# INTEGRATION OF CHEMICAL PROCESS OPERATION WITH ENERGY AND SYSTEMS INFRASTRUCTURE

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*Abstract*

Increased globalization, deregulation of energy markets, and environmental constraints, together with associated uncertainty, have created a highly dynamic and uncertain process manufacturing environment. Responding effectively to this increased variation and uncertainty is critical for a company to remain competitive. In this paper, we consider the plant infrastructure in relation to the energy and global market infrastructures. We describe changes to the plant infrastructure system in order to function more effectively in the current manufacturing environment, as well as key research advances that are aligned to addressing challenges faced by present day plant operation.

*Keywords*

Process operation, process control, energy systems, integration, decision-making hierarchy

## Introduction

Chemical and manufacturing industries continuously face multiple challenges: changes in overall economic environment, uncertainty in market drivers, rising energy costs, supply chain constraints, globalization, inflation, and hyper-competition, among others. The prevalent scenario is the survival of the fittest. All these challenges usually result in lower company profitability and lower return on investments if no corrective actions are taken.

One of the ways to not only mitigate the impact of these challenges, but to maintain a competitive edge is the adoption of new work processes, methods, initiatives, and technologies aimed to improve plant operational efficiency, agility, and reliability (e.g., reduction in energy consumption and higher plant up-time). To achieve this in a consistent way, industries need to strategize their operations, and take actions across multiple areas of the organization. For such a strategy to be effective, companies need to look both inwards and outwards. Enterprises are highly complex integrated entities, not only within a company (inwards), but also with suppliers, customers, competitors, government, etc. (outwards).

Successful attainment of these objectives requires appropriate infrastructure, organizational paradigms, and methodologies within process manufacturing enterprises, as well as an appropriate set of technology tools that can be deployed within this framework. In this paper, we discuss recent advances both within industry and the process systems engineering (PSE) research community, that are aligned with addressing the above-described challenges.

## Business Needs as Drivers for Operations Structure and Infrastructure Organization

Plant operations processes, organizations and infrastructure are, themselves, highly integrated complex

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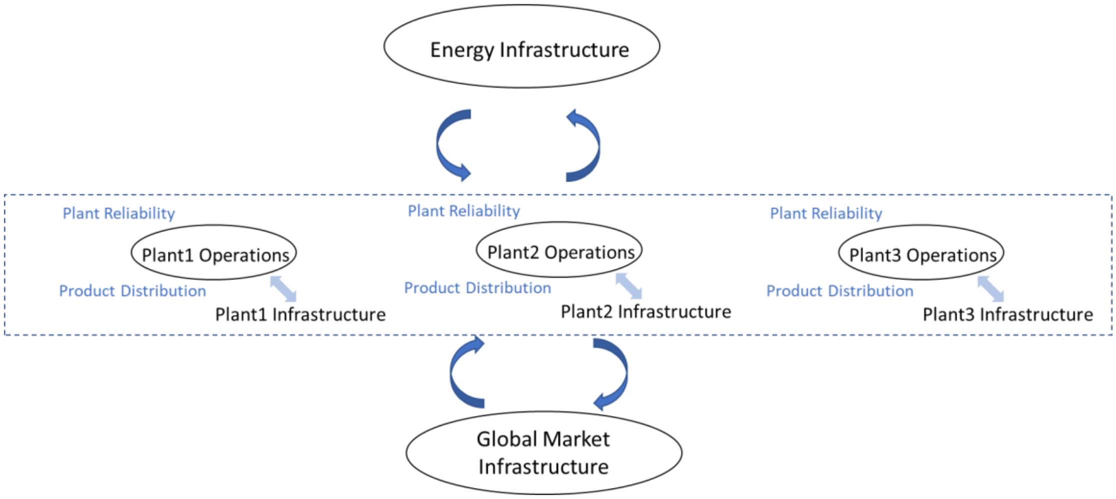


