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The quest towards the integration of process control, process operations, and process operability –Industrial need or academic curiosity?

Efstratios N. Pistikopoulos [a,b,*], Sahithi Srijana Akundi [a,b], Dustin Kenefake [a,b]
Nikolaos A. Diangelakis [c]

[a] *Texas A&M Energy Institute, Texas A&M University, College Station, TX, 77843, USA*
[b] *Texas A&M Department of Chemical Engineering, Texas A&M University, College Station, TX, 77843, USA*
[c] *School of Chemical and Environmental Engineering, Technical University of Crete, Chania, Crete, GR 73100, Greece*

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ABSTRACT

Historically, process control, process scheduling, and process operational functions (such as safety and maintenance) have been considered independently, in isolation, and/or in a sequential manner from an overall process automation perspective — primarily reflecting the widely accepted difference in their corresponding time scales like days/hours for scheduling, seconds/minutes for control, etc. However, the current trend towards real-time decision-making under increasingly dynamic and volatile business, market, and supply chain environments has intensified the need for an 'integration of scales' in terms of temporal and spatial considerations. The joint FOCAPO/CPC conference series over the last decade is an example of increasing evidence, at least within academic circles, of such a paradigm shift. It should not come as a surprise that there is increasing evidence of business and industrial needs in this direction. Moreover, significant advancements have been achieved in the development of solutions that effectively address the imperative of scale integration. Here, we will attempt to provide a road map of the evolution of the process systems engineering field towards the unification of control, operations, and operability, through industrial and research activities over the last twenty years. We aim to elucidate the following questions: When does the need for such an integration of scales arise? Which types of industrially relevant problems and applications can be considered for such an approach? Where do we stand regarding methodological developments and solution strategies as enablers and tools for such an integration? If desired, what would be the ideal framework and potentially the target software platform for achieving such a unification?

1. Introduction and overview

The chemical industry has been undergoing a sweeping transformation, propelled by the intricate interplay of dynamic market conditions, technological advancements, and evolving societal expectations. This era of unprecedented change has necessitated a relentless pursuit of operational excellence, prompting substantial research efforts and advances in the broad theme of real-time decision-making and optimization. Notably, the areas of production scheduling and capacity planning have emerged as critical focal points for optimizing decision-making processes, enabling chemical enterprises to respond effectively to market demands and achieve competitive advantage (Baldea and Harjunkoski, 2014). The field of Process Systems Engineering (PSE) has long been at the forefront of shaping the chemical industry by focusing on the fundamental research of designing economically viable plants and maximizing their operational performance through innovative modeling, simulation, and optimization techniques and tools, to improve efficiency, reliability, and profitability.

The urgent need to reduce carbon emissions, minimize waste generation, and develop environmentally friendly processes has further prompted a shift towards more responsible and sustainable operations. By integrating quantitative methods, advanced modeling techniques, and sustainability metrics, frameworks, and tools that enable comprehensive decision-making, accounting for economic, environmental, and social dimensions are emerging (Pistikopoulos et al., 2021a). The need for an integrated, holistic approach has never been more important, with the view to systematically coordinate the different layers of decision-making, analyze their interactions, and provide solutions that seamlessly look at the different scales of decision-making regarding control, scheduling, and ultimately design.

* Corresponding author at: Texas A&M Energy Institute, Texas A&M University, College Station, TX, 77843, USA.
E-mail address: stratos@tamu.edu (E.N. Pistikopoulos).

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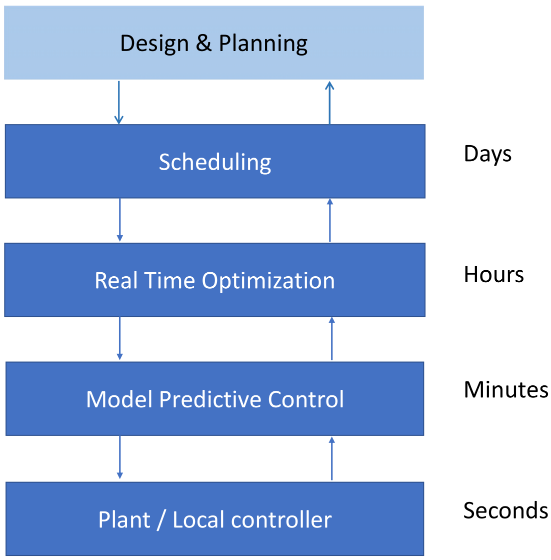


Fig. 1. The conventional decision-making hierarchy offers a structured approach to optimize industrial processes. While it provides a logical sequence for decision-making, it also has limitations regarding sub-optimality and iterative adjustments.

Traditionally, such operational decisions have been implemented over different time horizons ranging respectively from several days/weeks to minutes/seconds in a hierarchical manner, as shown in Fig. 1.

These decision layers are typically isolated and their interactions may be neglected. Each layer's objective(s), time scales, and sources of uncertainty are usually treated via different models and based on various data streams. On the other hand, the notion of Enterprise-wide optimization (EWO) focuses on harmonizing and optimizing operations at all levels, by explicitly recognizing the interdependencies and opportunities for the integration of information and decision-making across the diverse functions within a company's supply chain (Grossmann, 2012; Rafiei and Ricardez-Sandoval, 2020).

Such integration of scales is typically driven by various factors such as smart manufacturing (Edgar and Pistikopoulos, 2018), real-time optimization (Baldea and Harjunkoski, 2014), digital transformation (Coito et al., 2022), standardization, and increasing need for safety, sustainability, and cost-competitive resilience (Pistikopoulos et al., 2021a). While such integration of scheduling, control, and design may facilitate improved decision-making and operational performance, it presents numerous challenges attributed to various factors, including:

