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Economic Benefit from Progressive Integration of Scheduling and Control for Continuous Chemical Processes

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Abstract: Performance of integrated production scheduling and advanced process control with disturbances is summarized and reviewed with four progressive stages of scheduling and control integration and responsiveness to disturbances: open-loop segregated scheduling and control, closed-loop segregated scheduling and control, open-loop scheduling with consideration of process dynamics, and closed-loop integrated scheduling and control responsive to process disturbances and market fluctuations. Progressive economic benefit from dynamic rescheduling and integrating scheduling and control is shown on a continuously stirred tank reactor (CSTR) benchmark application in closed-loop simulations over 24 h. A fixed horizon integrated scheduling and control formulation for multi-product, continuous chemical processes is utilized, in which nonlinear model predictive control (NMPC) and continuous-time scheduling are combined.

Keywords: scheduling; model predictive control; dynamic market; market fluctuations; process disturbances; nonlinear; integration

1. Introduction

Production scheduling and advanced process control are related tasks for optimizing chemical process operation. Traditionally, implementation of process control and scheduling are separated; however, research suggests that opportunity is lost from separate implementation [1–3]. Many researchers suggest that economic benefit may arise from integrating production scheduling and process control [4–10]. Though integration may provide economic benefit, scheduling and control integration presents several challenges which are outlined in multiple reviews on integrated scheduling and control (ISC) [3,11–14]. Some of the major challenges to integration mentioned in review articles include time-scale bridging, computational burden, and human factors such as organizational and behavioral challenges.

1.1. Economic Benefit from Integrated Scheduling and Control

Many complex, interrelated elements factor into the potential benefit from the integration of scheduling and control, including the following [3,11]:

(i) Rapid fluctuations in dynamic product demand;
(ii) Rapid fluctuations in dynamic energy rates;
(iii) Dynamic production costs;

(iv) Benefits of increased energy efficiency;
(v) Necessity of control-level dynamics information for optimal production schedule calculation.

In the current economic environment, demand and selling prices for the products and inputs of chemical processes can change significantly over the course of not only months and years, but on the scales of weeks, days, and hours [3,11,12]. Energy rates often fluctuate hourly, with peak pricing during peak demand hours and rate cuts during off peak hours (sometimes even negative rate cuts occur during periods of excess energy production) [11]. An optimal schedule is intrinsically dependent upon market conditions such as input material price, product demand and pricing, and energy rates [12]. Therefore, when market conditions change, the optimal production sequence or schedule may also change. Since the time scale at which market factors fluctuates has decreased, the time scale at which scheduling decisions must be recalculated should also decrease [3,12].

Frequent recalculation of scheduling on a time scale closer to that of advanced process control (seconds to minutes) leads to a greater need to integrate process dynamics into the scheduling problem [3]. According to a previous review [11], process dynamics are important for optimal production scheduling because (i) transition times between any given products are determined by process dynamics and process control; (ii) process dynamics may show that a calculated production sequence or schedule is operationally infeasible; and (iii) process disturbances may cause a change in the optimal production sequence or schedule.

1.2. Previous Work

Significant research has been conducted on the integration of production scheduling and advanced process control [3,11]. This section summarizes evidence for economic benefit from integration, upon which this work builds. Previous research showing the benefits of combined scheduling and control is explored and previous research done to show the economic benefits of combined over segregated scheduling and control is examined. The reviewed articles are summarized in Table 1. This work focuses on research demonstrating benefit over a baseline comparison of segregated scheduling and control (SSC).

Table 1. Economic benefit of integrated scheduling and control (ISC) over segregated scheduling and control (SSC) (CSTR: continuously stirred tank reactor; MMA: methyl methacrylate; DR: demand response; FRB: fluidized bed reactor; RTN: resource task network; ASU: air separation unit; HIPS: high-impact polystyrene; PFR: plug flow reactor; SISO: single-input single-output; MIMO: multiple-input multiple-output).

Author	Shows Benefit of ISC over SSC	Batch Process	Continuous Process	Example Application (s)
Baldea et al. (2015) [15]			X	CSTR
Baldea et al. (2016) [16]			X	MMA
Baldea (2017) [17]			X	DR chemical processes and power generation facilities
Beal (2017) [18]			X	CSTR
Beal (2017) [19]			X	CSTR
Beal (2017a) [20]			X	CSTR
Cai et al. (2012) [21]		X		Semiconductor production
Capon-Garcia et al. (2013) [6]		X		2 different batch plants (1-stage, 3-product & 3-stage, 3-product)
Chatzidoukas et al. (2003) [22]	X		X	gas-phase polyolefin FBR.
Chatzidoukas et al. (2009) [23]	X		X	catalytic olefin copolymerization FBR
Chu & You (2012) [24]			X	MMA
Chu & You (2013) [25]			X	CSTR
Chu & You (2013a) [26]		X		polymerization with parallel reactors & 1 purification unit (RTN)
Chu & You (2013b) [27]	X	X		5-unit batch process
Chu & You (2013c) [28]	X	X		sequential batch process
Chu & You (2014) [29]		X		batch process (reaction task, filtration task, reaction task)

Table 1. *Cont.*

Author	Shows Benefit of ISC over SSC	Batch Process	Continuous Process	Example Application (s)
Chu & You (2014a) [30]		X		8-unit batch process
Chu & You (2014b) [31]	X	X		8-unit batch process
Dias et al. (2016) [32]			X	MMA
Du et al. (2015) [33]			X	CSTR & MMA
Flores-Tlacuahuac & Grossmann (2006) [34]			X	CSTR
Flores-Tlacuahuac (2010) [8]			X	Parallel CSTRs
Gutiérrez-Limón et al. (2011) [35]			X	CSTR
Gutiérrez-Limón et al. (2016) [36]			X	CSTR & MMA
Gutiérrez-Limón & Flores-Tlacuahuac (2014) [37]			X	CSTR
Koller & Ricardez-Sandoval (2017) [38]			X	CSTR
Nie & Bieglier (2012) [7]	X	X		flowshop plant (batch reactor, filter, distillation column)
Nie et al. (2015) [39]		X	X	polymerization with parallel reactors & 1 purification unit
Nystrom et al. (2005) [40]			X	industrial polymerization process
Nystrom et al. (2006) [4]			X	industrial polymerization process
Patil et al. (2015) [41]			X	CSTR & HIPS
Pattison et al. (2016) [42]	X		X	ASU model
Pattison et al. (2017) [10]			X	ASU model
Prata (2008) et al. [43]			X	medium industry-scale model
Terrazas-Moreno et al. (2008) [44]			X	MMA (with one CSTR) & HIPS
Terrazas-Moreno & Flores-Tlacuahuac (2007) [45]			X	HIPS & MMA
Terrazas-Moreno & Flores-Tlacuahuac (2008) [9]			X	HIPS & MMA
You & Grossmann (2008) [46]			X	medium and large polystyrene supply chaiins
Zhuge & Ierapetritou (2012) [47]			X	CSTR & PFR.
Zhuge & Ierapetritou (2014) [48]		X		simple and complex batch processes
Zhuge & Ierapetritou (2015) [49]			X	SISO & MIMO CSTRs
Zhuge & Ierapetritou (2016) [50]	X		X	CSTR & MMA

1.2.1. Integrating Process Dynamics into Scheduling

Mahadevan et al. suggest that process dynamics should be considered in scheduling problems. To avoid the computational requirements of mixed-integer nonlinear programming (MINLP), they include process dynamics as costs in the scheduling problem [51]. Flores-Tlacuahuac and Grossman implement process dynamics into scheduling directly in a mixed-integer dynamic optimization (MIDO) problem with a continuous stirred tank reactor (CSTR). Chatzidoukas et al. demonstrated the economic benefit of implementing scheduling in a MIDO problem for polymerization, solving product grade transitions along with the scheduling problem [22]. Economic benefit has also been shown for simultaneous selection of linear controllers for grade transitions and scheduling, ensuring that the process dynamics from the controller selection are accounted for in the scheduling problem [23]. Terrazas-Moreno et al. also demonstrate the benefits of process dynamics in cyclic scheduling for continuous chemical processes [45]. Capon-Garcia et al. prove the benefit of implementing process dynamics in batch scheduling via an MIDO problem [6]. MIDO batch scheduling optimization with dynamic process models is shown to be more profitable than a fixed-recipe approach. Chu and You also demonstrate enhanced performance from batch scheduling with simultaneous solution of dynamic process models over a traditional batch scheduling approach [27,28,31]. Economic benefit from integrating process dynamics into batch and semi-batch scheduling has also been demonstrated via mixed-logic dynamic optimization in state equipment networks and solution with Benders decomposition in resource task networks [7,39]. Potential for economic benefit from integrating process dynamics into design, scheduling, and control problems has also been demonstrated [41,44,52]. Computational reduction of incorporating process dynamics into scheduling has been investigated successfully, maintaining benefit from the incorporation of process dynamics into scheduling while reducing dynamic model order [10,15,16,33,42].