*Figure 1. Island Operations and Infrastructure Mode*

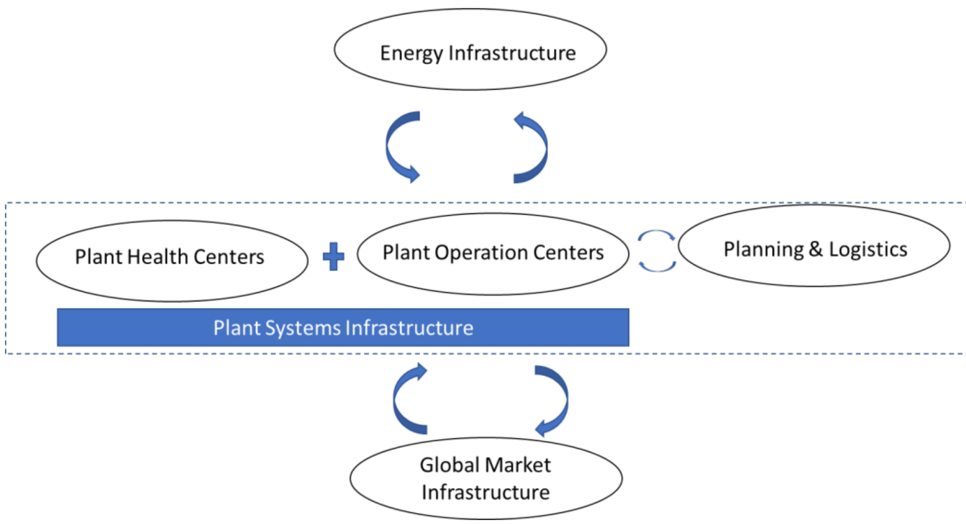


*Figure 2. Integrated and Remote Plant Operations and Infrastructure*

entities, that need to evolve to remain competitive accordingly to industry specific business models.

For example, in the industrial gas segment the following requirements have driven the smart manufacturing evolution (Flores-Cerrillo et al., 2020):

• Supply Reliability – Industrial gas customers require very high supply reliability. In many situations, high product availability is a contractual obligation. As a result, high equipment reliability and plant availability are key principles of the industrial gas business. Smart manufacturing initiatives consisting of the development of new IoT solutions that combine low-cost sensing with machine learning methods can provide new insights into machinery performance and avoid failures.

• Energy Efficiency - Industrial gas processes are not only highly energy intensive, but also highly integrated processes and systems that depend on energy suppliers and varying customer demand. The industrial gas business consumes about 2% of the US manufacturing industries overall energy consumption, so a 1% improvement in energy efficiency has large business and sustainability implications. Smart Manufacturing can leverage advanced plant automation to maximize overall process efficiency.

• Remote Accessibility - Given the utility nature of the business, industrial gas plants are typically located adjacent to other chemical customer facilities. As a result, the fleet base is highly distributed. Because of this, global remote access and robust digital tools are widely leveraged so that the appropriate experts can easily monitor and control plant performance remotely.

## Industrial Strategy

### *Smart Manufacturing & Digitalization*

Forward looking chemical and manufacturing industries have made considerable effort and progress in adopting and implementing Smart Manufacturing and Digital transformational initiatives. This has facilitated manufacturers to transform from being only product providers to be end-to-end solution partners through the integration of manufacturing and business solutions. Machine learning and artificial intelligence have broadened the overall functioning of the manufacturing industry.

Smart Manufacturing is a set of technologies and processes that maximizes data and connectedness to optimize highly integrated plant operations, including safety, reliability, and efficiency. However, to be successful in the Digitalization/Smart Manufacturing journey, companies need to have the right organizational structures, resources, and a strong foundation of global platforms.

### *Operations Structure and Infrastructure /Platforms Evolution*

To be successful, an industry/company not only needs new smart manufacturing/digital technologies like the ones mentioned above, but also, it needs to set the right organizational structures and foundational platforms.

We have seen that in different industry sectors, plant operations organizations and associated infrastructure have evolved as illustrated in Figures 1 & 2.

Figure 1 illustrates the Island plant operations and infrastructure mode, in which each plant is responsible for their plant operations, performance and reliability. Plant infrastructure is tailored to each plant facility.