- *Interdisciplinary Collaboration:* Integrating scheduling, design, and control requires collaboration among experts from different disciplines, including operations research, control engineering, and system design. Bridging the gaps between these disciplines and establishing effective communication and understanding can be challenging.
- *Complexity and Scale:* Real-world systems are often complex and large-scale, involving numerous components, constraints, and interactions. Managing the complexity and developing scalable integration approaches that can handle the sheer volume of data and decision variables is a significant challenge.
- *Dynamic and Uncertain Environments:* Many systems operate in dynamic and uncertain environments where parameters, demands, and constraints change over time. Developing integration methods that can adapt and respond to such dynamic changes, while considering uncertainty, is a complex task.
- *Conflicting Objectives:* Scheduling, design, and control often involve optimizing multiple conflicting objectives. For example, scheduling decisions may aim to minimize the makespan, while control decisions focus on stability and efficiency. Balancing these conflicting objectives and finding optimal or near-optimal solutions is a challenge.
- *Real-Time Decision-Making:* Integrating scheduling, design, and control in real-time decision-making scenarios requires efficient algorithms and methods that can process large amounts of data and provide timely solutions. Achieving low computational complexity and real-time responsiveness is crucial.
- *Information and Data Integration:* Integration requires the seamless exchange and integration of information and data across scheduling, design, and control domains. Ensuring the compatibility, consistency, and accuracy of data from different sources and formats is a challenge.
- *Software and System Integration:* Integrating scheduling, design, and control often involves the integration of different software tools and systems. Ensuring compatibility, interoperability, and efficient communication between these systems can be challenging, especially when they are developed by different vendors or based on different technologies.
- *Human Factors:* Integrating scheduling, design, and control systems also involves considering human factors, such as user interfaces, decision support systems, and human–machine interactions. Designing intuitive and user-friendly interfaces that facilitate effective human involvement in decision-making is a challenge.
- *Implementation and Deployment:* Transitioning from research and development to practical implementation and deployment of integrated systems is a challenge. Incorporating the integrated approach into existing systems, managing system upgrades, and ensuring smooth operation require careful planning and coordination.
- *Cost and Resource Constraints:* Integrating scheduling, design, and control should consider practical constraints, such as limited resources, budget constraints, and cost considerations. Finding cost-effective solutions that optimize system performance while respecting these constraints is a challenge.

Addressing these challenges requires a comprehensive and systematic approach that considers the specific requirements and characteristics of the integrated system. This alongside the increasing need for the integration of scales led to various attempts in the development of generalized step-by-step frameworks. There are various methodologies proposed for such an integration, as discussed in the following.

2. Integration of scales

Due to the numerous drawbacks of the conventional decision-making framework, various opportunities for the integration of scales were studied. These are graphically denoted in Fig. 2. The subsequent subsections provide a detailed explanation of these opportunities, followed by an exploration of the challenges and benefits associated with them.

2.1. Integration of scheduling and control

Scheduling is a critical decision-making process with significant importance in process industries. Its primary objective is to efficiently allocate limited resources to processing tasks over time, ensuring the fulfillment of demands and facilitating profitable operations. These scheduling problems can be modeled based on the specific characteristics and constraints of the process, allowing for the proposal of different objective functions such as maximizing profit or minimizing make-span. Through this modeling, the optimal sequence of tasks and resource allocation can be determined.

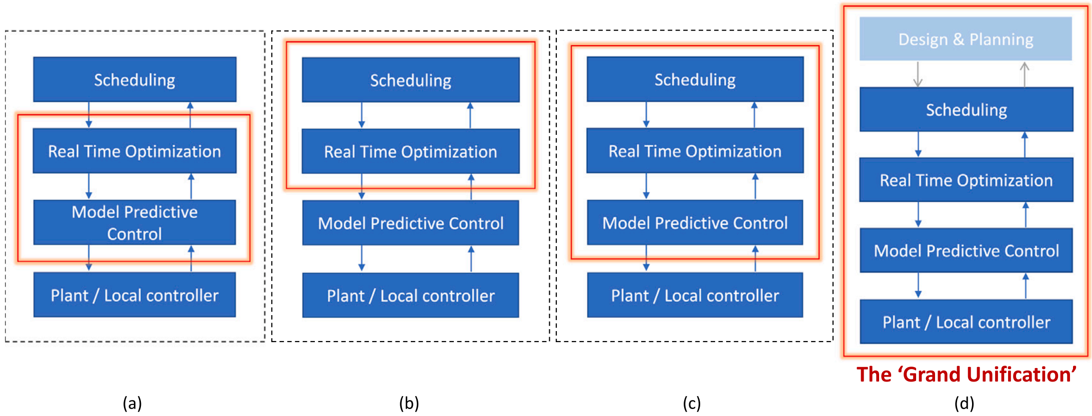


Fig. 2. Various opportunities for integration of scales, which facilitates a comprehensive understanding of the system and enables better alignment of decisions with strategic goals, operational requirements, and broader socio-economic and environmental considerations. (a) Integrating a real-time optimization layer that considers real-time measurements to dynamically adjust control variables and optimize system performance within predefined constraints and model predictive control layer thereby having hours and minutes time scale into consideration (b) Integrating scheduling layer which operates in days with real-time optimization layer which operates in hours (c) Integrating the top three layers of the conventional hierarchy thereby allowing the impact of lower level changes on the higher level and vice versa (d) The Grand unification of layers which poses the ultimate complexity in integrating and also expects to provide the best decision-making solutions.

On the other hand, process control also serves as a decision-making process aimed at managing the qualitative aspects of processes by adjusting their operating conditions. Advanced control techniques are gaining prominence across industries and are recognized by major companies as key elements for energy conservation, maximizing throughput, and achieving cost-efficient production (Dias and Ierapetritou, 2016; Baldea and Harjunkoski, 2014).

Traditionally, production scheduling and dynamic optimization problems in chemical processes have been approached separately. However, there exist variables that establish a connection between these two areas. For instance, the states at the beginning and end of transient periods, the duration of transient and steady-state periods, and the quantity of material in production stages are all linking variables. This linkage between scheduling and dynamic optimization implies that they cannot be completely isolated from each other (Zhuge, 2015). Another reason why integrating scheduling and control problems are challenging is due to the fundamental difference in the time horizons they address. Scheduling focuses on long-term calculations that span hours or days, while control actions operate on much shorter time scales, usually within seconds to a few minutes. This disparity in time frames presents a significant obstacle when attempting to combine scheduling and control processes (Baldea and Harjunkoski, 2014). By adopting an integrated approach, information can be shared between the scheduling and dynamic optimization levels, enabling integrated decision-making that enhances the profitability of process operations.

