Combined Scheduling and Control with Diurnal Constraints and Costs Using a Discrete Time Formulation

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Abstract

Integrated scheduling and control is a new approach that seeks to unify the objectives of the various layers of optimization in manufacturing. Recent efforts in this field have used a continuous-time, slot-based formulation. This work investigates combining scheduling and control using a novel discrete-time formulation, utilizing the full process model through the entire horizon. This discrete-time form lends itself to optimization with time-dependent constraints and costs. This work demonstrates the value of time-based parameters in this paradigm by applying cooling constraints and energy costs of a sample diurnal cycle. A psuedo-binary variable method is presented to ease the computational burden of this approach. The formulation is applied with a generic CSTR system in open-loop simulations over a 48-hour horizon.

Keywords

Optimization, Combined Scheduling and Control, Discrete-time, Diurnal constraints.

1 Introduction and Background

Current process control and optimization strategies are typically divided into major sections including base layer controls, advanced controls, real-time optimization, and planning and scheduling (Soderstrom and Hedengren, 2010). Each of these levels works at a different time scale, ranging from milliseconds to seconds for base controls, up to weeks or months at the planning and scheduling level.

In an effort to simplify models and decrease computation time, each of these layers receives a minimal amount of information to fulfill an objective. However, this lack of information creates lost opportunities. For example, the "optimal solution" determined by the scheduler is sometimes impossible to implement in practice e.g. in the required time to transition between products in continuous manufacturing (Capón-García et al., 2013). Further, the objectives of individual optimizations can sometimes counter each other (such as a controller goal to reach a set point against a scheduler goal to maximize profits) (Harjunkoski et al., 2009).

This control structure is largely an artifact of the development of process control and the computational limits during these developmental periods (Baldea and Harjunkoski, 2014). Thus, each field has grown within an isolated domain, without much coordination, sometimes at the expense of truly optimal solutions (Baldea and Harjunkoski, 2014).

With ever-increasing computational power, the segregation of optimization is being reanalyzed and extended through efforts such as model predictive control (MPC) for supply chain management (Subramanian et al., 2014), economic MPC (Ellis et al., 2014; Angeli et al., 2012), Dynamic Real-time Optimization (DRTO) (Pontes et al., 2015; Harjunkoski et al., 2014; Biegler et al., 2015), and combined nonlinear estimation and control (Hedengren et al., 2014; Lima et al., 2013).

Economic Model Predictive Control (EMPC) mixes the benefits of the optimization layers with an objective function centered around profit or reducing operating expenses, rather than reaching a setpoint, and is therefore reminiscent of a scheduler. However, EMPC

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requires a very short time horizon to be able to solve in real-time for closed-loop control situations (Ellis et al., 2014).

Similarly, Dynamic Real-Time Optimization (DRTO) has an economic objective function. DRTO is solved more frequently than scheduling problems and leverages the predictive power inherent in a first-principles model to calculate intermediate set points used by MPC for optimal product transitions (Pontes et al., 2015; Ellis et al., 2014).

These past efforts have proven valuable in practice (Soderstrom and Hedengren, 2010). Now, researchers are attempting to take this blend of benefits one step further by more directly integrating control and scheduling. In light of ever-increasing computational potential, an integrated optimization scheme is the future of process control. The suggestions and early implementations of fully combining scheduling and control go back at least a decade (Flores-Tlacuahuac and Grossmann, 2006).

Approaches to the integration are sometimes viewed in two classes: top-down (adding scheduling to the control paradigm) or bottom-up (adding control to the scheduling paradigm) (Baldea and Harjunkoski, 2014). Some researchers have investigated incorporating explicit process dynamics in the scheduling model with differential and/or algebraic constraints (Flores-Tlacuahuac and Grossmann, 2006), even for multi-product parallel CSTRs (Flores-Tlacuahuac and Grossmann, 2010). Another approach has been named the scale-bridging model (SBM), which is a simplified model of the process that encompasses most of the important dynamics that can be used in the scheduling framework (Du et al., 2015; Baldea et al., 2015, 2016). Prata et al. (2008) showed the benefit of integrating scheduling and control to optimize transition times in a polymerization reactor, and also found that the optimization problem grows rapidly with increasing number of products. Zhuge and Ierapetritou (2012) showed the value of a closed loop implementation of simultaneous scheduling and control over an open loop implementation to reject disturbances. Others have taken a more theoretical approach by employing the Benders' decomposition framework to particular problems (Chu and You, 2013) or by using Dinkelbach's algorithm to find a global optimum in online implementations (Chu and You, 2012). Still others have explored the integration of scheduling and control in batch processes (Capón-García et al., 2013; Nie et al., 2012).