1.2.2. Reactive Integrated Scheduling and Control

Research indicates that additional benefit arises from ISC responsive to process disturbances, which are a form of process uncertainty. This is in congruence with recent work by Gupta and Maravelias demonstrating that increased frequency of schedule rescheduling (online scheduling) can improve process economics [53–55]. Many previous works considering reactive ISC are outlined in Table 2. For a complete review of ISC under uncertainty, the reader is directed to a recent review by Dias and Ierapetritou [32]. Zhuge and Ierapetritou demonstrate increased profit from closed-loop implementation (over open-loop implementation) of combined scheduling and control in the presence of process disturbances [47]. The schedule is optimally recalculated when a disturbance is encountered. Zhuge and Ierapetritou also present methodology to reduce the computational burden of ISC to enable closed-loop online operation for batch and continuous processes. They propose using multi-parametric model predictive control for online batch scheduling and control [48], fast model predictive control coupled with reduced order (piece-wise affine) models in scheduling and control for continuous processes [49], and decomposition into separate problems for continuous processes [50]. Chu and You demonstrate the economic benefit of closed-loop moving horizon scheduling with consideration of process dynamics in batch scheduling [29]. Chu and You also investigate the reduction of computational burden to enable online closed-loop ISC for batch and continuous processes. They investigate utilization of Pareto frontiers to decompose batch scheduling into an online mixed-integer linear programming (MILP) problem and offline dynamic optimization (DO) problems [26]. Investigation of a solution via mixed-integer nonlinear fractional programming and Dinkelbach's algorithm coupled with decomposing into an online scheduling and controller selection and offline transition time calculation [24].

Table 2. Works considering reactive ISC.

Authors	Product Price Disturbance	Product Demand Disturbance	Process Variable Disturbance	Other Disturbances
Baldea et al. (2016) [16]	X	X		
Baldea (2017) [17]			X	
Cai et al. (2012) [21]			X	
Chu & You (2012) [24]			X	
Du et al. (2015) [33]				
Flores-Tlacuahuac (2010) [8]		X		
Gutiérrez-Limón et al. (2016) [36]		X		
Kopanos & Pistikopoulos (2014) [56]			X	
Liu et al. (2012) [57]	X	X		
Patil et al. (2015) [41]			X	
Pattison et al. (2017) [10]		X	X	
Touretzky & Baldea (2014) [58]				Weather & energy price
You & Grossmann (2008) [46]		X		
Zhuge & Ierapetritou (2012) [47]			X	
Zhuge & Ierapetritou (2015) [49]			X	

Closed-loop reactive ISC responds to process uncertainty in a reactive rather than preventative manner [59]. Preventative approaches to dealing with process uncertainty in ISC have also been investigated. Chu and You investigated accounting for process uncertainty in batch processes in a two-stage stochastic programming problem solved by a generalized Benders decomposition [28]. The computational requirements of the problem prevent online implementation. Dias and Ierapetritou demonstrate the benefits of using robust model predictive control in ISC to optimally address process uncertainty in continuous chemical processes [32].

1.2.3. Responsiveness to Market Fluctuations

As mentioned in Section 1.1, a major consideration affecting the profitability of ISC is rapidly fluctuating market conditions. If the market changes, the schedule should be reoptimized to new market demands and price forecasts. This is again congruent with recent work demonstrating benefit from frequent re-scheduling [53–55]. Literature on ISC reactive to market fluctuations is relatively limited in scope. Gutierrez-Limon et al. demonstrated integrated planning, scheduling, and control responsive to fluctuations in market demand on a CSTR benchmark application [36,37]. Pattison et al. investigated ISC with an air separation unit (ASU) in fast-changing electricity markets, responding optimally to price fluctuations [42]. Pattison et al. also demonstrated theoretical developments with moving horizon closed-loop scheduling in volatile market conditions [10]. Periodic rescheduling to account for fluctuating market conditions was implemented successfully on an ASU application.

1.3. Purpose of This Work

This work aims to provide evidence for the progressive economic benefits of combining scheduling and control and operating combined scheduling and control in a closed-loop responsive to disturbances over segregated scheduling and control and open-loop formulations for continuous chemical processes. This work demonstrates the benefits of integration through presenting four progressive stages of integration and responsiveness to disturbances. This work comprehensively demonstrates the progression of economic benefit from (1) integrating process dynamics and control level information into production scheduling and (2) closed-loop integrated scheduling and control responsive to market fluctuations. Such a comprehensive examination of economic benefit has not been performed to the authors' knowledge. This work also utilizes a novel, computationally light decomposed integration method employing continuous-time scheduling and nonlinear model predictive control (NMPC) as the fourth phase of integration. This method is outlined in detail in another work [60]. Although the phases of integration presented in this work are not comprehensively representative of integration methods presented in the literature, the concepts of integration progressively applied in the four phases are applicable across the majority of formulations in the literature.

2. Phases of Progressive Integration

This section introduces the four phases of progressive integration of scheduling and control investigated in this work. Each phase is outlined in the appropriate section.

2.1. Phase 1: Fully Segregated Scheduling and Control

A schedule is created infrequently (every 24 h in this work) and a controller seeks to implement the schedule throughout the 24 h with no other considerations. In this format, the schedule is open-loop, whereas the control is closed-loop. The controller acts to reject disturbances and process noise to direct the process to follow the predetermined schedule (see Figure 1).

This work considers an NMPC controller and a continuous-time, slot-based schedule (Section 2.5). For this phase, the schedule is uninformed of transition times as dictated by process dynamics and control structure. All product grade transitions are considered to produce a fixed amount of off-specification material and to require the same duration.

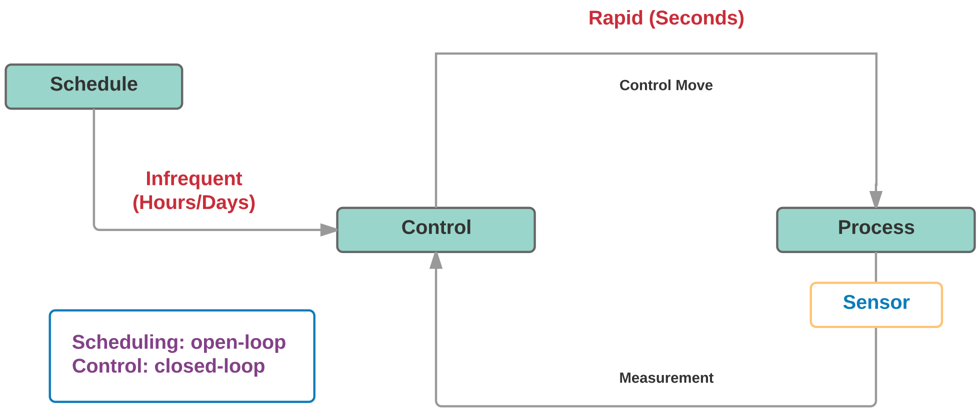


Figure 1. Phase 1: Open-loop scheduling determined once per day with no consideration of process dynamics. Closed-loop control implemented to follow the schedule.

2.2. Phase 2: Reactive Closed-Loop Segregated Scheduling and Control

Phase two is a closed-loop implementation of completely segregated scheduling and control. The formulation for Phase 2 is identical to that of Phase 1 with the exception that the schedule is recalculated in the event of a process disturbance or market update (see Figure 2).

2.3. Phase 3: Open-Loop Integrated Scheduling and Control

For phase 3, the schedule is calculated infrequently, similar to phase 1 (every 24 h in this work). However, information about the control structure and process dynamics in the form of transition times are fed to the scheduling algorithm to enable a more intelligent decision. Scheduling remains open-loop while the controller remains closed-loop to respond to noise and process disturbances while implementing the schedule (see Figure 3).

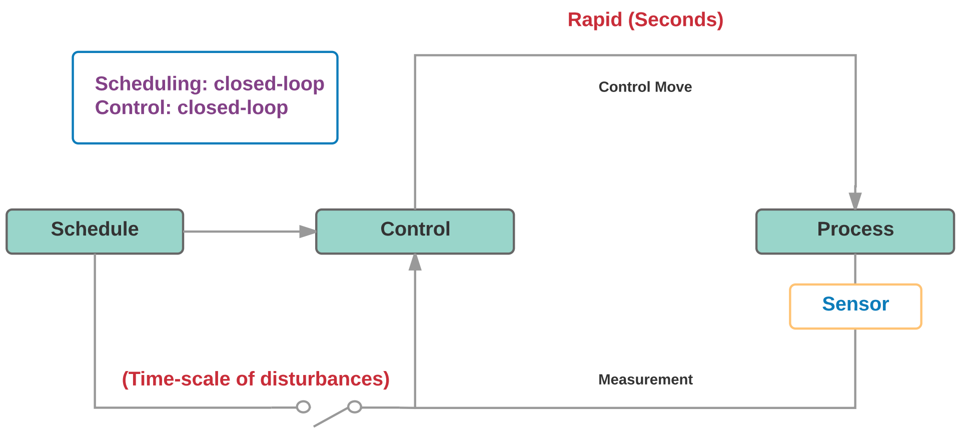


Figure 2. Phase 2: Dual-loop segregated scheduling and control. Scheduling is recalculated reactively in the presence of process disturbances above a threshold or updated market conditions. Closed-loop control implements the schedule in the absence of disturbances.