The integration of process scheduling and control poses several challenges. These challenges encompass the need for synchronization and coordination between scheduling and control decisions, the incorporation of real-time production data for dynamic decision-making, the complexity arising from resource constraints and uncertainties, and the integration of feedback control strategies into scheduling algorithms. Additionally, challenges related to system scalability, computational efficiency, and the integration of advanced technologies such as artificial intelligence and machine learning are also explored.

Current research emphasizes the considerable advantages associated with integrating process scheduling and control within manufacturing environments. The integration of these systems enables the reduction of production lead times by optimizing the sequencing and coordination of operations. By incorporating real-time data and feedback control, it becomes possible to enhance resource utilization, improve product quality, and enhance the adaptability of production processes to changing circumstances. Consequently, this integration contributes to improved manufacturing efficiency, increased throughput, and heightened customer satisfaction. Extensive ongoing research in this field, along with a focus on process design, is evident and can be observed in Tables 1a and 1b.

In the pursuit of effectively integrating process scheduling and control, researchers have explored a wide array of methodologies and technologies. One line of investigation centers around the development of optimization models and algorithms that take a holistic approach to consider both scheduling and control objectives. By enabling synchronized decision-making, these models and algorithms aim to optimize the overall system performance by carefully examining the interplay between scheduling and control variables. Advanced control strategies, including model predictive control and adaptive control, undergo rigorous scrutiny to evaluate their effectiveness in managing dynamic production conditions and enhancing process performance. Leveraging real-time data and adaptive algorithms, these strategies dynamically adapt control actions and optimize process operations in response to changing circumstances.

Moreover, the research delves into the significance of real-time data acquisition and analysis, Internet of Things (IoT) technologies, and digital twins in supporting the seamless integration of scheduling and control systems (Andrés-Martínez and Ricardez-Sandoval, 2022a). Real-time data acquisition and analysis play a pivotal role in providing valuable insights into the present state of the production process, empowering timely decision-making. Through the facilitation of seamless communication and data exchange between various components of the manufacturing system, IoT technologies enable efficient coordination between scheduling and control functions. Additionally, digital twins, which serve as virtual replicas of physical assets and processes, prove to be invaluable tools in simulating and optimizing production operations. Leveraging digital twins, researchers and practitioners can conduct virtual experiments and optimize system performance within a risk-free environment, thus furthering the integration of scheduling and control. Section 3 of the research paper provides an in-depth analysis and categorization of methodologies, presenting a comprehensive assessment of different approaches and their respective advantages and limitations.

2.2. Integration of operability and control

Process operability plays a crucial role in the efficient and successful operation of industrial processes. It encompasses a broad spectrum of factors that impact the ability to control, monitor, and maintain a process in a safe and reliable manner. Achieving effective process operability necessitates the integration of various elements such as design considerations, instrumentation, control systems, maintenance strategies, and human factors. By prioritizing operability, organizations

Table 1a
Integration of scheduling and control — indicative list.

Gutiérrez-Limón et al. (2012b), Terrazas-Moreno et al. (2005), Zachar and Daoutidis (2019) and Dowling et al. (2018)	Bi-level optimization for simultaneous scheduling and control
Gutiérrez-Limón et al. (2014), Adloor and Vassiliadis (2020), Al Ismaili et al. (2018), Kelley et al. (2018) and Maravelias (2021)	Simultaneous planning, scheduling, and control via mixed-integer programming formulations
Burnak et al. (2020b), Diangelakis et al. (2017), Charitopoulos et al. (2019) and Zhuge and Ierapetritou (2014)	Simultaneous process scheduling and control via Multi-parametric programming
Frankl et al. (2012), Elixmann et al. (2010), Prata et al. (2008), Petersen et al. (2017) and Charitopoulos et al. (2017b)	Integrated scheduling and control of continuous processes
Beal et al. (2017a), Nie et al. (2015) and Touretzky et al. (2016)	Integrated scheduling and control via discrete-time formulations
Misra and Gudi (2018), Chu and You (2014), Huercio et al. (1995), Capón-García et al. (2013), Overturf et al. (1978) and Maravelias and Grossmann (2004)	Integrated scheduling and control for batch processes
Mitra et al. (2010)	Resiliency based integration of scheduling and control
Risbeck et al. (2018), McAllister et al. (2019), Zhuge and Ierapetritou (2012) and Dias et al. (2018)	Closed-loop implementation of scheduling and control
Subramanian et al. (2013)	Scheduling and control for supply chain management
Dias and Ierapetritou (2016), Rodríguez Vera and Ricárdez-Sandoval (2021), Hossein Sahraei and Ricardez-Sandoval (2014) and Dering and Swartz (2022)	Integrated scheduling and control using MPC/under uncertainties
Dias and Ierapetritou (2020) and Simkoff and Baldea (2020)	Data-driven scheduling and control models
Du et al. (2015)	Integration via time-scale bridging methods

Table 1b
Integration of design with scheduling/control — indicative list.

Burnak et al. (2019a, 2018a) and Burnak et al. (2020a)	Integration of process design, control, and scheduling using multi-parametric programming
Papageorgiou et al. (1993), Realff et al. (1996), Jayaraman et al. (2000), Burnak et al. (2020a), Grossmann et al. (1996), Vaselenak et al. (1987) and Bhatia and Biegler (1996)	Integrated design, planning and scheduling of batch processes
Fisher et al. (1988) and Al-Mutairi and El-Halwagi (2010)	Interactions between design, control, and operability
Seferlis and Georgiadis (2004)	Integration of design and control via controller parametrization
Iftakher et al. (2022), Georgiadis et al. (2001) and Panjwani et al. (2005)	Integrated design and control of reactive distillation processes
Tsolas and Hasan (2021) and Guillén-Gosálbez and Grossmann (2009)	Resilience-based optimal design and operation of supply chain networks
Allman et al. (2019), Palys et al. (2023), Elms and El-Halwagi (2010), Stefanis et al. (1997), Avraamidou and Pistikopoulos (2019) and Bhatia and Biegler (1997)	Scheduling based optimal design of process systems
Georgiadis (1998), Zhou et al. (2013), Liu et al. (2013), You and Grossmann (2007) and Logsdon (1990)	Integrated design and operation of process systems
Ierapetritou and Pistikopoulos (1996)	Global optimization of integrated stochastic planning, scheduling and design problems
Flores-Tlacuahuac and Biegler (2005)	Simultaneous design and control under uncertainty
Biegler et al. (1997)	Large-scale optimization of design and control of process systems

can optimize production levels, mitigate risks, and ensure the well-being of personnel and the environment. Ongoing research in process operability focuses on developing and refining methodologies, technologies, and best practices that enhance the operability of complex systems. This includes advancements in process control algorithms, intelligent monitoring systems, risk assessment, and management techniques, as well as training programs and the design of human–machine interfaces. The aim is to continually improve the operability of processes, ensuring their stability and reliability under various operational conditions. Table 2 provides a comprehensive list of academic research groups actively engaged in studying the integration of control with operability. These groups contribute to advancing knowledge and expertise in the field, driving innovation, and promoting the adoption of effective operability practices across industries.