One development that will increase the available information to the optimizers is the continuing transition to a smart electrical grid. As the electricity grid transitions to a "smart grid," stakeholders will be empowered to perform energy transactions (Farhangi, 2010). Industrial plants could also take advantage of the variable cost of electricity.

Demand Response (DR) seeks to manage both volatile demand and renewable energy in order to increase efficiency of the electrical grid. DR incentivizes consumers to behave in ways that benefit the electrical grid as well as themselves by utilizing variable pricing to reduce consumption during peak hours when the reliability of the grid is jeopardized (U S Department of Energy, 2006). Generation should match consumption in order to maintain grid reliability (Mendoza-Serrano and Chmielewski, 2013). DR is a major reason why variability of energy prices is expected to increase (Deng et al., 2015). Industrial manufacturing processes can benefit from DR by decreasing energy consumption when the cost of electricity is high and increasing consumption when electricity costs are low.

Although residential makes up the largest portion of electrical grid consumers, tremendous opportunities exist for industrial participants (Mendoza-Serrano and Chmielewski, 2013). Previous efforts to quantify the benefits of DR for the industrial sector include petroleum refining (Mendoza-Serrano and Chmielewski, 2013), chemical processing (Feng et al., 2015), and gas production (Air Separation Unit) (Huang et al., 2011).

This work utilizes a Continuously Stirred Tank Reactor (CSTR) with a first-order, irreversible reaction to illustrate the benefits of adjusting operations based on periodic electricity price changes. Previous efforts to implement DR in chemical manufacturing processes required capital equipment. This work utilizes a standard CSTR and requires no additional capital equipment. Moreover, the periodic constraint of effective maximum cooling is added to the model. During the heat of the day, effective maximum cooling is reduced compared to nighttime operation. Periodic constraints for Nonlinear Model Predictive Control (NMPC) have been previously formulated (Huang et al., 2011). In this work, periodic constraints of both effective maximum cooling and electricity price are utilized in the optimization.

2 Test System

In this section we present the CSTR model used in this work. The model is applicable in various industries from food/beverage to oil and gas and chemicals. The notable assumptions of a CSTR include:

- Continuous flow in and out
- Well mixed
- Constant density

The model shown in Eqs. 1 to 4 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. The fluid in the cooling jacket undergoes an external, arbitrary cooling process where ΔH_{cool} is the effective cooling rate.

$$\frac{dC_A}{dt} = \frac{q}{V}(C_{A0} - C_A) - k_0 e^{-E_A/RT} C_A \tag{1}$$

$$\frac{dT}{dt} = \frac{q}{V}(T_f - T) - \frac{1}{\rho C_p} k_0 e^{\frac{-E_A}{RT}} C_A \Delta H_r - \frac{UA}{V\rho C_p}(T - T_c) \tag{2}$$

$$\frac{dT_c}{dt} = \frac{q_{cool}}{V_j}(T_{cin} - T_c) + \frac{UA}{V_j \rho C_p (T - T_c)} \tag{3}$$

$$\Delta H_{cool} = \rho C_{p.cool} q_{cool} (T_c - T_{cin}) \tag{4}$$

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, q_{cool} is the flowrate of coolant, V_j is the volume of the cooling jacket, T is the temperature of reactor, T_c is the temperature of cooling jacket, T_{cin} is the temperature of cooling return line and $C_{p.cool}$ is the cooling fluid heat capacity, Table 1 lists the CSTR parameters used.

This system is a simple test problem used to demonstrate this method. However, this formulation can be easily applied to various systems by simply replacing this model with an applicable system model.