Figure 2 illustrates a modern integrated and remote plant operations architecture with global systems infrastructure and platforms. The advantages of an integrated operations organization are multiple: high demand experts can be leveraged among multiple facilities, learnings from one facility can be leveraged to other ones, optimal resource utilization (a single resource can monitor and remote-control multiple facilities). Advantages of global infrastructures and platforms are also great differentiators: same or few technology stack options across the enterprise, small team of global experts to maintain, optimize and improve platforms, data availability to everyone, fast deployment of advanced machine learning solutions and IoT systems, among many others.

Sustaining these systems becomes a key enabler for some of the innovations described in the next sections.

## PSE Tools and Paradigms

In this section, we briefly review some key advances in PSE research that either seek to directly address the challenges of the modern-day process plant operating environment as described above, or can be harnessed to this end as enabling technologies. The discussion of research advances will be mostly in relation to the hierarchical decision-making paradigm that is prevalent in large chemical and petrochemical plants, and illustrated in Figure 3. We note that not all of the layers are necessarily present in every application, and that communication between the layers is generally not as seamless as may be inferred from the idealized diagram. While the hierarchical decision-making paradigm represents, for the most part, the status quo, it does exhibit challenges such as inconsistency of modeling or process representation at the different levels, and lack of coordination between them. Spatial and temporal integration across various functions and decision-making levels have been identified as key challenges in enterprise-wide optimization (Grossmann, 2005).

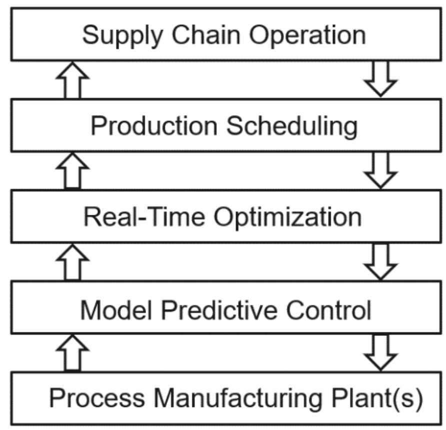


*Figure 3. Decision-making hierarchy in process manufacturing operation*

In the description that follows, we highlight some key advances in the technologies associated with the individual decision-making levels, then briefly describe advances in integration between the levels of the hierarchy. This is followed by a brief discussion of research developments in the areas of data analytics, AI and machine learning.

### *Advances at decision-making levels*

Model predictive control (MPC) is a model-based control algorithm in which a future input trajectory is calculated such that a performance criterion, based on the inputs and predicted plant response, is optimized. The inputs corresponding to the current time interval are applied to the plant, and the calculation process repeated, taking plant feedback into account. Advances to MPC have continued since its initial development about four decades ago, including extension to nonlinear models, stability analysis, incorporation of uncertainty, multiparametric formulations, economic MPC formulations, and inclusion of discrete decisions (Qin and Badgwell, 2003; Rawlings et al., 2022; Bemporad et al., 2002; Amrit et al., 2013; Bemporad and Morari, 1999). Concurrent with these extensions have been advances in computational and implementation strategies to enable applications involving large-scale, nonlinear models (Biegler, 2018; Zavala and Biegler, 2009).

While the entire plant decision-making hierarchy can, in principle, be replaced by a single MPC system, this is clearly impractical due to the times scale differences, high dimension, and problem complexity, in addition to considerations of reliability. An open question is how much of the decision-making should be delegated to the MPC system.

Real-time optimization (RTO) involves the adjustment of plant operating conditions to ideally coincide with the plant economic optimum (Marlin and Hrymak, 1997; Darby et al., 2011). The traditional approach utilizes a first-principles steady-state model, and follows a sequence of data reconciliation, model updating, and optimization at each RTO execution. The reliance on a steady-state model, however, limits the RTO execution frequency, resulting in suboptimal performance for plants with slow dynamics and or frequent transitions. This has led to the utilization of dynamic models at the RTO level (Kadam et al., 2002; Tosukhowong et al, 2004). A DRTO formulation in which the predicted response of the plant includes the action of the plant's MPC system was proposed by Jamaludin and Swartz (2017), and extended in Li and Swartz (2019) to the dynamic economic coordination of distributed MPC systems.