Traditionally, process control is responsible for regulating and optimizing process variables, while process operability ensures efficient and safe operation. However, recent research has shed light on the potential advantages of integrating these two aspects to achieve superior industrial performance. Current research studies explore the synergistic relationship between process control and operability, examining the potential benefits that arise from their integration (Downs and Ogunnaike, 1995). The integration of process control and operability yields significant benefits. One key observation is that improved process stability leads to enhanced product quality, increased production efficiency, and reduced variability. By integrating these two aspects, organizations can implement proactive maintenance strategies, mitigating the risk of equipment failures and unplanned shutdowns. Additionally, incorporating human factors considerations into control system design enhances operator situational awareness, minimizing the likelihood of human error and improving overall safety (Wu et al., 2018). By merging process control and operability, industrial processes can achieve heightened performance and optimize their operations. This integration paves the way for enhanced product quality, improved efficiency, reduced variability, proactive maintenance, and enhanced safety.

There are several challenges identified in integrating process control and operability. These include the need for compatible control and operability objectives, the availability and reliability of real-time process data, the development of robust control strategies that account for process disturbances, and the consideration of human factors in control system design. Challenges related to system complexity, scalability, and the integration of advanced technologies, such as artificial intelligence and machine learning, are also explored. The current-day research investigates various methodologies and technologies that facilitate this integration of process control and operability. This includes the development of advanced control algorithms, such as model predictive control and adaptive control, that consider operability constraints. Real-time monitoring techniques, such as fault detection and diagnosis systems, are examined for their ability to enhance process reliability and safety. The role of data analytics and predictive maintenance practices in improving operability and reducing downtime is also explored. More about the classification of methodologies is discussed in Section 3.

Table 2
Operability and Safety — indicative list.

Pistikopoulos et al. (2021b)	Challenges and opportunities in the integration of design, operability, and control of intensified and modular process systems
Tian and Pistikopoulos (2018)	Integration of process intensification systems with guaranteed flexibility and safety performances
Mesquita et al. (2021)	Development of novel control strategy using process operability and biometric control algorithms for batch bio-processes
Fisher and Douglas (1985)	Evaluation of process operability during the initial design phase
Wang et al. (1996)	Safety and operability analyses of processes using neural network learning algorithms
Georgiadis et al. (2002)	Interactions of design, control, and operability in reactive distillation systems
Longwell (1994)	Dynamic modeling for control and operability
Al-Mutairi et al. (2008)	Integration of inherently safer process design and scheduling
Albalawi et al. (2018) and Wu et al. (2019)	Safety via model predictive control

3. Classification of methodologies

3.1. Integration of scheduling, control and, design

Engell and Harjunkoski (2012) provide insights into the initial efforts made to integrate scheduling and control, along with the various challenges encountered, including technical, business-related, and psychological aspects. The classification of integrated scheduling and control (iSC) problems can be broadly categorized into two approaches: *top-down bottom-up*.

3.1.1. Top-down integration

The top-down approach in integrated scheduling and control (iSC) involves incorporating control decisions into the scheduling problem by integrating the dynamic process model or a control scheme like Model Predictive Control (MPC) or Proportional–Integral (PI) controllers. When the dynamic model is included as additional constraints in the scheduling problem, it is referred to as integrated scheduling and dynamic optimization (Prata et al., 2008). Solving this iSC problem yields an optimal schedule and a corresponding open-loop control policy for implementation. For continuous systems, time-slot-based scheduling formulations are commonly used, where each slot represents production and transition times (Flores-Tlacuahuac and Grossmann, 2006). Batch systems utilize state equipment network (SEN) and state-task network (STN) structures for integration (Nie et al., 2012). As the scheduling level involves discrete decisions, the iSC problem is typically formulated as a Mixed-Integer Dynamic Optimization (MIDO) problem. Since chemical processes are often described by conservation equations, the dynamic model includes nonlinear terms. Consequently, the MIDO problem is transformed into a Mixed-Integer Nonlinear Programming (MINLP) problem after discretizing the dynamic equations. However, the presence of nonlinear terms can significantly increase the complexity of the integrated model, especially when nonconvexities arise. As a result, solving the MINLP problem becomes computationally demanding and challenging for large-scale applications, necessitating practical and efficient solution strategies (Koller and Ricardez-Sandoval, 2017). To alleviate computational costs, initialization of the solution procedure close to the optimal or sub-optimal solution can be beneficial. However, obtaining accurate initial guess values is generally difficult. Various techniques have been proposed to decompose, initialize, and reformulate the integrated problem for both batch and continuous chemical and manufacturing systems. These include approaches such as Bender decomposition (Chu and You, 2013b) and community detection for continuous systems and bi-level programming for batch systems (Chu and You, 2014). In the case of multi-product continuous systems, integer variables can be avoided by using a switching system formulation.

To incorporate the closed-loop behavior of the system in the integrated scheduling and control (iSC) problem, the Model Predictive Control (MPC) formulation can be added as constraints in the scheduling problem, leading to bi-level optimization formulations (Palma-Flores and Ricardez-Sandoval, 2022). This approach has also been employed in the integration of design and control. However, integrating the MPC formulation increases the complexity of the model, particularly when considering integer decisions in the formulations. Various strategies have been explored to reduce the size of the integrated model. Several techniques aim to reduce the complexity of the integrated model, including linear state space representations (Burnak et al., 2018b), latent variables (Tsay and Baldea, 2020), piece-wise affine (PWA) model approximations (Zhuge and Ierapetritou, 2015), linear metamodels (Charitopoulos et al., 2019), and time scale-bridging models (Baldea et al., 2015). However, in some cases, extensive plant/MPC simulations are necessary to identify accurate low-order representations of the integrated model. Additionally, some of these reduction techniques may encounter difficulties when dealing with discrete variables. Applications of these reduction techniques can be found in multi-product continuous systems such as continuously stirred tank reactors (CSTR) and multitask batch systems. An alternative strategy involves deriving the optimality conditions of the MPC and integrating them into the scheduling model (Simkoff and Baldea, 2019; Remigio and Swartz, 2020). This formulation introduces a set of complementarity constraints, requiring proper reformulation to avoid numerical issues. This approach has been applied to multi-product CSTRs, as demonstrated in the work by Andrés-Martínez and Ricardez-Sandoval (2022a).