Table 1. Reactor Parameter Values

Parameter	Value
V	$400m^3$
q_{cool}/V_{jacket}	$5hr^{-1}$
E_A/R	$8750K$
$\frac{UA}{V\rho C_p}$	$0.523hr^{-1}$
k_0	$1.8e10hr^{-1}$
T_f	$350K$
C_{A0}	$1mol/L$
$\frac{\Delta H_r}{\rho C_p}$	$-209\frac{Km^3}{mol}$

3 Problem Formulation

In this example, one reactor can make multiple products by varying the concentrations of A and B in the outlet stream. The manipulated variables in this optimization were ΔH_{cool} and q, which are bounded by $2MW \leq \Delta H_{cool}$ and $100\,m^3/hr \leq q \leq 120\,m^3/hr$. The sample problem used three products over a 48-hour horizon. The product descriptions are shown in Table 2, where the product specification tolerance is $\pm 0.005\,mol/L$.

Table 2. Product specifications.

Product	C_A (mol/L)	Max Demand (m^3)	Price (\$/100 m^3)
1	0.35	1920	24
2	0.12	2400	27
3	0.25	2880	21

Four test cases were considered to develop the integration of time-based parameters:

1. Static pricing and cooling constraints
2. Static pricing, diurnal cooling constraint function
3. Static cooling constraint, diurnal pricing function
4. Diurnal pricing and cooling constraint functions

Case 1 is the standard, time-independent case that should largely replicate results of a continuous-time, slot-based formulation.

The diurnal cycles of energy price and effective cooling constraints were generalized by simple sinusoidal curves, as shown in Figure 1. The energy price varies between \$10-\$90 per MWh, with the static price representing the average of \$50 per MWh. The effective cooling constraint represents the amount of cooling done that affects the system; in other words, the cooling done minus losses to the environment, etc. Therefore, higher ambient temperature during the day reduces effective cooling to the reactor because of heat loss to the environment, while more cooling is possible during the colder night.

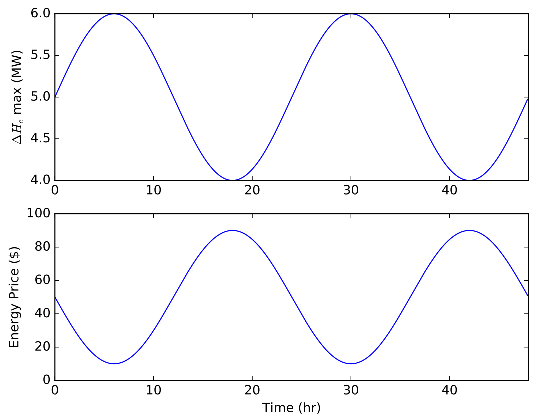


Figure 1. Plots of maximum effective cooling constraint and time-of-day pricing over 48 hours.

The objective function is shown in Eq. 5, where B is the binary variable that determines if product p is produced at time t, Π is the price of product p and E is the price of energy consumed at time t.

$$\begin{aligned} \text{maximize} \quad & \sum_t \sum_p (q_t \Pi_p B_{p,t}) - E_t \\ \text{s.t.} \quad & \text{Process Model} \quad \text{(Eqs. 1 - 4)} \end{aligned} \tag{5}$$

Pseudo-Binary Variables

Fine time resolution dictates a large number of integer variables. To avoid the extra computation required by mixed-integer nonlinear programming (MINLP) solvers, this work utilized a pseudo-binary variable approach for B. Using Eq. 6, the gradient-based solver is provided a gradient to recognize the location of products. In Eq. 6, h represents the max height of the function and must exceed 1, tol is the product tolerance (ie ± 0.01) and $C_{A,prod}$ is the specified concentration of the desired product. In this format, the function exceeds 1 in the range of product specifications and within (0,1) elsewhere. Equation 7 then caps the function to 1, creating a binary range.

$$f(C_A) = h10^{log(1/h)/tol^2 (C_{A,prod} - C_A)^2} \tag{6}$$

$$B(C_A) \leq f(C_A), \quad B \in [0, 1] \tag{7}$$

To force B closer to a binary form, the height (h) can be increased, as shown in Figure 2. In this work, h was manually increased and solved again, with each solution initializing the next. However, this method is related to, but has the opposite effect of, the barrier method used in interior point solvers. It is the authors' opinion that this form would be better implemented within a solver where (h) could be updated on a per-iteration basis. This is a point of future work.