This work considers a continuous-time schedule with process dynamics incorporated via transition times estimated by NMPC. Transitions between products are simulated with a dynamic process model and nonlinear model predictive controller implementation. The time required to transition between products is minimized by the controller, and the simulated time required to transition is fed to the scheduler as an input to the continuous-time scheduling formulation (Section 2.5).

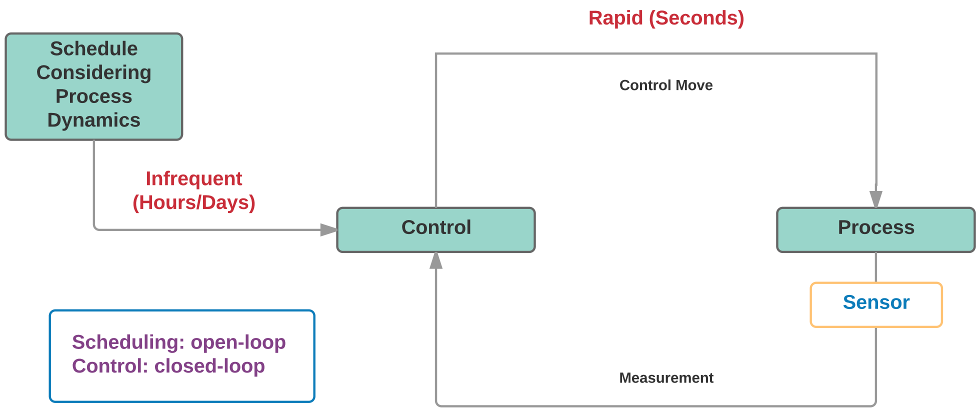


Figure 3. Phase 3: Open-loop scheduling determined once per day with consideration of process dynamics and control structure in the form of grade transition information. Closed-loop control implemented to follow the schedule.

2.4. Phase 4: Closed-Loop Integrated Scheduling and Control Responsive to Market Fluctuations

Phase 4 represents closed-loop implementation of ISC responsive to both market fluctuations and process disturbances. This work utilizes the formulation for computationally light online scheduling and control for closed-loop implementation introduced in another work by the authors [60]. As in phase 3, a continuous-time schedule is implemented with NMPC-estimated transition times as inputs to the scheduling optimization; however, the ISC algorithm is implemented not only once at the beginning of the horizon as in phase 3, but triggered by updated market conditions or process disturbances above a threshold (see Figure 4). This enables the ISC algorithm to respond to fluctuations in market conditions as well as respond to measured process disturbances in a timely manner to ensure that production scheduling and control are updated to reflect optimal operation with current market conditions and process state.

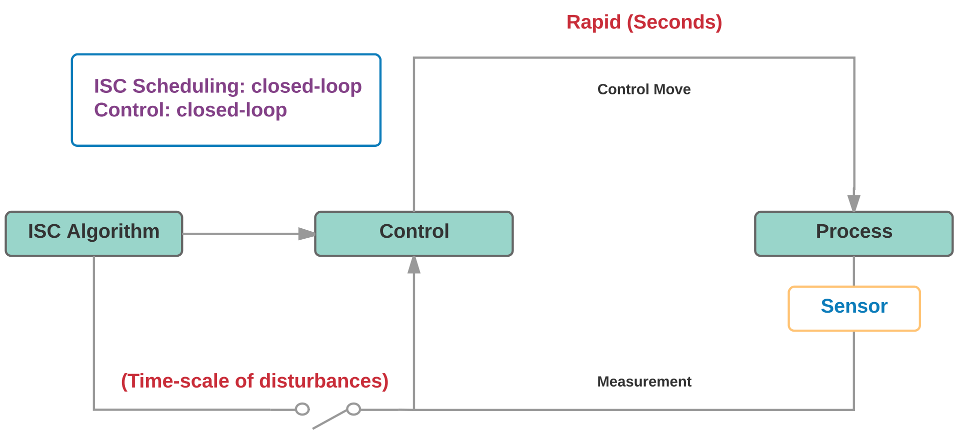


Figure 4. Phase 4: Closed-loop combined scheduling and control responsive to both process disturbances and updated market information.

The formulation for phase 4 builds on the work of Zhuge et al. [49], which justifies decomposing slot-based ISC into two subproblems: (1) NLP solution of transition times and transition control profiles and (2) MILP solution of the slot-based, continuous-time schedule. The formulation in [60] expands the work of Zhuge et al. by combining a look-up transition time table with control profiles and transition times between known product steady-state conditions, calculated offline and stored in memory, with transitions from current conditions to each product. The transitions from current conditions or most recently received process measurements are the only transition times and transition control profiles required to be solved at each iteration of combined scheduling and control (Equations (2)–(8)). This reduces the online problem to few nonlinear programming (NLP) dynamic optimization problems and an MILP problem only, eliminating the computational requirements of MINLP. This work also introduces the use of nonlinear models in this form of decomposition. Zhuge et al. use piecewise affine (PWA) models, whereas this work harnesses full nonlinear process dynamics to calculate optimal control and scheduling.

This work also builds on the work of Pattison et al., who demonstrate closed-loop moving horizon combined scheduling and control to respond to market updates [10]. This formulation, however, does not use simplified dynamic process models for scheduling, but rather maintains nonlinear process dynamics while reducing computational burden via problem decomposition into offline and online components and further decomposition of the problem into computationally light NLP and MILP problems, solvable together without the need for iterative alternation [60].

The continuous-time scheduling formulation, as introduced in Section 2.5, will produce sub-optimal results if the number of products exceeds the optimal number of products to produce in a prediction horizon. The number of slots is constrained to be equal to the number of products, causing the optimization to always create n production slots and n transitions even in cases in which $<n$ slots would be most economical in the considered horizon for scheduling and control. To eliminate this sub-optimality, an iterative method is introduced to leverage the computational lightness of the MILP continuous-time scheduling formulation. The number of slots in the continuous-time schedule is selected iteratively based on improvement to the objective function (profit), beginning from one slot. As previously mentioned, transition times and control profiles between steady-state products are stored in memory, requiring no computation in online operation. Additionally, the transitions from current measured state to each steady-state product ($\tau_{0'i}$) are calculated once before iterations are initiated. Thus, the iterative method only iterates the MILP problem, not requiring any recalculation of grade transition NLP dynamic optimization problems. This decomposition is computationally light and allows for a fixed-horizon non-cyclic scheduling and control formulation. This non-cyclic fixed-horizon approach to combined scheduling and control enables response to market fluctuations in maximum demand and product price, whereas traditional continuous-time scheduling requires a makespan (T_M) to meet a demand rather than producing an optimal amount of each product within a given fixed horizon. Additional details for this formulation are included in another paper [60].

2.5. Mathematical Formulation

This continuous-time optimization used in phases 1–3 seeks to maximize profit and minimize grade transitions (and associated waste material production) while observing scheduling constraints. The objective function is formulated as follows:

$$\begin{aligned} \max_{z_{i,s}, t_i^s, t_i^f \forall i,s} \quad & J = \sum_{i=1}^{n} \Pi_i \omega_i - \sum_{i=1}^{n} c_{storage,i} \omega_i \sum_{s=1}^{m} z_{i,s} (T_M - t_s^f) - W_\tau \sum_{s=1}^{m} \tau_s, \\ \text{s.t.} \quad & \text{Equations (2)–(8)}, \end{aligned} \tag{1}$$

where T_M is the makespan, n is the number of products, m is the number of slots ($m = n$ in these cyclic schedules), $z_{i,s}$ is the binary variable that governs the assignment of product i to a particular slot s, t_s^s is the start time of the slot s, t_s^f is the end time of slot s, Π_i is the per unit price of product i, W_τ is an optional weight on grade transition minimization, τ_s is the transition time within slot s, $c_{storage,i}$ is the per unit cost of storage for product i, and ω_i represents the amount of product i manufactured,

$$\omega_i = \sum_{s=1}^{m} \int_{t_s^s + \tau_s}^{t_s^f} z_{i,s} q \, dt, \tag{2}$$

and where q is the production volumetric flow rate and τ_s is the transition time between the product made in slot $s-1$ and product i made in slot s. The time points must satisfy the precedence relations:

$$t_s^f > t_s^s + \tau_s \qquad \forall s > 1, \tag{3}$$

$$t_s^s = t_{s-1}^f \qquad \forall s \neq 1, \tag{4}$$

$$t_m^f = T_M, \tag{5}$$

which require that a time slot be longer than the corresponding transition time, impose the coincidence of the end time of one time slot with the start time of the subsequent time slot, and define the relationship between the end time of the last time slot (t_n^f) and the total makespan or horizon duration (T_M).