3.1.2. Bottom-up integration

The bottom-up approach in the integration of scheduling and control (iSC) involves incorporating scheduling decisions into the control formulation. One common strategy is to use an economic objective function within the Model Predictive Control (MPC) scheme, resulting in an economic MPC (EMPC) formulation (Heidarinejad et al., 2012). While EMPC has potential and attractiveness, stability and feasibility considerations need to be revised as they may differ from traditional MPC (Ellis et al., 2014). EMPC does not necessarily operate the system at a specified steady state or target value; instead, it optimizes the process economics in a time-varying manner, leading to frequently changing set-points and scheduling decisions based on process economics and external perturbations. Additionally, EMPC may not account for discrete decisions such as sequencing relations. Nonetheless, EMPC is regarded as a promising bottom-up approach for efficient iSC in various applications, including chemical process networks (Ellis and Christofides, 2014), inventory management (Subramanian et al., 2014), and continuously stirred tank reactors (CSTRs) (Santander et al., 2016).

Rescheduling schemes have been proposed as extensions of iSC formulations to handle disturbances and unexpected events. Some studies propose online solutions to the iSC problem to correct deviations from desired state values. However, computational time constraints may make this approach impractical for large-scale models. Consequently, techniques to reduce model complexity, such as linear state space representations and multi-parametric programming, have been applied to develop iSC schemes suitable for efficient online implementation (Zhuge and Ierapetritou, 2014). Frameworks involving a nested decision-making structure with two loops have also been proposed for continuous and batch systems (Nie et al., 2015; Maravelias and Grossmann, 2004; Overturf et al., 1978). In the outer loop, rescheduling is performed by solving an iSC problem (either full-space or reduced

Table 3
Industrial applications.

Bindlish (2018)	Scheduling, optimization, and control of power for industrial co-generation plants
Baldea et al. (2015)	Development of frameworks for integrating scheduling and control operations in manufacturing plants
Kenefake et al. (2022), Dias et al. (2018) and Kelley et al. (2022)	Integration of scheduling and model predictive control in the air separation unit operations
Guillén-Gosálbez et al. (2010)	Integration of planning and scheduling in hydrogen supply networks
Chu and You (2013a)	Integration of scheduling and closed-loop control online for MMA polymer manufacturing process
Nie et al. (2015), Maravelias and Grossmann (2004) and Overturf et al. (1978)	Scheduling and control for chemical batch processes
Elixmann et al. (2010)	Integration of scheduling and control for reactive distillation systems and wastewater treatment systems
Pravin et al. (2020)	Scheduling and control framework for the integration of renewable energy sources for fuel cell systems
Sahraei and Ricardez-Sandoval (2014)	Scheduling and control of CO2 emission capture from coal-based power plant
Mathur et al. (2021, 2020)	Robust online scheduling for cascaded hydro-power systems
Risbeck et al. (2020)	Online scheduling for large HVAC systems
Subramanian et al. (2013)	Scheduling and control methods for supply chain management
Biegler (2018)	Integrated dynamic scheduling policies for polyol processes
Touretzky and Baldea (2014)	Integrated scheduling and control for energy storage buildings

order) to determine optimal set-point values, which are then tracked using either MPC or explicit MPC in the inner loop.

A state space representation has been developed for scheduling, allowing the application of control theory concepts such as Model Predictive Control (MPC) and Economic MPC (EMPC) for rescheduling and online scheduling tasks (Subramanian et al., 2012; McAllister et al., 2019). This unified state-space formulation for integrated scheduling and control (iSC) considers the closed-loop properties of the system (Risbeck et al., 2019). The state space representation provides a natural description of the scheduling process as a dynamic system, offering more accurate scheduling models when used individually or integrated with planning and/or control. This approach has potential applications in multi-product continuous and batch systems, although model reduction techniques may be necessary for large-scale problems.

While the closed-loop implementation of iSC decisions can handle uncertainties at the control level in a reactive or preventive manner, uncertainties in the iSC formulation have received limited attention. Promising frameworks for handling uncertainties in the iSC model include two-stage stochastic programming, chance-constrained optimization, and robust optimization (Ierapetritou and Pistikopoulos, 1996). These approaches have been tested on multitask batch systems with uncertain kinetic parameters and initial conditions, as well as on a multi-product continuously stirred tank reactor (CSTR) with uncertain demand (Gutiérrez-Limón et al., 2012b). However, solving the resulting formulations can be challenging and may require decomposition techniques like Bender decomposition. Another approach for addressing uncertainties is the use of back-off terms to approximate their effects. These terms can be estimated through Monte Carlo simulations. An iterative procedure is employed to update the back-off terms until a convergence criterion is met. This approach has been applied to multi-product continuous systems, including process design and multi-product, multi-unit batch systems (Nie et al., 2015; Maravelias and Grossmann, 2004; Overturf et al., 1978). However, for large-scale problems, the computational cost can be significant due to the intensive calculations involved in Monte Carlo simulations.

In recent years, the integration of scheduling and control (iSC) strategies has been observed in various industrial applications. Bindlish (2018) demonstrated the simultaneous solution of scheduling, real-time optimization, and control of power for industrial co-generation plants. They employed a first-principle, steady-state, non-linear model that was continuously tuned with plant data. This model was utilized for online optimization, followed by the implementation of scheduler results using a model-predictive controller. A nested decision-making framework was applied by Dias et al. (2018). to an Air Separation Unit. The framework consisted of an inner loop with an online model-predictive controller and an outer loop as a closed-loop simulation optimization problem. This approach allowed for the integration of scheduling and control in a coordinated manner. Baldea et al. (2015) illustrated the iSC solution strategy for manufacturing plants using a scheduling-oriented model-predictive controller. They incorporated a scale-bridging model that provided an explicit description of the closed-loop process dynamics. This approach allowed for a comprehensive integration of scheduling, control, planning, and design aspects. Table 3 provides an extensive and comprehensive list of industrial applications where scheduling, control, planning, and design have been integrated. It showcases the diverse range of industries and processes in which iSC strategies have been implemented. Table 4 presents a comprehensive classification of the different approaches that have been utilized in investigating iSC over the past few years. This classification helps to categorize and understand the various methodologies and techniques employed in the field of integrated scheduling and control.