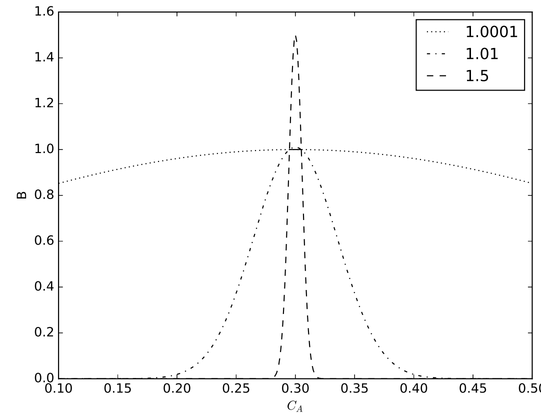


Figure 2. Plot showing convergence of pseudo-binary variable.

This function is suitable for this use because product specification variables are typically within a known, relatively small bound. Thus, the function f can provide a gradient through the entire range with initially small h.

4 Results

The results of each of the four test cases are described below. Each case has two plots. The first shows the system state variables, the second shows the maximum $\Delta H_{cool}(MW)$ constraint with the system ΔH_{cool} and (in cases 2 and 4) the energy price curve is overlayed with the right axis showing price units.

Case 1

This case is the first known implementation of scheduling using the full process model through the entire horizon and is the only known implementation of a combined scheduling and control formulation with discrete time. This case proves that this formulation is successful in combining scheduling and control.

This first test case produces the maximum amount of product 2 (the most profitable). Product 2 ($C_A = 0.12$) is produced at a lower rate because of the constant energy constraint.

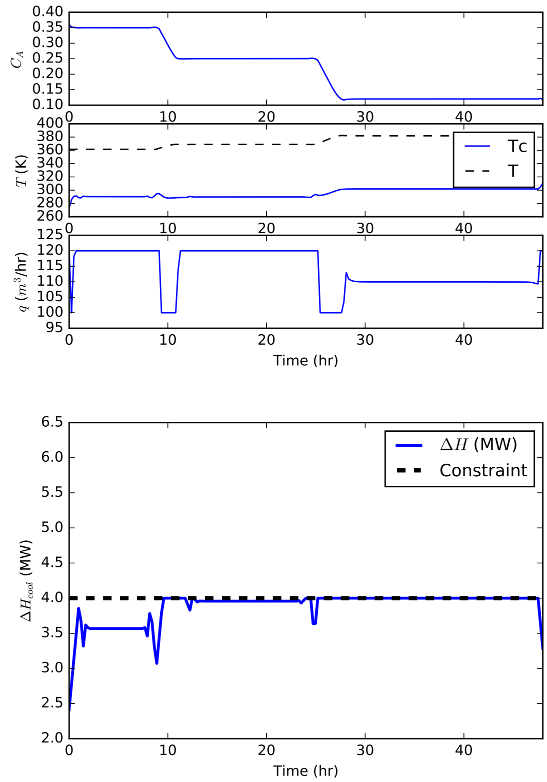


Figure 3. Case 1: Static pricing and cooling constraints.