Products are assigned to each slot using a set of binary variables, $z_{i,s} \in \{0,1\}$, along with constraints of the form:

$$\sum_{s=1}^{m} z_{i,s} = 1 \qquad \forall i, \tag{6}$$

$$\sum_{i=1}^{n} z_{i,s} = 1 \qquad \forall s, \tag{7}$$

which ensure that one product is made in each time slot and each product is produced once.

The makespan is fixed to an arbitrary horizon for scheduling. Demand constraints restrict production from exceeding the maximum demand (δ_i) for a given product, as follows:

$$\omega_i \leq \delta_i \qquad \forall i. \tag{8}$$

The continuous-time scheduling optimization requires transition times between steady-state products ($\tau_{i'i}$) as well as transition times from the current state to each steady-state product if initial state is not at steady-state product conditions ($\tau_{0'i}$).

Transition times are estimated using NMPC via the following objective function:

$$\begin{aligned} \min_{u} \quad & J = (x - x_{sp})^T W_{sp} (x - x_{sp}) + \Delta u^T W_{\Delta u} + u^T W_u, \\ \text{s.t.} \quad & \text{nonlinear process model} \\ & x(t_0) = x_0, \end{aligned} \tag{9}$$

where W_{sp} is the weight on the set point for meeting target product steady-state, $W_{\Delta u}$ is the weight on restricting manipulated variable movement, W_u is the cost for the manipulated variables, u is the vector of manipulated variables, x_{sp} is the target product steady-state, and x_0 is the start process state from which the transition time is being estimated. The transition time is taken as the time at which and after which $|x - x_{sp}| < \delta$, where δ is a tolerance for meeting product steady-state operating conditions. This formulation harnesses knowledge of nonlinear process dynamics in the system model to find an optimal trajectory and minimum time required to transition from an initial concentration to a desired concentration. This method for estimating transition times also effectively captures the actual behavior of the controller selected, as the transition times are estimated by a simulation of actual controller implementation. This work uses $W_{\Delta u} = 0$ and $W_u = 0$.

3. Case Study Application

As shown in prior work, there are many different strategies for integrating scheduling and control. A novel contribution of this work is a systematic comparison of four general levels of integration through a single case study. In this section, the model and scenarios used to demonstrate progressive economic benefit from the integration of scheduling and control for continuous chemical processes are presented.

3.1. Process Model

This section presents a standard CSTR problem used to highlight the value of the formulation introduced in this work. The CSTR model is applicable in various industries from food/beverage to oil and gas and chemicals. Notable assumptions of a CSTR include:

- Constant volume;
- Well mixed;
- Constant density.

The model shown in Equations (10) and (11) is an example of an exothermic, first-order reaction of $A \Rightarrow B$, where the reaction rate is defined by an Arrhenius expression and the reactor temperature is controlled by a cooling jacket:

$$\frac{dC_A}{dt} = \frac{q}{V}(C_{A0} - C_A) - k_0 e^{-E_A/RT} C_A, \tag{10}$$

$$\frac{dT}{dt} = \frac{q}{V}(T_f - T) - \frac{1}{\rho C_p} k_0 e^{\frac{-E_A}{RT}} C_A \Delta H_r - \frac{UA}{V\rho C_p}(T - T_c). \tag{11}$$

In these equations, C_A is the concentration of reactant A, C_{A0} is the feed concentration, q is the inlet and outlet volumetric flowrate, V is the tank volume (q/V signifies the residence time), E_A is the reaction activation energy, R is the universal gas constant, UA is an overall heat transfer coefficient times the tank surface area, ρ is the fluid density, C_p is the fluid heat capacity, k_0 is the rate constant, T_f is the temperature of the feed stream, C_{A0} is the inlet concentration of reactant A, ΔH_r is the heat of reaction, T is the temperature of reactor and T_c is the temperature of cooling jacket. Table 3 lists the CSTR parameters used.

Table 3. Reactor parameter values.

Parameter	Value
V	100 m^3
E_A/R	8750 K
$\frac{UA}{V\rho C_p}$	2.09 s^{-1}
k_0	7.2×10^{10} s^{-1}
T_f	350 K
C_{A0}	1 mol/L
$\frac{\Delta H_r}{\rho C_p}$	−209 K m^3 mol^{-1}
q	100 m^3/h

In this example, one reactor can make multiple products by varying the concentrations of A and B in the outlet stream. The manipulated variable in this optimization is T_c, which is bounded by 200 K $\leq T_c \leq$ 500 K and by a constraint on manipulated variable movement as $\Delta T_c \leq$ 2 K/min.

3.2. Scenarios

The sample problem uses three products over a 24-h horizon. The product descriptions are shown in Table 4, where the product specification tolerance (δ) is ±0.05 mol/L.

Table 4. Product specifications.

Product	C_A (mol/L)	Max Demand (m^3)	Price (\$/m^3)	Storage Cost (\$/h/m^3)
1	0.10	1000	22	0.11
2	0.30	1000	29	0.1
3	0.50	1000	23	0.12

The transition times between products, as calculated by NMPC using Equation (9), is shown in Table 5.

Table 5. Transition Times Between Products (h).

Starting Product	Final Product 1	2	3
1	0	0.50	0.833
2	0.50	0	0.50
3	0.417	0.833	0

Three scenarios are applied to each phase of progressive integration of scheduling and control:

(A) Process disturbance (C_A);
(B) Demand disturbance;
(C) Price disturbance.

Scenarios A–C maintain the specifications in Table 4 but introduce process disturbances, demand disturbances, and price disturbances, respectively (see Table 6). Scenario A introduces a process disturbance to the concentration in the reactor (C_A) of 0.15 mol/L, ramping uncontrollably over 1.4 h. Scenario B introduces a market update with a 20% increase in demand for product 2. Scenario C shows a market update with fluctuations in selling prices for products 2 and 3. The starting concentration for each scenario is 0.10 mol/L, the steady-state product conditions for product 1.

Table 6. Scenario descriptions.

Scenario	Time (h)	Disturbance		
		Product 1	Product 2	Product 3
A	2.2–3.8	0.15 mol/L		
B	3.1	+0 m^3	+200 m^3	+0 m^3
C	2.1	+0 $/$m^3$	−9 $/$m^3$	+6 $/$m^3$

4. Results

The results of implementation of each phase for each scenario are discussed and presented in this section. Each problem is formulated in the Pyomo framework for modeling and optimization [61,62]. Nonlinear programming dynamic optimization problems are solved via orthogonal collocation on finite elements [63] with 5 min time discretization and the APOPT and COUENNE MINLP solvers are utilized to solve all mathematical programming problems presented in this work [64,65]. For comparative purposes, profits are compared to those of Phase 3 due to its centrality in performance.

4.1. Scenario A: Process Disturbance

In Scenario A, phase 1 has a poor schedule due to a lack of incorporation of process dynamics into scheduling. The durations of grade transitions, as dictated by process dynamics, are unaccounted for. However, the production amounts or production durations for each product are optimized based on selling prices. The order is selected based on storage costs, clearly leading to longer grade transitions than necessary. The schedule maximizes production of higher-selling products 2 and 3. Phase 1 does not recalculate the schedule after the process disturbance, holding to pre-determined transition timing.

Phase 2 follows the same pattern as phase 1 due to its lack of incorporation of process dynamics. Phase 2 recalculates a schedule after the process disturbance, but because it does not account for process dynamics, it cannot determine that it would be faster to transition to Product 3 from the disturbed process state than to return to Product 2. Thus, the production sequence remains sub-optimal. However, the recalculated schedule enables more profitable Product 2 to be produced than in Phase 1 as the timing of transition to Product 1 is delayed due to the disturbance by the recalculation. Phase 2 illustrates benefit that comes from frequent schedule recalculation rather than from scheduling and control integration.

Phase 3 does not react optimally to the process disturbance because it has a fixed schedule, but its initial schedule is optimal due to the incorporation of process dynamics and the resultant minimization of grade transition durations. Phase 3 illustrates benefit originating solely from scheduling and control integration, without schedule recalculation. Phase 4 optimally reschedules with understanding of transition behavior from the disturbed state to each steady-state operating condition, transitioning to Product 2 immediately after the disturbance. Phase 4 demonstrates the premium benefits of both reactive or frequent rescheduling and from scheduling and control integration.

The simulation results of scenario A are shown in Figure 5 and Table 7.

Table 7. Results: Scenario A.

