical and not overly conservative.

5.2. "I want it now!" Responsiveness and agility

As mentioned above, a key element of smart manufacturing is to match production to demand through prediction and real-time control. This has two elements: the ability to decide on a course of action based on the information received, and the ability to achieve that outcome.

Within PSE, the second element is tackled by focusing on controllability: Can these actions be achieved according to the model, and how can this actually be done? Much work has been done on controllability in the PSE community (see recent reviews in Refs. [21,22]). These methods are not yet adequate for large problems with nonlinearities, and it is difficult to incorporate heuristic knowledge from experienced practitioners. Process control is now dominated by model-based control [23], which permits integrated operations, although the computational burden can become significant. It is typical for real-time optimizers to work with steady-state models to determine optimal strategies and then implement them using model-based controllers to ensure coordinated and responsive systems. Although these are mature technologies, they may not have been tested for the more agile requirements expected in the future, in which customer demands are much more varied and frequently changing.

While a considerable amount of historic trend data has been collected on operations, the chemical industry does not incorporate large demand databases directly into their control systems. However, this is being done now in many consumer product industries, including the food industry. The resulting responsiveness is creating new challenges in ensuring robustness [24]. Data repositories provide trends in demand, and are reliable when changes are regular and relatively smooth. However, challenges occur as a result of big events such as failures or large market shifts in response to political changes, for example. Does matching production to demand by using control measures have the potential to make systems more sensitive, or will it make them unstable? It will also be a major challenge to ensure that the required accuracy of data-driven models is suitable for each specific area. Accuracy requirements (e.g., regarding demand or the quality of raw materials or products) will vary considerably for different areas.

PSE researchers have performed numerous studies for supply chain research using discrete optimization models. In a recent review, scholars considered supply chain optimization to be particularly relevant for high-value low-volume products [25]. Although they did not identify any single method as the best one, the reviewers concluded that decomposition and hierarchical algorithms have consistently provided good results. The process industries will gradually see more connections between customer data and demand-driven manufacture. Li et al. [26] showed how a data-driven global optimization framework can be used for the planning process of an entire petrochemical complex. Sahay and Ierapetritou [27] showed how agent-based technology can be used to optimize multi-enterprise supply chains.

Many practical issues of implementation confront user companies. For example, enterprises need methods and tools that are able to handle company interfaces across the supply chain as well as the broad range of commercial and contractual relationships that exist.

For example, vaccine production can require rapid response in an emergency, while retaining the safety and quality of the product over an effective timespan. Personalized medicine will require very small-scale production, and may require an entirely new type of business model and technical solution.

5.3. "Can you guarantee it?" Robustness and security

Along with speed and agility, customers also want certainty: of supply, of quality, and of safety. The discussion in the literature of design under uncertainty addresses part of this issue, in that the designs that are produced allow for all predicted uncertainties, resulting in rather conservative designs. Of course, our models are approximations based on assumptions of the physics and chemistry involved, and have parameters that can be inaccurate or flawed. However, even assuming that we have considered all possible uncertainties, things can still go wrong: Elements in the manufacturing process break down, communication systems fail, predictions are wrong, and so on.

There is a rich seam of work exploring fault detection in process plants [28]. Fault detection is likely to become more important as we use increasingly sophisticated instruments to get better quality measurements that also have a greater propensity to either predict with bias or fail altogether. Hazard detection must be incorporated directly into the systems because operating close to optimal conditions usually puts extra pressure on operations, resulting in a greater likelihood of failure.

Issues of data robustness and security are a new aspect to be considered. Can we guarantee data accuracy and ensure security from competitors and other agents seeking to cause difficulties? As instruments increase their local intelligence, and as greater interconnectedness occurs through the Internet of things, the potential for security breaches also grows, as shown by recent hacking cases. Although PSE researchers have not traditionally worked in this area, computer scientists have made major strides in cybersecurity, as most countries consider cybersecurity to be a major national priority. By working closely with our colleagues in computer science, PSE researchers can ensure that developments in cybersecurity inform our methods and software.

5.4. "What do you want?" Selling molecules, mixtures, or function?

