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Combined Model Predictive Control and Scheduling with Dominant Time Constant Compensation

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Abstract

Linear model predictive control is extended to both control and optimize a product grade schedule. The proposed methods are time scaling of the linear dynamics based on throughput rates and grade-based objectives for product scheduling based on a mathematical program with complementarity constraints. The linear model is adjusted with a residence time approximation to time-scale the dynamics based on throughput. Although nonlinear models directly account for changing dynamics, the model form is restricted to linear differential equations to enable fast online cycle times for large-scale and real-time systems. This method of extending a linear time-invariant model for scheduling is designed for many advanced control applications that currently use linear models. Simultaneous product switching and grade target management is demonstrated on a reactor benchmark application. The objective is a continuous form of discrete ranges for product targets and economic terms that maximize overall profitability.

Keywords: scheduling, model predictive control, dynamic pricing, time scaling, complementarity constraints

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1. Introduction

Time-of-day energy pricing for electricity and natural gas pose a challenge and opportunity for industrial scale manufacturing processes. In many manufacturing processes in which Model Predictive Control (MPC) is well-established, such as downstream refining and petrochemicals, there is lost opportunity when advanced process control only operates at certain conditions but must be turned off when unit production is lowered [1]. A challenge with changing production rates is that the dynamics of a process often change dramatically with throughput. Empirical models identified at high throughput rates are often inaccurate and lead to poor control performance at low production rates. An opportunity with time-of-day pricing is to temporarily reduce the consumption of energy-intensive processes for periods when the energy costs are sufficiently high. During off-peak periods, the production rate is increased or more energy-intensive product grades are produced to take advantage of low energy costs. With typical daily cycles in energy costs, a cyclical operation forms that the original advanced control system may not be designed to follow. When production targets are not set to maximize to production constraints, MPC may switch to maximize energy efficiency or other secondary objectives. Set point targets traditionally come from a real-time optimization (RTO) application that optimizes a steady state operating point for the plant [2].

Segregated control and scheduling structure is historically due to computational factors that limit application complexity [3]. As a result, the control and scheduling fields have grown independently and without coordination, leading to a loss of opportunity from combining the applications [2, 4]. By combining process scheduling of set points with control, the inefficiencies of application layering are avoided. One such inefficiency that results from application layering is the infeasibility on the control layer of individual solutions pass from the supervisory layer [5]. Scheduling applications frequently do not consider grade transition times because of the large combinatorial look-up table that would be required to consider all possible transitions. Additionally, objectives

31 of individual solutions can oppose each other. For example, the controller does
32 not consider the most economical route to reach a target set point given by the
33 scheduler or steady-state optimizer [6].

34 The computational barriers for combined control and scheduling are dimin-
35 ished with improved computer hardware and adaptation of algorithms to the
36 hardware. Algorithmic barriers are being overcome with a number of key con-
37 tributions that are opening several fronts of development [7, 8]. Hardware or
38 network resources such as multi-core, cloud-based, and graphics processing units
39 (GPUs) provide access to previously inaccessible computing power. However,
40 advanced architectures such as GPUs for optimization impose some limitations
41 on the type of problems that can be solved because the algorithms have not yet
42 been adapted to take full advantage of the architecture [9].

43 Economic MPC (EMPC) [10, 11] uses an objective function that maximizes
44 a profit function rather than targeting a set point as in standard MPC. Including
45 the profit function directly in the MPC application ensures that decisions are
46 directly driven by economic considerations. The profit function also provides
47 guidance on product scheduling, although work on EMPC up to this point
48 has focused on single products. The drawback of this approach is that EMPC
49 generally requires a short time horizon such that the longer horizon required for
50 scheduling constraints and objectives cannot be met [10]. MPC for supply chain
51 management [12] is an alternative strategy that extends the control horizon to
52 schedule product movement through a distribution network.