Phase	Description	Profit		Production (m^3)		
		($)	(%)	Product 1	Product 2	Product 3
1	Segregated, Fixed Schedule	3114	(−38%)	367	858	908
2	Segregated, Reactive Schedule	3942	(−21%)	317	900	992
3	Integrated, Fixed Schedule	4983	(+0%)	308	1000	983
4	Integrated, Reactive Schedule	7103	(+43%)	308	1000	983

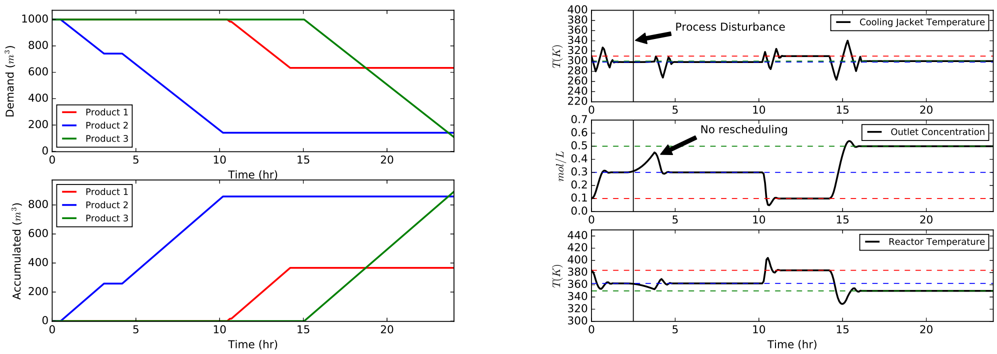
Table 8. Results: Scenario B.

Phase	Description	Profit		Production (m^3)		
		($)	(%)	Product 1	Product 2	Product 3
1	Segregated, Fixed Schedule	6033	(−19%)	367	967	908
2	Segregated, Reactive Schedule	7446	(+0.1%)	133	1200	908
3	Integrated, Fixed Schedule	7441	(+0%)	317	1000	992
4	Integrated, Reactive Schedule	8676	(+17%)	308	1200	800

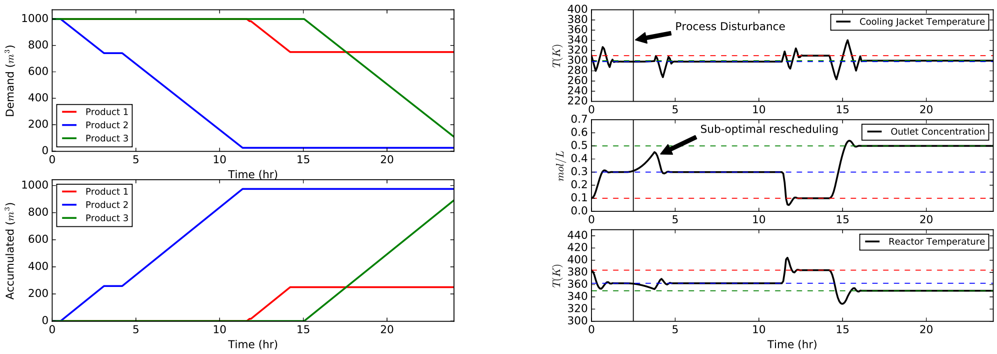
4.2. Scenario B: Market Update Containing Demand Fluctuation

As in Scenario A, the production order for Phases 1 and 2 is sub-optimal due to a lack of incorporation of process dynamics in scheduling, or a lack of integration of scheduling and control. Phase 2 improves performance over Phase 1 by reacting to the market update and producing more profitable Product 2, which had a surge in demand, illustrating again the benefits of reactive scheduling. Phase 3 integrates control with scheduling, resulting in an optimal initial schedule minimizing transition durations. The benefits from integrating scheduling and control (Phase 3) and the benefits of reactive scheduling (Phase 2) are approximately the same in Scenario B, differing in profit by only a negligible amount. However, incorporating both reactive scheduling and scheduling and control integration (Phase 4) leads to a large increase in profits. The initial and recalculated schedules in Phase 4 have optimal production sequence, utilizing process dynamics information to minimize grade transition durations. Additionally, recalculation of the integrated scheduling and control problem after the market update allows for increased production of the highest-selling product, leading to increased profit.

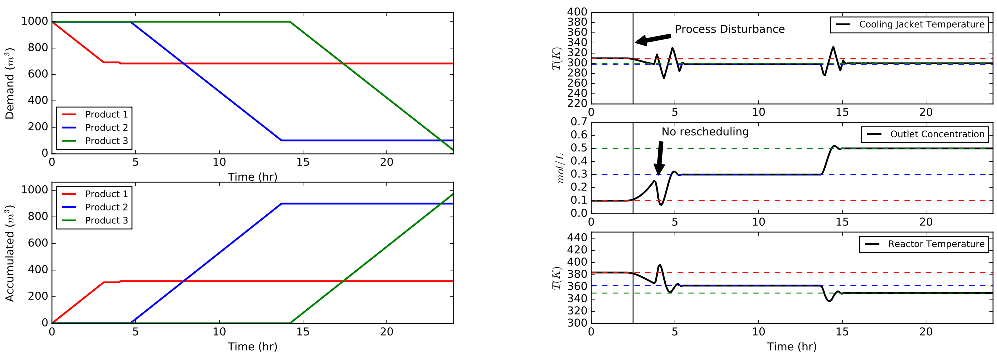
The simulation results of scenario B are shown in Figure 6 and Table 8.



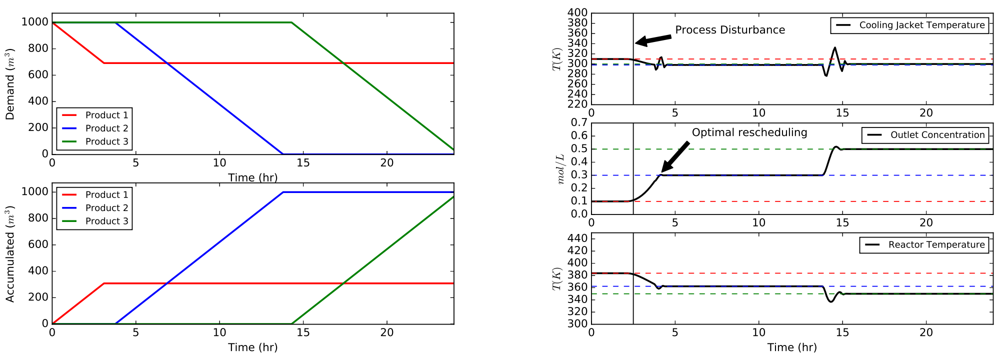
(**a**) Phase 1: Segregated, Fixed Schedule



(**b**) Phase 2: Segregated, Reactive Schedule

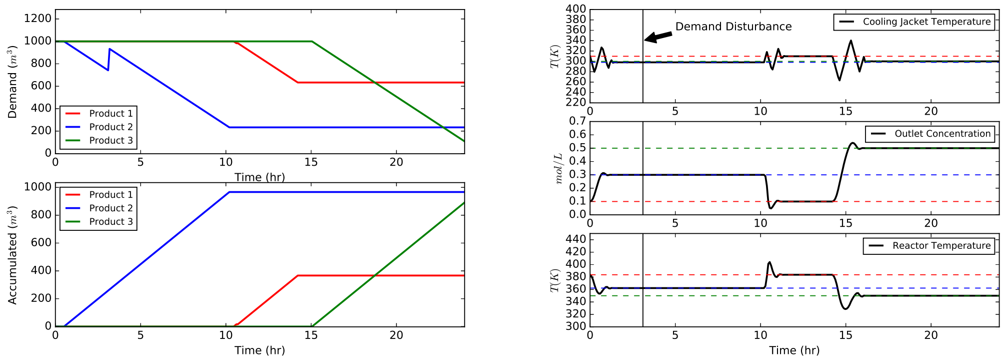


(**c**) Phase 3: Integrated, Fixed Schedule

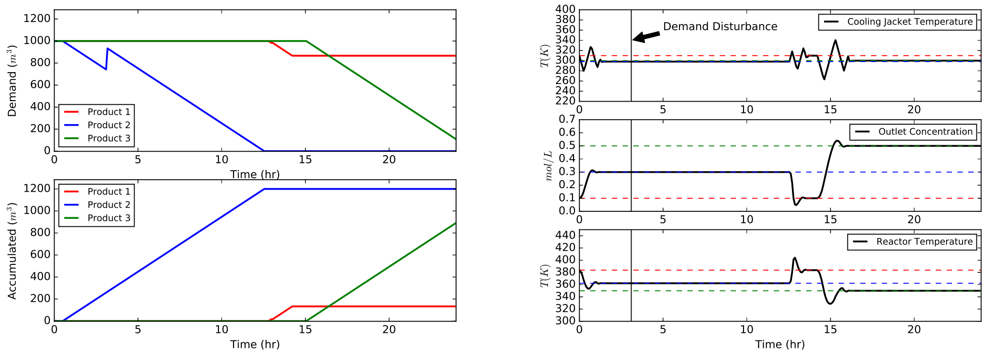


(**d**) Phase 4: Integrated, Reactive Schedule

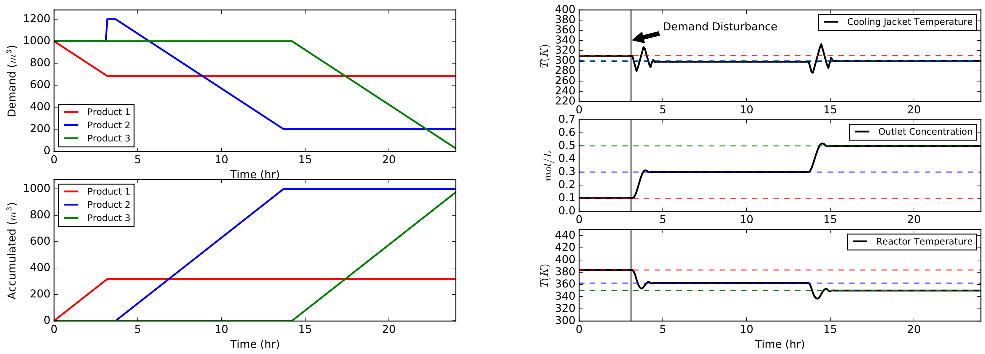
Figure 5. Scenario A: Process disturbance.