Case 2

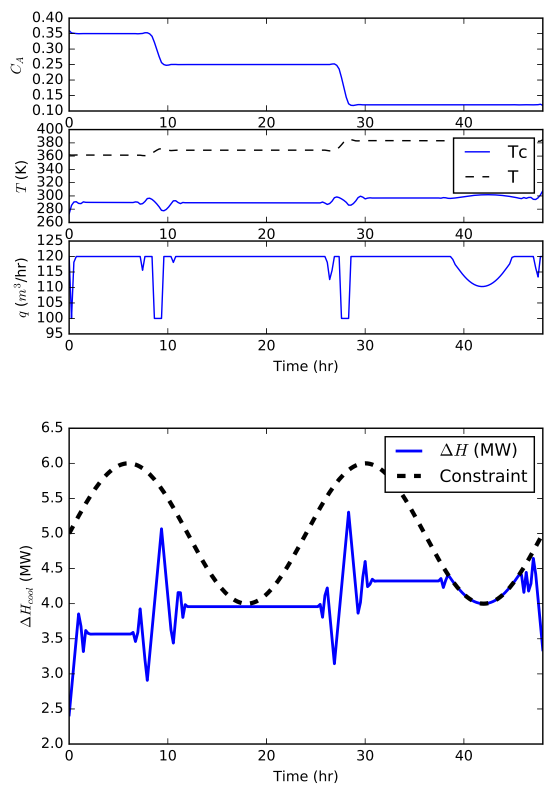


Figure 4. Static pricing, diurnal cooling constraints.

The diurnal cooling constraint curve applied in case 2 allows product 2 to be produced at a higher rate. The rate is decreased during the hottest part of the day, reaching the production rate of case 1 for only a brief period. Further, the transitions between products occur at different times when the max cooling constraint is higher because the extra cooling allows transitions to occur more quickly.

The profit for this case increased ˜20% over case 1. This shows the value of considering time-dependent constraints in combined scheduling and control. This benefit further justifies a discrete-time formulation for the ease of applying these constraints.

Case 3

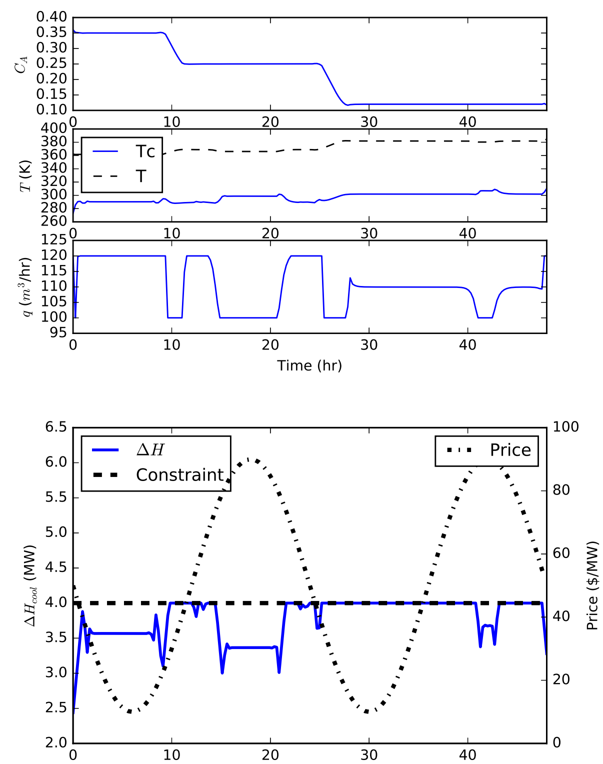
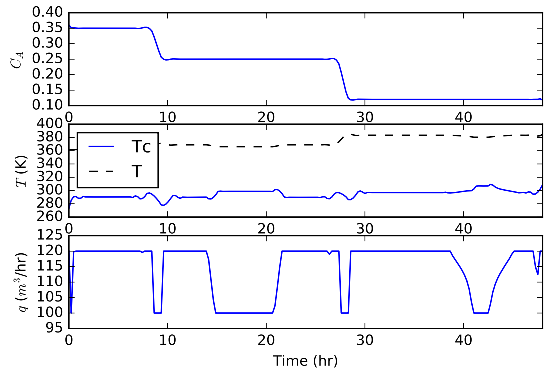


Figure 5. Static cooling constraint, diurnal energy price.

Case 3 largely follows case 1, except that production rates decrease when energy prices peak. Energy costs too much during these times and production generates negative revenue so the optimizer minimizes production to the lower bound of q ($100\ m^3/hr$). Also, the transitions occur at slightly different times to compensate for different production rates and to transition during times of cheaper energy.

The profit in this case increased only slightly (˜2%), but lowering the lower bound of q would easily increase this benefit. Again, time-dependent parameters are shown to be worth considering.