53 Dynamic Real-Time Optimization (DRTO) also has an economic objective
54 function but augments a steady state Real-Time Optimization (RTO) with se-
55 lect differential equations that capture the salient and dominant dynamics of
56 a process [13, 14, 15]. One drawback of RTO is that the process must be at
57 steady-state [16] to perform data reconciliation. RTO has traditionally been
58 applied to processes that do not have grade transitions but are dominated by
59 changing economics, disturbances, and slow dominant dynamics. With dynam-
60 ics included, DRTO can be solved more frequently than RTO applications and
61 can be solved during periods of transient disturbances, during startup, or during

62 shutdown periods. RTO calculations are typically performed every hour to ev-
 63 ery day while DRTO optimizes the transition between steady-state conditions.
 64 Like EMPC, DRTO does not manage multiple sequential product campaigns as
 65 a scheduler.

66 Complete integration of scheduling and control requires an extended pre-
 67 diction horizon to plan the production sequence as well as near-term control
 68 actions. Two integration approaches are referred to as top-down (add control
 69 and dynamics to a scheduling application) or bottom-up (add scheduling to a
 70 control algorithm) [3]. An early top-down implementation includes differential
 71 and algebraic equations in the scheduling application [17]. Another method is
 72 the scale-bridging model (SBM) in which a simplified model of process dynamics
 73 is embedded in the scheduling application [18, 19, 20]. A benefit of this method
 74 is disturbance rejection [21]. Algorithms include Benders’ decomposition [22]
 75 for problems that have a large-scale structured form and Dinkelbach’s algorithm
 76 [23] for non-convex problems that require global optimization methods. Applica-
 77 tions of combined scheduling and control include batch processes [5, 24], polymer
 78 reactors [25], parallel Continuously Stirred Tank Reactors (CSTRs) [26], and an
 79 electrical grid that responds to current and future price signals [27].

80 Variable electrical pricing incentivizes reduced consumption during peak
 81 hours [28]. It is desirable to match generation to consumption, but the adop-
 82 tion of more renewable energy requires producers and consumers to respond
 83 to price signals [29, 30, 31]. Energy producers may expose consumers to time-
 84 of-day pricing to discourage consumption during peak hours [32]. Scheduling
 85 operation of chemical processing [33, 34], oil refining [35], and air separation
 86 [36] are some examples of industrial units that can shed electrical load during
 87 peak hours, typically in the middle of the day. Many cooling-limited processes
 88 also operate more efficiently at night [34]. Periodic constraints can be used to
 89 optimize a typical daily cycle.

90 Prior work in scheduling and control integration has been centered around
 91 slot-based, continuous-time scheduling formulations. The benefit of discrete-
 92 time formulation has been shown [34]. However, the non-linear discrete-time

93 formulation proved computationally difficult. The purpose of this work is to
 94 restrict the dynamic model to linear form while capturing benefits of the inte-
 95 gration of scheduling and control. There is a large installed base of advanced
 96 controls that utilize linear models [1]. A unique aspect of this work is a time-
 97 scaling algorithm that adjusts the linear dynamic model based on residence
 98 time calculations with a theoretical foundation for first-order systems. The
 99 time-scaling approximation is applied to higher order, finite impulse response
 100 models that are common in industrial practice. These linear models are used in
 101 the combined scheduling and control application.

102 2. Time-Scaling with First-Order Systems

103 It is well known that linear MPC performance degrades with changes in the
 104 actual process time constant or gain [37]. This effect has been quantified for
 105 MPC where there is model mismatch in the time constant or gain of a first
 106 order system. A simple example is where the actual system is described by a
 107 single differential equation as $\tau_p \frac{dy}{dt} = -y + K_p u$ with a process time constant
 108 of $\tau_p = 1$ and a process gain of $K_p = 1$. An MPC controller with objective
 109 $\sum_{i=1}^{20} |y_i - 5|$ drives the response from a set point of 0 to 5. The controller
 110 model is similar to the process but with variable model time constant of τ_m and
 111 gain K_m in the equation $\tau_m \frac{dy}{dt} = -y + K_m u$. Common industrial practice is that
 112 acceptable MPC performance can be achieved with gain mismatch less than 30%
 113 ($0.7 \leq K_m \leq 1.3$) and time constant mismatch less than 50% ($0.5 \leq \tau_m \leq 1.5$)
 114 [37]. The dominant time constant for many industrial processes is characterized
 115 by the volume (V) divided by the volumetric flowrate (q) as $\tau_p = V/q$. The
 116 explicit solution to the first order equation is given by Equation 1.