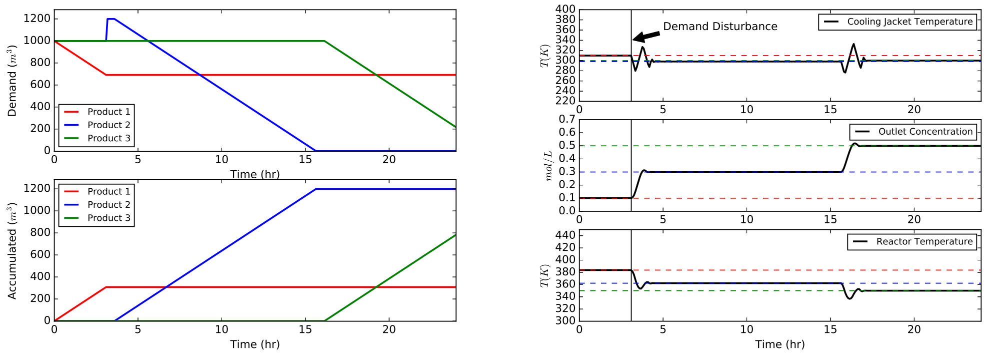
(**a**) Phase 1: Segregated, Fixed Schedule



(**b**) Phase 2: Segregated, Reactive Schedule

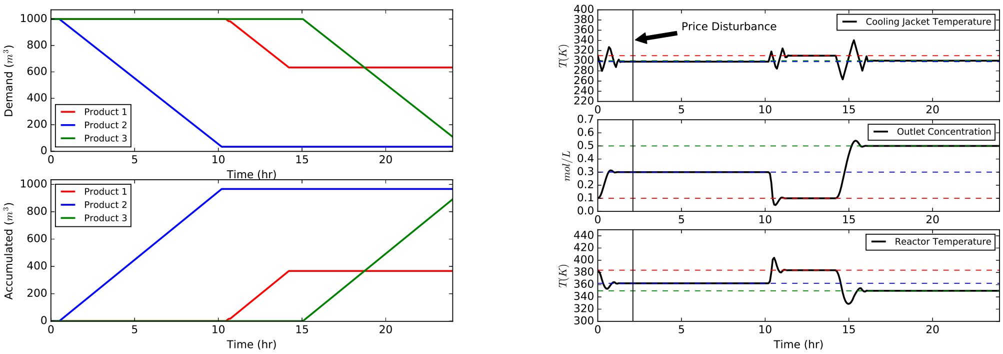


(**c**) Phase 3: Integrated, Fixed Schedule

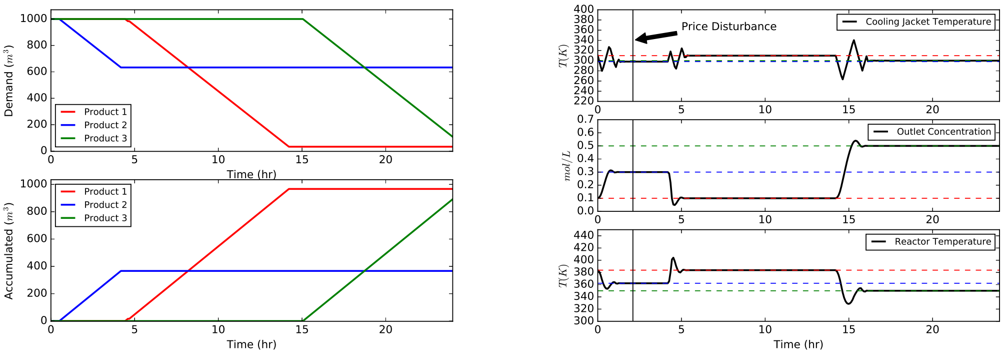


(**d**) Phase 4: Integrated, Reactive Schedule

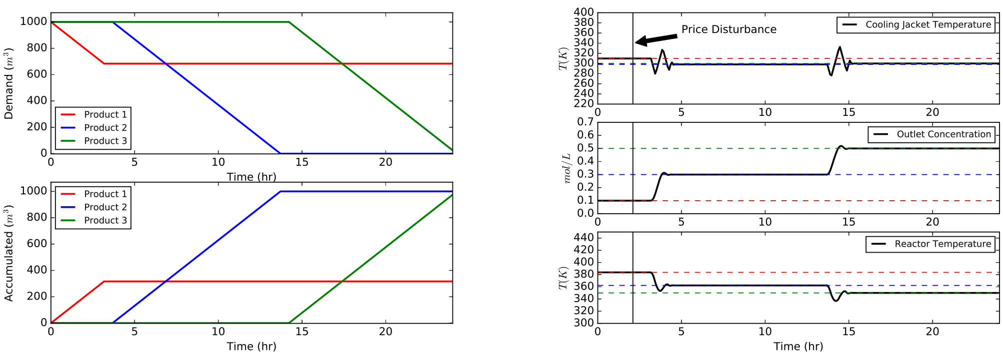
Figure 6. Scenario B: Market update (demand disturbance).



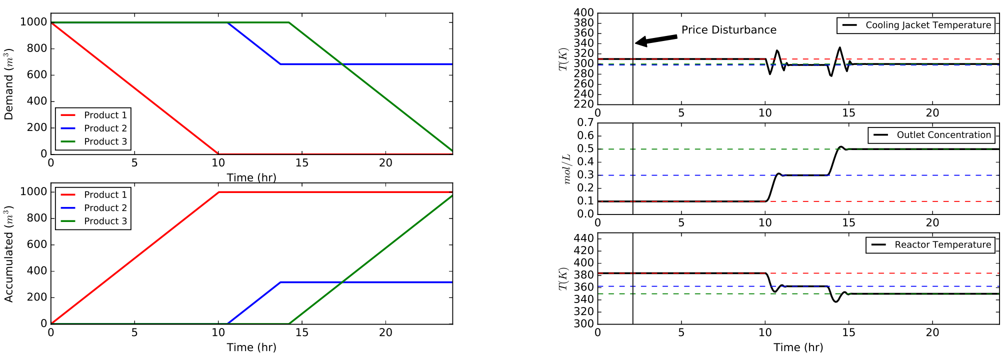
(**a**) Phase 1: Segregated, Fixed Schedule



(**b**) Phase 2: Segregated, Reactive Schedule



(**c**) Phase 3: Integrated, Fixed Schedule



(**d**) Phase 4: Integrated, Reactive Schedule

Figure 7. Scenario C: Market update (price disturbance).

4.3. Scenario C: Market Update Containing New Product Selling Prices

As in Scenarios A and B, the production order for Phases 1 and 2 is sub-optimal due to a lack of incorporation of process dynamics in scheduling. However, reactive rescheduling after the price fluctuation information is made available results in a large profit increase from Phase 1 to Phase 2, demonstrating the strength of reactive scheduling even without scheduling and control integration.

Phases 3 and 4 have an optimal production sequence due to the integration of scheduling and control, leading to higher profits than the corresponding segregated phases. This illustrates again the benefits of scheduling and control integration. Like Phase 2, Phase 4 reschedules when the updated market conditions are made available, producing less of product 2 and more of products 1 and 3 due to the price fluctuations. This leads to a leap in profit compared to Phase 3. Phase 4 with both scheduling and control integration and reactive or more frequent scheduling is again the most profitable phase.

The simulation results of scenario C are shown in Figure 7 and Table 9.

Table 9. Results: Scenario C.

Phase	Description	Profit		Production (m^3)		
		($)	(%)	Product 1	Product 2	Product 3
1	Segregated, Fixed Schedule	3758	(−16%)	367	967	908
2	Segregated, Reactive Schedule	4879	(+9%)	967	367	908
3	Integrated, Fixed Schedule	4466	(+0%)	317	1000	992
4	Integrated, Reactive Schedule	5662	(+27%)	1000	317	992

5. Conclusions

This work summarizes and reviews the evidence for the economic benefit from scheduling and control integration, reactive scheduling with process disturbances and market updates, and from a combination of reactive and integrated scheduling and control. This work demonstrates the value of combining scheduling and control and responding to process disturbances or market updates by directly comparing four phases of progressive integration through a benchmark CSTR application and three scenarios with process disturbance and market fluctuations. Both ISC and reactice resecheduling show benefit, though their relative benefits are dependent on the situation. More complete integration (applying ISC in closed-loop control, rather than just the scheduling) demonstrates the most benefit.