Case 4



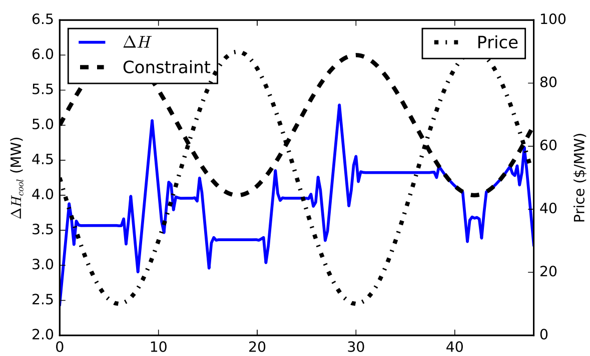


Figure 6. Diurnal constraint and price.

Case 4 implements the positive effects of cases 2 and 3 — the transitions occur at different places, production rate of product 2 is maximized and production at peak energy prices is decreased. The overall profit is the highest of the 4 cases.

Summarized Results

Table 3. Economic Summary of Results

Case	Product Production (m^3)			Profit
	1	2	3	($)
1	1105	2288	1748	4632
2	1004	2328	2144	5656
3	1132	2264	1584	4712
4	1004	2304	2012	5684

In summary, transitions are treated differently (different net costs, start times and durations) with time-dependent constraints. These considerations can have a significant economic impact, with diurnal constraints increasing profits ˜20% in this example.

It is also anticipated that, under the right circumstances, the scheduler may go so far as to switch products in response to these diurnal cycles, forcing extra transitions that would not be possible in current implementations of slot-based combined scheduling and control formulations where the number of slots frequently equals the number of products. In other cases, the scheduler may order products differently with time-based constraints in consideration. Further, this method is easily applied to other time-dependent parameters beyond diurnal cycles, such as feed stock price predictions.

5 Conclusion

This work applied a novel, discrete-time formulation of combined scheduling and control. This method provided a schedule of sequential products using the full model dynamics through the entire horizon. The discrete-time formulation easily allowed the implementation of time-based parameters. This work applied time-dependent parameters of diurnal cycles of energy price and maximum effective cooling of a CSTR. This optimization improved open-loop scheduling profit prediction over 20%. This work also implemented a psuedo-binary approach to assist the gradient-descent solvers.

This work motivates continued investigation into discrete-time formulations and time-dependent parameters in considering both transitions and product manufacturing. In particular, the pseudo-binary approach should be implemented as part of an interior point solver. As this method matures, other objectives, such as on-time delivery, should be incorporated in the objective.

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References

Angeli, D., Amrit, R., and Rawlings, J. B. (2012). On Average Performance and Stability of Economic Model Predictive Control. *IEEE Transactions on Automatic Control*, 57(7):1615–1626.

Baldea, M., Du, J., Park, J., and Harjunkoski, I. (2015). Integrated production scheduling and model predictive control of continuous processes. *AIChE Journal*, 61(12):4179–4190.

Baldea, M. and Harjunkoski, I. (2014). Integrated production scheduling and process control: A systematic review. *Computers and Chemical Engineering*, 71:377–390.

Baldea, M., Touretzky, C. R., Park, J., and Pattison, R. C. (2016). Handling Input Dynamics in Integrated Scheduling and Control. In *2016 IEEE International Conference on Automation, Quality and Testing, Robotics (AQTR)*, pages 1–6.

Biegler, L., Yang, X., and Fischer, G. (2015). Advances in sensitivity-based nonlinear model predictive control and dynamic real-time optimization. *Journal of Process Control*, 30:104–116.

Capón-García, E., Guillén-Gosálbez, G., and Espuña, A. (2013). Integrating process dynamics within batch process scheduling via mixed-integer dynamic optimization. *Chemical Engineering Science*, 102:139–150.

Chu, Y. and You, F. (2012). Integration of scheduling and control with online closed-loop implementation: Fast computational strategy and large-scale global optimization algorithm. *Computers and Chemical Engineering*, 47:248–268.

Chu, Y. and You, F. (2013). Integration of production scheduling and dynamic optimization for multi-product CSTRs: Generalized Benders decomposition coupled with global mixed-integer fractional programming. *Computers and Chemical Engineering*, 58:315–333.

Deng, R., Yang, Z., Chow, M.-Y., and Chen, J. (2015). A Survey on Demand Response in Smart Grids: Mathematical Models and Approaches. *IEEE Transactions on Industrial Informatics*, 11(3):1–1.