Production scheduling is largely concerned with determining the quantities of products to be manufactured, when to produce them, and in what sequence. It is applicable to both batch and continuous processes, the former typically also requiring determination of equipment and resource usage and the timing thereof. Comprehensive reviews of scheduling optimization formulations may be found in Floudas and Lin (2005) and Mendez et al. (2006). Key advances have been made in recent years in formulation paradigms to improve computational efficiency, and in online scheduling. The latter includes event triggered reactive scheduling (Kopanos et al., 2008; Li and Ierapetritou, 2008; Kopanos and Pistikopoulos, 2014; Henning, 2017), and periodic online scheduling (Gupta and Maravelias, 2016, 2017; Mathur at al., 2020). Mathur et al. (2021) propose a robust online scheduling scheme that mitigates uncertainty through both two-stage stochastic programming and feedback.

*Integration between decision-making levels*

While replacing the entire hierarchy depicted in Fig. 3 by a single-layer formulation may be impractical, integration between subsets of the layers has been, and continues to be, studied. Economic MPC, in which the traditional MPC set-point tracking and move suppression objective is replaced by an economic objective, or combination of an economic and performance objective (Amrit at al., 2011; Amrit at al., 2013), can be considered as an integration of the RTO and MPC layers. The DRTO formulation of Jamaludin and Swartz (2017), on the other hand, retains the two-level DRTO-MPC structure, but utilizes within the DRTO layer, the prediction of the closed-loop response of the plant under the action of constrained MPC.

A second area of integration that has grown considerably in recent years is integrated scheduling and control (ISC). This has been motivated largely by the dynamic environment in which process manufacturing plants operate, where process dynamics have an increasingly significant impact on the scheduling decisions (Baldea et al., 2015). ISC, broadly speaking, considers plant dynamics in scheduling decisions, and includes several different formulation and implementation paradigms. This includes calculation of control inputs along with scheduling decisions that are applied directly to the plant (Prata et al., 2008), calculation of reference state values in the ISC formulation that are tracked by a plant MPC (Zhuge and Ierapetritou, 2014), and calculation of scheduling decisions that account for the closed-loop plant response under constrained MPC, with the optimal operation communicated to the plant through MPC set-point trajectories (Remigio and Swartz, 2020).

*Advances in Data Analytics, AI and Modeling*

The confluence of advances in computer hardware, cloud storage capabilities, wireless communication technologies, and numerical computation have created fertile ground for the paradigms of Smart Manufacturing (Davis et al., 2012) and Industry 4.0 (Zheng et al., 2021), where there has been a surge in industrial uptake. There has been parallel growth in related research areas of data analytics, surrogate modeling, artificial intelligence, and machine learning. The highly multidisciplinary nature of these areas provides a vast terrain of approaches to draw upon, but also comes with the caveat that methods and applications in a particular domain may not directly translate to applications in process manufacturing. However, potential opportunities and PSE-relevant applications are steadily being explored.

Perspectives on machine learning for process data analytics are given in Qin and Chiang (2019). Surrogate modeling (Bhosekar and Ierapetritou, 2018; Wilson and Sahinidis, 2017) have significant potential for expanding the domain of model-based decision making through reduced computation times. The application of reinforcement learning to control is discussed in Spielberg et al. (2019) and Sin et al. (2019), while Hubbs et al. (2020) present a deep reinforcement learning approach to chemical production scheduling. An overview of machine learning, with implications for the PSE field, is given in Lee at al. (2018).

## Conclusion

The process manufacturing landscape has shifted significantly in recent years to an environment of increased global competition, energy price fluctuations, high degrees of variability, and increased uncertainty. In this paper, we have the outlined shifts in the process manufacturing infrastructure in response to these changes, as well as developments in process systems engineering research that are aligned to addressing these challenges. The tumultuous manufacturing environment shows no signs of abating, calling for continued research and industry-university partnerships to respond to this new normal.

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