Directions for Future Work

This work demonstrates the benefit of ISC through four phases of progressive integration using continuous-time scheduling and NMPC on a CSTR case study with three scenarios. This work introduces a benchmark problem with an application (CSTR) and three scenarios on which to benchmark the performance of a scheduling and control formulation. The development of additional benchmark problems applicable to a wider variety of industrial scenarios is proposed as an important potential subject of future work. With increasing research in ISC, benchmark problems for formulation performance comparison of integrated scheduling and control formulations as well as for comparison against a baseline segregated scheduling and control formulation are increasingly important. Benchmark applications and scenarios applicable to batch processes, multi-product continuous processes, and other processes with scenarios representative of probable industrial occurrences should be developed.

This work is applicable to continuous processes considering a single process unit. Progressive integrations proving economic benefit of scheduling and control integration should also be applied to batch processes and continuous processes considering multiple process units. Additionally, this work utilized continuous-time scheduling and NMPC in a decomposed ISC formulation. This formulation inherently considered only steady-state production with no external or dynamic factors (such as time-of-day pricing or dynamic constraints) during production periods. Discrete-time

ISC formulations [18–20,66,67] have been shown to effectively incorporate external and dynamic factors, such as cooling constraints and time-of-day energy pricing. This incorporation enables demand response to time-of-day pricing by reducing or increasing production during periods of steady-state product manufacturing and moving the time of transitions to take advantage of times with relaxed constraints (such as relaxed cooling constraints on exothermic processes). A study of economic benefit of discrete-time formulations as compared to continuous-time formulations for ISC is a potential subject of future work.

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Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

ISC	integrated scheduling and control
SSC	segregated scheduling and control
MINLP	mixed-integer nonlinear programming
NLP	nonlinear programming
CSTR	continuous stirred tank reactor
MIDO	mixed-integer dynamic optimization
MILP	mixed-integer linear programming
NMPC	nonlinear model predictive control
ASU	air separation unit
MMA	methyl methacrylate reactor
FBR	fluidized bed reactor
RTN	resource task network
HIPS	high impact polystyrene reactor
ASU	cryogenic air separation unit
SISO	single-input single-output
PFR	plug flow reactor
PWA	piecewise affine
DR	demand response

References

1. Backx, T.; Bosgra, O.; Marquardt, W. Integration of Model Predictive Control and Optimization of Processes. In Proceedings of the ADCHEM 2000 International Symposium on Advanced Control of Chemical Processes, Pisa, Italy, 14–16 June 2000; pp. 249–260.
2. Soderstrom, T.A.; Zhan, Y.; Hedengren, J. Advanced Process Control in ExxonMobil Chemical Company: Successes and Challenges. In Proceedings of the AIChE Spring Meeting, Salt Lake City, UT, USA, 7–12 Novembrer 2010; pp. 1–12.
3. Baldea, M.; Harjunkoski, I. Integrated production scheduling and process control: A systematic review. *Comput. Chem. Eng.* **2014**, *71*, 377–390.
4. Nyström, R.H.; Harjunkoski, I.; Kroll, A. Production optimization for continuously operated processes with optimal operation and scheduling of multiple units. *Comput. Chem. Eng.* **2006**, *30*, 392–406.
5. Chatzidoukas, C.; Perkins, J.D.; Pistikopoulos, E.N.; Kiparissides, C. Optimal grade transition and selection of closed-loop controllers in a gas-phase olefin polymerization fluidized bed reactor. *Chem. Eng. Sci.* **2003**, *58*, 3643–3658.
6. Capón-García, E.; Guillén-Gosálbez, G.; Espuña, A. Integrating process dynamics within batch process scheduling via mixed-integer dynamic optimization. *Chem. Eng. Sci.* **2013**, *102*, 139–150.

7. Nie, Y.; Biegler, L.T.; Wassick, J.M. Integrated scheduling and dynamic optimization of batch processes using state equipment networks. *AIChE J.* **2012**, *58*, 3416–3432.
8. Flores-Tlacuahuac, A.; Grossmann, I.E. Simultaneous scheduling and control of multiproduct continuous parallel lines. *Ind. Eng. Chem. Res.* **2010**, *49*, 7909–7921.
9. Terrazas-Moreno, S.; Flores-Tlacuahuac, A.; Grossmann, I.E. Lagrangean heuristic for the scheduling and control of polymerization reactors. *AIChE J.* **2008**, *54*, 163–182.
10. Pattison, R.C.; Touretzky, C.R.; Harjunkoski, I.; Baldea, M. Moving Horizon Closed-Loop Production Scheduling Using Dynamic Process Models. *AIChE J.* **2017**, *63*, 639–651.
11. Engell, S.; Harjunkoski, I. Optimal operation: Scheduling, advanced control and their integration. *Comput. Chem. Eng.* **2012**, *47*, 121–133.
12. Harjunkoski, I.; Maravelias, C.T.; Bongers, P.; Castro, P.M.; Engell, S.; Grossmann, I.E.; Hooker, J.; Méndez, C.; Sand, G.; Wassick, J. Scope for industrial applications of production scheduling models and solution methods. *Comput. Chem. Eng.* **2014**, *62*, 161–193.
13. Harjunkoski, I.; Nyström, R.; Horch, A. Integration of scheduling and control—Theory or practice? *Comput. Chem. Eng.* **2009**, *33*, 1909–1918.
14. Shobrys, D.E.; White, D.C. Planning, scheduling and control systems: Why cannot they work together. *Comput. Chem. Eng.* **2002**, *26*, 149–160.
15. Baldea, M.; Du, J.; Park, J.; Harjunkoski, I. Integrated production scheduling and model predictive control of continuous processes. *AIChE J.* **2015**, *61*, 4179–4190.
16. Baldea, M.; Touretzky, C.R.; Park, J.; Pattison, R.C. Handling Input Dynamics in Integrated Scheduling and Control. In Proceedings of the 2016 IEEE International Conference on Automation, Quality and Testing, Robotics (AQTR), Cluj-Napoca, Romania, 19–21 May 2016; pp. 1–6.
17. Baldea, M. Employing Chemical Processes as Grid-Level Energy Storage Devices. *Adv. Energy Syst. Eng.* **2017**, 247–271, doi:10.1007/978-3-319-42803-1_9.
18. Beal, L.D.R.; Clark, J.D.; Anderson, M.K.; Warnick, S.; Hedengren, J.D. Combined Scheduling and Control with Diurnal Constraints and Costs Using a Discrete Time Formulation. In Proceedings of the FOCAPO/CPC, Tucson, Arizona, 8–12 January 2017.
19. Beal, L.D.; Petersen, D.; Grimsman, D.; Warnick, S.; Hedengren, J.D. Integrated Scheduling and Control in Discrete-Time with Dynamic Parameters and Constraints. *Comput. Chem. Eng.* **2008**, *32*, 463–476.
20. Beal, L.D.; Park, J.; Petersen, D.; Warnick, S.; Hedengren, J.D. Combined model predictive control and scheduling with dominant time constant compensation. *Comput. Chem. Eng.* **2017**, *104*, 271–282.
21. Cai, Y.; Kutanoglu, E.; Hasenbein, J.; Qin, J. Single-machine scheduling with advanced process control constraints. *J. Sched.* **2012**, *15*, 165–179.
22. Chatzidoukas, C.; Kiparissides, C.; Perkins, J.D.; Pistikopoulos, E.N. Optimal grade transition campaign scheduling in a gas-phase polyolefin FBR using mixed integer dynamic optimization. *Comput. Aided Chem. Eng.* **2003**, *15*, 744–747.
23. Chatzidoukas, C.; Pistikopoulos, S.; Kiparissides, C. A Hierarchical Optimization Approach to Optimal Production Scheduling in an Industrial Continuous Olefin Polymerization Reactor. *Macromol. React. Eng.* **2009**, *3*, 36–46.
24. Chu, Y.; You, F. Integration of scheduling and control with online closed-loop implementation: Fast computational strategy and large-scale global optimization algorithm. *Comput. Chem. Eng.* **2012**, *47*, 248–268.
25. Chu, Y.; You, F. Integration of production scheduling and dynamic optimization for multi-product CSTRs: Generalized Benders decomposition coupled with global mixed-integer fractional programming. *Comput. Chem. Eng.* **2013**, *58*, 315–333.
26. Chu, Y.; You, F. Integrated Scheduling and Dynamic Optimization of Sequential Batch Proesses with Online Implementation. *AIChE J.* **2013**, *59*, 2379–2406.
27. Chu, Y.; You, F. Integrated Scheduling and Dynamic Optimization of Complex Batch Processes with General Network Structure Using a Generalized Benders Decomposition Approach. *Ind. Eng. Chem. Res.* **2013**, *52*, 7867–7885.
28. Chu, Y.; You, F. Integration of scheduling and dynamic optimization of batch processes under uncertainty: Two-stage stochastic programming approach and enhanced generalized benders decomposition algorithm. *Ind. Eng. Chem. Res.* **2013**, *52*, 16851–16869.