3.2. Integration of operability and control

There has been a growing interest in coordinating control with safety considerations, recognizing that traditional approaches to process safety, such as process design modifications, may overlook important factors that impact process operational safety. These factors include the complex multi-variable interactions of process components and variables, limitations on the capacity of control actuators, and the influence of safety or relief system responses on the effectiveness of the process control system. To address these challenges, researchers have proposed various approaches. One such approach involves incorporating thresholds based on a state-based Safeness Index, as developed by Albalawi et al. (2017), to serve as triggers for safety system activation. By integrating these thresholds into the design of safety systems, coordination between safety and control can be achieved. The same Safeness Index, with different thresholds, can also be utilized in the design of model-predictive controllers (MPC) to enhance coordination between safety and control designs (Wu et al., 2019; Albalawi et al., 2018). Control designs have been developed by Mhaskar et al. (2012), Mhaskar (2006), Lao et al. (2013), Kettunen et al. (2008), Prakash et al. (2002), Bø and Johansen (2014), Xue and El-Farra (2016) and Allen and El-Farra (2017) to handle safety-related issues, particularly in the context of faults. These control designs aim to detect and respond to faults in the system, ensuring safe and reliable operation. The integration of safety and control has also been explored through dynamic risk assessment, which plays a crucial role in providing real-time evaluation and mitigation of potential hazards. By dynamically assessing risks, safety measures can be promptly adjusted or implemented in response to changing process conditions, thereby enhancing overall safety performance and ensuring the protection of personnel, assets, and the environment. The integration of safety considerations with process control represents a significant advancement in ensuring safe and efficient operation. By considering both the inherent risks associated with the process and the effectiveness of control measures, this integrated approach enhances overall safety performance and helps mitigate potential hazards in real-time.

Most of these methodologies presented in the classification handle the linearities in a great way but there is still a struggle in handling non-linearities (Chu and You, 2014; Gutiérrez-Limón et al., 2012a) (See Table 4 for categorization), and uncertainties within the systems (Santander and Baldea, 2021). There have been considerable works on handling nonlinear systems via methods like model reduction, surrogate, and hybrid modeling. Further, uncertainties are gaining prevalence in recent academic research. Another major challenge that is being addressed in the current-day research is the scaling up of the integration methodologies to the industrial stage.

Although significant progress has been made in integrating design, control, scheduling, and operational functions such as safety and resilience, it is important to note that a universally accepted methodology or protocol for the integration of these aspects does not currently exist. Furthermore, there is currently no commercially available software or prototype system that fully supports such integration. To address this challenge, Pistikopoulos and Diangelakis (2016) proposed the PAROC framework as a step towards resolving this issue. The PAROC framework provides a systematic approach to integrating the different aspects of process operations. It aims to bridge the gap between design, control, scheduling, and other operational functions. While the PAROC framework is discussed in detail in Section 4, it is important to note that further research and development are still needed to establish a comprehensive and widely accepted methodology for the integration of design, control, scheduling, and operational functions. The absence of a commercially available software or prototype system underscores the ongoing efforts to address this challenge and highlights the need for continued advancements in this field.

Table 4
Grand classification of methodologies.