Du, J., Park, J., Harjunkoski, I., and Baldea, M. (2015). A time scale-bridging approach for integrating production scheduling and process control. *Computers & Chemical Engineering*, 79:59–69.

Ellis, M., Durand, H., and Christofides, P. D. (2014). A tutorial review of economic model predictive control methods. *Journal of Process Control*, 24(8):1156–1178.

Farhangi, H. (2010). The Path of the Smart Grid 18. *IEEE Power & Energy Mag.,*, (february):1828,.

Feng, J. Y., Brown, A., O'Brien, D., and Chmielewski, D. J. (2015). Smart grid coordination of a chemical processing plant. *Chemical Engineering Science*, 136:168–176.

Flores-Tlacuahuac, A. and Grossmann, I. E. (2006). Simultaneous Cyclic Scheduling and Control of a Multiproduct CSTR. *Industrial & Engineering Chemistry Research*, 45(20):6698–6712.

Flores-Tlacuahuac, A. and Grossmann, I. E. (2010). Simultaneous scheduling and control of multiproduct continuous parallel lines. *Industrial and Engineering Chemistry Research*, 49(17):7909–7921.

Harjunkoski, I., Maravelias, C. T., Bongers, P., Castro, P. M., Engell, S., Grossmann, I. E., Hooker, J., Méndez, C., Sand, G., and Wassick, J. (2014). Scope for industrial applications of production scheduling models and solution methods. *Computers and Chemical Engineering*, 62:161–193.

Harjunkoski, I., Nyström, R., and Horch, A. (2009). Integration of scheduling and controlTheory or practice? *Computers and Chemical Engineering*, 33:1909–1918.

Hedengren, J. D., Shishavan, R. A., Powell, K. M., and Edgar, T. F. (2014). Nonlinear modeling, estimation and predictive control in APMonitor. *Computers & Chemical Engineering*, 70:133–148.

Huang, R., Harinath, E., and Biegler, L. T. (2011). Lyapunov stability of economically oriented NMPC for cyclic processes. *Journal of Process Control*, 21(4):501–509.

Lima, F. V., Rajamani, M. R., Soderstrom, T. A., and Rawlings, J. B. (2013). Covariance and State Estimation of Weakly Observable Systems: Application to Polymerization Processes. *IEEE Transactions on Control Systems Technology*, 21(4):1249–1257.

Mendoza-Serrano, D. I. and Chmielewski, D. J. (2013). Demand Response for Chemical Manufacturing using Economic MPC. *Proceedings of 2013 American Control Conference (ACC)*, pages 6655–6660.

Nie, Y., Biegler, L. T., and Wassick, J. M. (2012). Integrated scheduling and dynamic optimization of batch processes using state equipment networks. *AIChE Journal*, 58(11):3416–3432.

Pontes, K. V., Wolf, I. J., Embiruçu, M., and Marquardt, W. (2015). Dynamic Real-Time Optimization of Industrial Polymerization Processes with Fast Dynamics. *Industrial & Engineering Chemistry Research*, 54(47):11881–11893.

Prata, A., Oldenburg, J., Kroll, A., and Marquardt, W. (2008). Integrated scheduling and dynamic optimization of grade transitions for a continuous polymerization reactor. *Computers and Chemical Engineering*, 32(3):463–476.

Soderstrom, T.A., Z. Y. and Hedengren, J. (2010). Advanced Process Control in ExxonMobil Chemical Company: Successes and Challenges. In *CAST Division, AIChE National Meeting*, Salt Lake City, UT.

Subramanian, K., Rawlings, J. B., and Maravelias, C. T. (2014). Economic model predictive control for inventory management in supply chains. *Computers & Chemical Engineering*, 64:71–80.

U S Department of Energy (2006). Benefits of Demand Response in Electricity Markets and Recommendations for Achieving Them. Technical Report February, US DOE.

Zhuge, J. and Ierapetritou, M. G. (2012). Integration of Scheduling and Control with Closed Loop Implementation. *Industrial & Engineering Chemistry Research*, 51(25):8550–8565.