29. Chu, Y.; You, F. Moving Horizon Approach of Integrating Scheduling and Control for Sequential Batch Processes. *AIChE J.* **2014**, *60*, 1654–1671.
30. Chu, Y.; You, F. Integrated Planning, Scheduling, and Dynamic Optimization for Batch Processes: MINLP Model Formulation and Efficient Solution Methods via Surrogate Modeling. *Ind. Eng. Chem. Res.* **2014**, *53*, 13391–13411.
31. Chu, Y.; You, F. Integrated scheduling and dynamic optimization by stackelberg game: Bilevel model formulation and efficient solution algorithm. *Ind. Eng. Chem. Res.* **2014**, *53*, 5564–5581.
32. Dias, L.S.; Ierapetritou, M.G. Integration of scheduling and control under uncertainties: Review and challenges. *Chem. Eng. Res. Des.* **2016**, *116*, 98–113.
33. Du, J.; Park, J.; Harjunkoski, I.; Baldea, M. A time scale-bridging approach for integrating production scheduling and process control. *Comput. Chem. Eng.* **2015**, *79*, 59–69.
34. Flores-Tlacuahuac, A.; Grossmann, I.E. Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR. *Ind. Eng. Chem. Res.* **2006**, *45*, 6698–6712.
35. Gutierrez-Limon, M.A.; Flores-Tlacuahuac, A.; Grossmann, I.E. A Multiobjective Optimization Approach for the Simultaneous Single Line Scheduling and Control of CSTRs. *Ind. Eng. Chem. Res.* **2011**, *51*, 5881–5890.
36. Gutierrez-Limon, M.A.; Flores-Tlacuahuac, A.; Grossmann, I.E. A reactive optimization strategy for the simultaneous planning, scheduling and control of short-period continuous reactors. *Comput. Chem. Eng.* **2016**, *84*, 507–515.
37. Gutiérrez-Limón, M.A.; Flores-Tlacuahuac, A.; Grossmann, I.E. MINLP formulation for simultaneous planning, scheduling, and control of short-period single-unit processing systems. *Ind. Eng. Chem. Res.* **2014**, *53*, 14679–14694.
38. Koller, R.W.; Ricardez-Sandoval, L.A. A Dynamic Optimization Framework for Integration of Design, Control and Scheduling of Multi-product Chemical Processes under Disturbance and Uncertainty. *Comput. Chem. Eng.* **2017**, *106*, 147–159.
39. Nie, Y.; Biegler, L.T.; Villa, C.M.; Wassick, J.M. Discrete Time Formulation for the Integration of Scheduling and Dynamic Optimization. *Ind. Eng. Chem. Res.* **2015**, *54*, 4303–4315.
40. Nyström, R.H.; Franke, R.; Harjunkoski, I.; Kroll, A. Production campaign planning including grade transition sequencing and dynamic optimization. *Comput. Chem. Eng.* **2005**, *29*, 2163–2179.
41. Patil, B.P.; Maia, E.; Ricardez-Sandoval, L.A. Integration of Scheduling, Design, and Control of Multiproduct Chemical Processes Under Uncertainty. *AIChE J.* **2015**, *61*, 2456–2470.
42. Pattison, R.C.; Touretzky, C.R.; Johansson, T.; Harjunkoski, I.; Baldea, M. Optimal Process Operations in Fast-Changing Electricity Markets: Framework for Scheduling with Low-Order Dynamic Models and an Air Separation Application. *Ind. Eng. Chem. Res.* **2016**, *55*, 4562–4584.
43. Prata, A.; Oldenburg, J.; Kroll, A.; Marquardt, W. Integrated scheduling and dynamic optimization of grade transitions for a continuous polymerization reactor. *Comput. Chem. Eng.* **2008**, *32*, 463–476.
44. Terrazas-Moreno, S.; Flores-Tlacuahuac, A.; Grossmann, I.E. Simultaneous design, scheduling, and optimal control of a methyl-methacrylate continuous polymerization reactor. *AIChE J.* **2008**, *54*, 3160–3170.
45. Terrazas-Moreno, S.; Flores-Tlacuahuac, A.; Grossmann, I.E. Simultaneous cyclic scheduling and optimal control of polymerization reactors. *AIChE J.* **2007**, *53*, 2301–2315.
46. You, F.; Grossmann, I.E. Design of responsive supply chains under demand uncertainty. *Comput. Chem. Eng.* **2008**, *32*, 3090–3111.
47. Zhuge, J.; Ierapetritou, M.G. Integration of Scheduling and Control with Closed Loop Implementation. *Ind. Eng. Chem. Res.* **2012**, *51*, 8550–8565.
48. Zhuge, J.; Ierapetritou, M.G. Integration of Scheduling and Control for Batch Processes Using Multi-Parametric Model Predictive Control. *AIChE J.* **2014**, *60*, 3169–3183.
49. Zhuge, J.; Ierapetritou, M.G. An Integrated Framework for Scheduling and Control Using Fast Model Predictive Control. *AIChE J.* **2015**, *61*, 3304–3319.
50. Zhuge, J.; Ierapetritou, M.G. A Decomposition Approach for the Solution of Scheduling Including Process Dynamics of Continuous Processes. *Ind. Eng. Chem. Res.* **2016**, *55*, 1266–1280.
51. Mahadevan, R.; Doyle, F.J.; Allcock, A.C. Control-relevant scheduling of polymer grade transitions. *AIChE J.* **2002**, *48*, 1754–1764.
52. Mojica, J.L.; Petersen, D.; Hansen, B.; Powell, K.M.; Hedengren, J.D. Optimal combined long-term facility design and short-term operational strategy for CHP capacity investments. *Energy* **2017**, *118*, 97–115.

53. Gupta, D.; Maravelias, C.T.; Wassick, J.M. From rescheduling to online scheduling. *Chem. Eng. Res. Des.* **2016**, *116*, 83–97.
54. Gupta, D.; Maravelias, C.T. On deterministic online scheduling: Major considerations, paradoxes and remedies. *Comput. Chem. Eng.* **2016**, *94*, 312–330.
55. Gupta, D.; Maravelias, C.T. A General State-Space Formulation for Online Scheduling. *Processes* **2017**, *4*, 69.
56. Kopanos, G.M.; Pistikopoulos, E.N. Reactive scheduling by a multiparametric programming rolling horizon framework: A case of a network of combined heat and power units. *Ind. Eng. Chem. Res.* **2014**, *53*, 4366–4386.
57. Liu, S.; Shah, N.; Papageorgiou, L.G. Multiechelon Supply Chain Planning With Sequence-Dependent Changeovers and Price Elasticity of Demand under Uncertainty. *AIChE J.* **2012**, *58*, 3390–3403.
58. Touretzky, C.R.; Baldea, M. Integrating scheduling and control for economic MPC of buildings with energy storage. *J. Process Control* **2014**, *24*, 1292–1300.
59. Li, Z.; Ierapetritou, M.G. Process Scheduling Under Uncertainty Using Multiparametric Programming. *AIChE J.* **2007**, *53*, 3183–3203.
60. Petersen, D.; Beal, L.D.R.; Prestwich, D.; Warnick, S.; Hedengren, J.D. Combined Noncyclic Scheduling and Advanced Control for Continuous Chemical Processes. *Processes* **2017**, *4*, 83, doi:10.3390/pr5040083.
61. Hart, W.E.; Watson, J.P.; Woodruff, D.L. Pyomo: Modeling and solving mathematical programs in Python. *Math. Program. Comput.* **2011**, *3*, 219–260.
62. Hart, W.E.; Laird, C.; Watson, J.P.; Woodruff, D.L. *Pyomo—Optimization Modeling in Python*; Springer Science+Business Media, LLC: Berlin/Heidelberg, Germany, 2012; Volume 67.
63. Carey, G.; Finlayson, B.A. Orthogonal collocation on finite elements for elliptic equations. *Chem. Eng. Sci.* **1975**, *30*, 587–596.
64. Hedengren, J.; Mojica, J.; Cole, W.; Edgar, T. APOPT: MINLP Solver for Differential Algebraic Systems with Benchmark Testing. In Proceedings of the INFORMS Annual Meeting, Pheonix, AZ, USA, 14–17 October 2012.
65. Belotti, P.; Lee, J.; Liberti, L.; Margot, F.; Wächter, A. Branching and bounds tightening techniques for non-convex MINLP. *Optim. Methods Softw.* **2009**, *24*, 597–634.
66. Floudas, C.A.; Lin, X. Continuous-time versus discrete-time approaches for scheduling of chemical processes: A review. *Comput. Chem. Eng.* **2004**, *28*, 2109–2129.
67. Sundaramoorthy, A.; Maravelias, C.T. Computational study of network-based mixed-integer programming approaches for chemical production scheduling. *Ind. Eng. Chem. Res.* **2011**, *50*, 5023–5040.