The business of the process industries is to manufacture chemical products. For a long time, we focused on producing molecules that were required for further processing, such as methanol and ethylene. The chemical industry was originally rooted in the production of dyestuffs—synthetic colors for the textile industry, used to replace expensive naturally occurring minerals. Dyestuffs produced an effect, or function, that customers were willing to pay for. This function sometimes came from a single molecule and was sometimes produced by a mixture. In fact, we still manufacture products with a specific, well-defined function; for example, gasoline is a complex hydrocarbon mixture with specific functional requirements such as octane number, flash point, and cloud point. The personal products industry has also been seeking to manufacture products with a specific function. In the future, will we be able to follow customer demands more closely based on data trends, predictions, and market intelligence? This problem contains many challenges. One challenge is our limited ability to predict function, and thus our limited ability to design mixtures to achieve specific functional demands by customers. Much progress has been made in the capability to design polymer blends, solvent mixtures, and electrolytes, leading to considerable commercial use of predictive methods [29,30]. Many challenges still exist regarding predicting the functional effect of complex mixtures of many substances and designing mixtures for specific functions that are desired by consumers, particularly when it is difficult to characterize the function itself using models. Many properties, such as taste, are very personal and difficult to predict.

Another challenge is the need to optimize the molecular characterization of the whole supply chain, from primary manufacture, through intermediates, and through to the final product. A supply chain may involve many enterprises that have different systems, different business models, and a need to keep their unique selling point (USP) and commercial secrets confidential, particularly around specific products. Can this be achieved?

Finally, the development of personalized medicine is a major upcoming change. Medicines will be tailored to personalized requirements based on diseases and their progression, metabolism, physical condition, and personal needs. Personalized medicine presents many challenges to medicine regulators; however, assuming that these challenges are resolved, it will require a considerably different manufacturing strategy with personalized specifications of function, dosage, and delivery. In order to optimize for customer needs, we can consider our ability to optimize function based on physiological models [31,32] integrated with production models.

5.5. "Please help!" The enablers: Modeling and mathematics

High-performance computing and communications have been crucial for PSE developments. However, mathematics has been the key enabler for PSE tools and techniques and will continue to be so for smart process manufacturing. The development of computational optimization techniques in the 1950s and 1960s led to powerful tools and techniques that are now in common use in the process industries and beyond. In the 1980s and 1990s, the development of discrete optimization as a reliable and tractable problem led to the development of mixed-integer nonlinear programming (MINLP) solution techniques [33], which led in turn to great progress in the whole area. Disjunctive programming now allows us to handle solutions to problems with logical conditions [34]. We still struggle with discontinuities and with finding globally optimal solutions [35], and handling a full range of dynamic scenarios is still a challenge. We need methods that allow the visualization of large-scale problems to help understand and verify solutions.

Another enabler is the ability to model large-scale problems with complex mixtures and complex geometries. Generally speaking, modeling tools are still the domain of experts. Although there has been progress in considering how best to automate the process modeling workflow and the modeling of units and systems [36,37], the tools remain difficult to use. Engineering education and training has embraced this problem; however, making the tools more intuitive and robust would certainly help.

Model accuracy is important, and strongly relies on the ability to predict the properties and functional performance of complex mixtures.

Finally, when tools interact with big data repositories (both historical repositories and those related to customer demands), model accuracy can be taken into account systematically, using methods for quantifying uncertainty, for example, in order to account for situations when data is unreliable. A large community of researchers in computer science are studying the issues involved in handling big data. This will involve new forms of data, such as huge volumes of images, text, and so on, and will require the tools of knowledge management [38].

Enabling methods is the work of PSE researchers, so the development of new methods will continue to be a big part of our work. We will also continue to work with and draw from colleagues in other disciplines, including computer science, mathematics, and physics. Smart process manufacturing confronts us with an increasingly cross-disciplinary set of challenges.

6. Discussion and conclusions

The process industries have already made progress in smart manufacturing ideas, with PSE researchers and practitioners as key enablers. I have referred to some of the key published research work. Many of these ideas have been put into practice. However, there is very little benchmarking in the public domain. The publication of such information is always controversial. There is a need for a consolidation of reports on the specific beneficial outcomes of plant-wide optimization—perhaps on an anonymized basis, or resulting from application at one or more industrial-scale plants and sites.

I have highlighted some of the challenges confronting the PSE research community in achieving the full benefits of smart manufacturing. Many of these challenges revolve around how information is shared and passed between the units, plants, and sites of all the enterprises involved in a specific supply chain. There are also challenges in ensuring that all key aspects are properly modeled, particularly where health, safety, and environmental concerns require accurate predictions of small but critical amounts at specific locations. Although we have some of the technology that is required for a rapid and agile response to customer demands, the process industry's relationship (direct or indirect) to the end user makes it a particular challenge. It is difficult to predict whether this shift will bring about entirely new business models.

A key message is that in order to enact smart manufacturing, the PSE research and practice community needs to collaborate with other disciplines. For the most part, the process industry is challenge-oriented, and teams are not based on traditional discipline boundaries. The education and training of engineers in universities is also becoming more cross-disciplinary. Collaboration will certainly be a key requirement for bringing about smart process manufacturing.

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