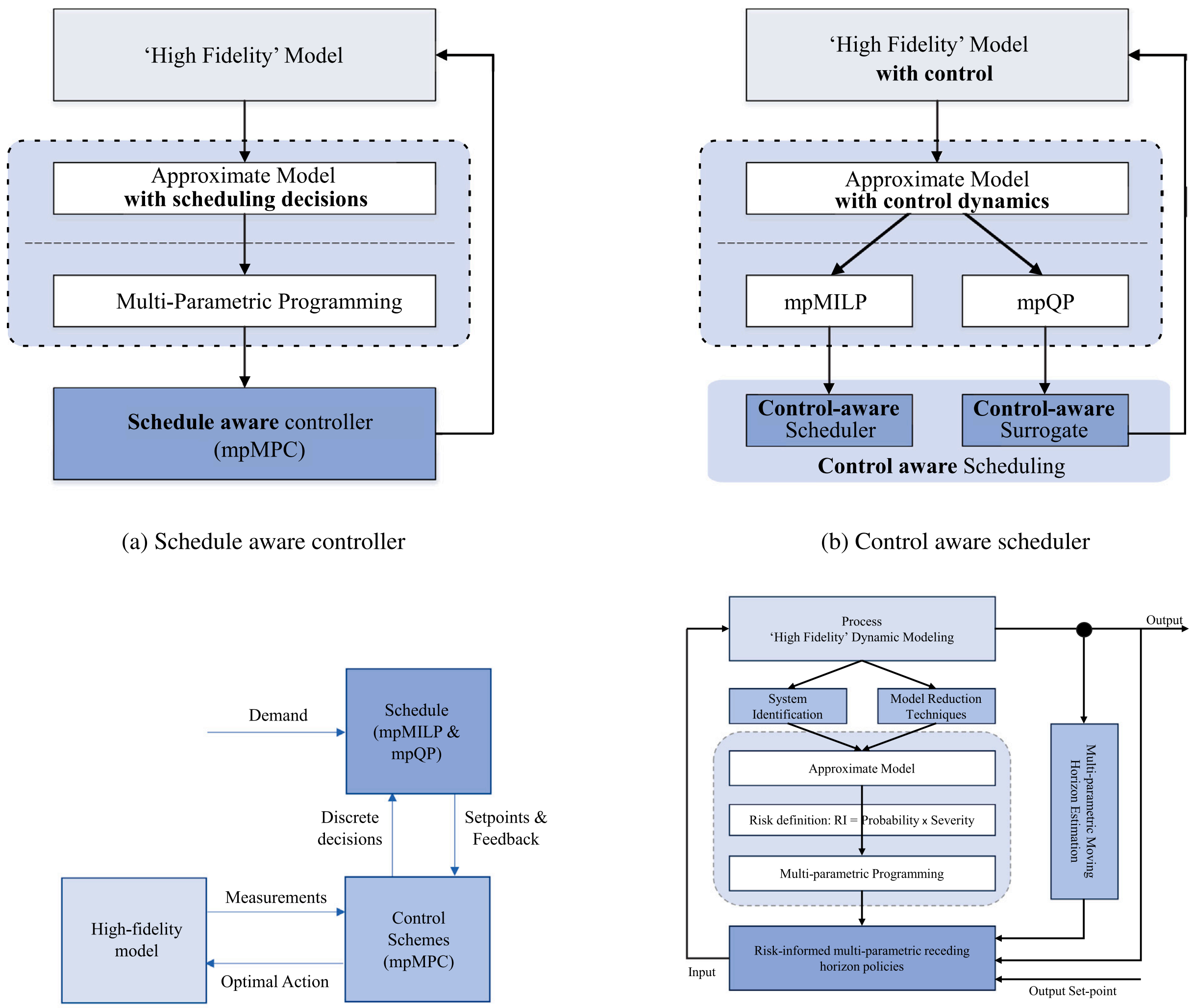
Author	Approach	Methodology
Gutiérrez-Limón et al. (2012a), Chu and You (2014), Pravin et al. (2020) and Misra and Gudi (2018)	Bottom-up	Simultaneous/Decomposition MIDO/MINLP open loop dynamics
Subramanian et al. (2013), Risbeck et al. (2019), McAllister et al. (2019), Touretzky and Baldea (2016), Santander and Baldea (2021), Baldea et al. (2016), Georgiadis et al. (2002) and Kopanos and Pistikopoulos (2014)	Bottom-up	Economic MPC/control theory in scheduling problems
Zhuge and Ierapetritou (2012), Elixmann et al. (2010), Prata et al. (2008) and Frankl et al. (2012)	Top-down	Simultaneous/Decomposition MIDO formulation to MINLP
Zhuge and Ierapetritou (2015), Dias et al. (2018), Zhuge and Ierapetritou (2014), Charitopoulos et al. (2017a,b), Sahraei and Ricardez-Sandoval (2014), Andrés-Martínez and Ricardez-Sandoval (2022b), Burnak et al. (2018b, 2020b, 2019a, 2020a) and Burnak et al. (2020c)	Top-down	Integration via mpMPC/NMPC/fast MPC
Dias and Ierapetritou (2020), Du et al. (2015), Baldea et al. (2015), Kelley et al. (2018), Tsay and Baldea (2020), Simkoff and Baldea (2020) and Dowling et al. (2018)	Bottom-up	Data-driven surrogate model and MINLP scheduling, Scale bridging control formulation in scheduling
Dias and Ierapetritou (2016), Vera and Ricárdez-Sandoval (2021), Ierapetritou and Pistikopoulos (1996), Raspanti et al. (2000) and Dering and Swartz (2022)	Bottom-up	Flexibility, feasibility, scheduling under uncertainty
Valdez-Navarro and Ricardez-Sandoval (2019) and Nie et al. (2015)	Top-down	MIDO formulations with Stochastic back-off formulation for uncertainty
Dowling et al. (2018)	Top-down	Decomposition algorithms with surrogate model and MILP scheduling
Al Ismaili et al. (2018) and Adloor and Vassiliadis (2020)	Top-down	Multistage mixed-integer optimal control formulation
Charitopoulos et al. (2019)	Bottom-up	Multi set-point mpMPC scheduling layer with MILP control layer
Huercio et al. (1995) and Muñoz et al. (2011)	Top-down	Simultaneous/decomposition algorithms using control/dynamics-aware scheduling models
Beal et al. (2017b), Diangelakis et al. (2017), Subramanian et al. (2012) and Maravelias (2021)	Bottom-up	Advanced control and MIP scheduling schemes

4. The PAROC framework for the integration of scales

The PAROC (PARametric Optimization and Control) framework is a methodology for developing and evaluating receding horizon optimization policies for process systems (Pistikopoulos et al., 2015; Burnak et al., 2020a; Pistikopoulos and Diangelakis, 2016). It involves creating a detailed high-fidelity model of the process, validating and analyzing it followed by the simplification of the model through model reduction methods. The framework leverages multi-parametric programming to solve optimization problems offline. Thus reducing the computational burden during real-time implementation. Various types of multi-parametric programming problems, such as multi-parametric linear programming (mpLP), multi-parametric quadratic programming (mpQP), multi-parametric nonlinear programming (mpNLP), multi-parametric mixed-integer linear programming (mpMILP), and multi-parametric mixed-integer quadratic programming (mpMIQP) are addressed, and state-of-the-art solvers are used in finding robust solutions (Kvasnica et al., 2004; Kenefake and Pistikopoulos, 2022; Oberdieck et al., 2016). Closed-loop validation ensures the accuracy and practicality of the developed control system by simulating its operation against the high-fidelity model, making it a powerful tool for optimizing and improving the performance of complex process systems in real-world applications. Some of the applications of interest for this review paper are the integration of scheduling and control and, the integration of operability and control. The remainder of this section discusses briefly the proposed frameworks for the integration of scales using PAROC.

4.1. PAROC for integration of scheduling and control

The integration of scheduling and control within the context of the PAROC framework represents a significant advancement in the optimization of complex dynamic systems. This methodology, as proposed by Diangelakis and Pistikopoulos (2017), follows a systematic two-step approach. Initially, a control strategy is established, where multi-parametric model predictive controllers (mp-MPC) are designed, treating the high-fidelity model as a single entity with manipulated control variables while considering external disturbances as uncontrollable factors (see Fig. 3(a)). Control variables are adjusted to control operational set points, optimizing system conditions and efficiency. Subsequently, an approximate linear state-space model is derived, incorporating the dynamics of the control system with the model, including changes in



(a) Schedule aware controller
(b) Control aware scheduler
(c) Closed-loop simultaneous scheduling and control
(d) Safety aware control

Fig. 3. PAROC framework for the integration of scales.

control variables induced by the control scheme. This approximate model serves as the foundation for a scheduling formulation, where MILP and QP problems are used to optimize economic scheduling (see Fig. 3(b)). Binary variables are employed to select suitable control schemes and operational conditions, reflecting the interplay between scheduling and control. Notably, the scheduling formulation operates with larger discretization time intervals, necessitating the development of a receding horizon optimization framework to align scheduling and control efforts. The final step involves closed-loop validation, where the integrated scheme is rigorously tested against the original high-fidelity model to ensure its effectiveness (see Fig. 3(c)). This framework was demonstrated via the implementation of Combined heat and power systems for simultaneous scheduling and control, which offers a holistic strategy for optimizing short and long-term processes, enhancing operational efficiency, and enabling informed decision-making in complex dynamic systems.

4.2. PAROC for integration of operability and control

In a research endeavor led by Ali et al. (2023), an innovative approach was developed within the PAROC framework to seamlessly integrate design optimization, explicit model predictive control (MPC), and dynamic risk assessment for real-time process safety management (see Fig. 3(d)). This comprehensive methodology encompasses several pivotal steps, commencing with the meticulous construction of high-fidelity models for both the process and safety systems, providing a profound understanding of system dynamics. The introduction of dynamic risk modeling allows for continuous real-time assessment of safety risks based on process variables. Multi-parametric programming is leveraged to calculate control strategies, accounting for design dependencies and safety–critical variable limits as path constraints within the MPC framework, thereby addressing complex multivariate interactions and uncertainties associated with fault probability and severity. The incorporation of dynamic optimization completes the loop, enabling the synthesis of optimal decisions that encompass design, operation, and risk control. This systematic and integrated approach proves invaluable in addressing the intricate challenges of complex process systems while providing control-aware fault prognosis and proactive risk mitigation. Practical validation through a real-world case study underscores its effectiveness in enhancing both process safety and operational efficiency.

Moreover, another noteworthy contribution by Vedant et al. (2021) involves the development of a software prototype with a primary focus on enhancing Process Intensification (PI) systems while concurrently addressing safety, flexibility, and control considerations. This comprehensive prototype comprises three distinct suites. The Synthesis

Suite systematically employs the Generalized Modular Representative Framework to generate promising PI configurations. The Simulation Suite intricately interfaces with a PI model library, facilitating the translation of synthesis outcomes into equipment-based process alternatives. Lastly, the Operability Suite conducts model-based assessments, ensuring the safe, flexible, and controllable performance of resulting PI systems across diverse operating conditions. These suites operate seamlessly through a user-friendly interface, promoting an environment where PI flowsheets can be generated without the constraints of predefined process schemes. Ultimately, this integrated framework not only enhances safety and control but also fosters operational excellence in the realm of Process Intensification systems, underscoring its significance in advanced process engineering research.

5. Concluding remarks

In the dynamic landscape of process engineering and industrial systems, the integration of scheduling and control has emerged as a pivotal frontier, demanding our unwavering attention. This comprehensive review has ventured deep into this intriguing domain, unveiling the intricate interplay between scheduling, control, and operability considerations. We have diligently examined the driving forces propelling this integration, the methodological frameworks employed therein, and the manifold advantages it proffers for the augmentation of system performance and operational efficiency.

Notably, a conspicuous trend that has gained substantial momentum in recent years pertains to the assimilation of operational functions, with a pronounced emphasis on safety and maintenance considerations, into the ambit of integrated scheduling and control (iSC). The overarching objective is manifest: the creation of systems that not only function optimally but also guarantee the safety of personnel and the longevity of industrial equipment. This holistic approach underscores the growing realization that process operability must no longer remain a peripheral concern but must be regarded as a fundamental cornerstone of effective industrial operations.

However, it would be remiss not to acknowledge the formidable challenges that loom on the horizon. The convergence of scheduling and control is no facile undertaking; it is a multifaceted puzzle comprised of intricate pieces. The confluence of multifarious facets, dimensions, and research disciplines necessitates a concerted effort on a grand scale. The symbiotic partnership between industry and academia must be actively fostered to unlock the full potential of integrated scheduling and control.

While formal methodologies have indeed been formulated, we cannot discount the abundant theoretical inquiries and practical impediments that persist in this realm. This arena of research remains in its nascent stages, and, akin to any burgeoning field, it demands incessant dedication and unceasing exploration. The industrial context further accentuates the urgency of bridging the chasm that exists between academia and industry. Through enhanced collaboration, we can attain deeper insights into the real-world ramifications of incorporating scheduling and control within industrial settings, thereby propelling practical efficacy to unprecedented heights.

In summation, our journey through segments of this review work has illuminated the pathway towards a more unified, efficient, and secure industrial milieu. Commencing with the initial exploration of the amalgamation of process control, process operations, and process operability, and culminating in the categorization of methodologies and the utilization of frameworks such as PAROC, we have borne witness to the intricate nexus of relationships that underlie this pivotal field of study.

As we find ourselves at the confluence of academia and industry, let us not underestimate the vast potential that beckons before us. The convergence of scheduling and control is not a mere academic curiosity; it is an imperious industrial imperative. By nurturing enhanced collaboration and by committing ourselves to surmounting theoretical and practical impediments, we can chart a course towards a future wherein integrated scheduling and control is not merely a conceptual construct but a transformative reality, redefining the operational paradigms of industries, assuring safety, optimizing performance, and attaining efficiency that transcends our present conceptions. In this synergy between academia and industry, we discern the pivotal key to unlocking the limitless possibilities of integrated scheduling and control. This calls for the research pathway towards the grand unification of process design, control, and scheduling, heralding an era of unprecedented innovation and industrial excellence (Burnak et al., 2019b).

CRediT authorship contribution statement

Efstratios N. Pistikopoulos: Conceptualization, Funding acquisition, Investigation, Methodology, Project administration, Supervision, Validation, Writing – review & editing. **Sahithi Srijana Akundi:** Conceptualization, Data curation, Formal analysis, Validation, Visualization, Writing – original draft, Writing – review & editing. **Dustin Kenefake:** Conceptualization, Validation, Writing – review & editing. **Nikolaos A. Diangelakis:** Conceptualization, Investigation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

As the author of the manuscript, I declare there are no potential conflicts of interest.

Data availability

No data was used for the research described in the article.

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