$$y[k+1] = \exp\left(\frac{-\Delta t}{\tau_p}\right) y[k] + \left(1 - \exp\left(\frac{-\Delta t}{\tau_p}\right)\right) K_p u[k] \quad (1)$$

117 where y is the output, u is the input, k is the discrete time step, and t is the
 118 time. The integrated sum of absolute errors is computed for combinations of
 119 K_m and τ_m , each between 0.1 and 5.0. The 3D contour plot shows the control

120 performance over the range of time constant and gain mismatch (see Figure
 121 1a). A mismatch in the gain (x-axis) and time constant (y-axis) are plotted
 122 versus the error. The vertical axis (z-axis) is the integrated absolute value of
 123 the objective function for a set point change from 0 to 5. A lower sum of absolute
 124 errors equates to better control performance with a minimum at $K_m = 1$ and
 125 $\tau_m = 1$ (no model mismatch) as shown in Figure 1b.

Figure 1: Performance degradation of MPC with model mismatch

126 Especially poor performance occurs when the model has a higher time-
 127 constant (slower) than the actual process. The model in MPC predicts that
 128 changes happen slower than are actually the case, leading to a controller that is
 129 more aggressive. This aggressiveness translates into overshoot of the set point
 130 or even instability. Likewise, a model with a lower gain than the actual process
 131 also exhibits poor control performance. The model predicts that larger changes
 132 in the Manipulated Variable (MV) are required to drive the process to the new
 133 set point. In reality, a smaller adjustment is required and the over-reaction
 134 of the controller leads to overshoot and possibly instability. A contour plot of
 135 the performance profile gives insight on the performance as shown in Figure
 136 2a. Figure 2b shows the performance with the time-scaled model. The parallel
 137 contour lines show that there is no performance degradation of the controller
 138 when τ_m changes such as a production rate decrease or increase. The abil-

ity of the MPC to function over all production rates is required for processes that respond to utility price or product demand signals. This simple example shows the increased effectiveness over a wider range of operating conditions with time-scaling while still preserving the linear model.

Figure 2: Contour plot of performance degradation of MPC. An objective below 7 is acceptable, between 7-30 is marginal, and above 30 (red line) is poor performance.

This result nearly agrees with industry observations, shown with dashed box in Figure 2. Another feature of this result is that the combination of high mismatch in time-constant (τ_m) and low mismatch in gain (K_m) combine to form a region of poor control performance. Acceptable or marginal performance is also possible if both τ_m and K_m are both too high or too low. If there is low mismatch in time-constant (τ_m) and high mismatch in gain (K_m), the controller degradation is manifest as sluggishness and only incremental moves in the MV but not instability.

The time scaling approach adjusts either the controller cycle time or the discrete model time step based on the change in unit throughput q relative to the nominal throughput $\bar{q}$. $\bar{\tau}_p$ is the nominal time constant associated with $\bar{q}$. The modified process time constant is $\tau_p = q \times (\bar{\tau}_p/\bar{q})$ which now has a linear relationship to q . If the process model is not easily adjusted, the cycle time Δt of the controller is adjusted to $\Delta t \times (q/\bar{q})$ to compensate for the changing process dynamics. For first-order systems, this gives an exact representation of

the nonlinear dynamics without modifying the original linear model.

3. Selective Time-Scaling

Multi-variate and higher-order systems may have certain MV to CV relationships that are known to scale with changing unit throughput while others are invariant to throughput changes. Prior work has focused on decomposition of fast and slow dynamics [38] or variable time-delay of measurements [39, 40]. For systems with multiple MVs and CVs, only the relationships that are sensitive to throughput are scaled. These can be identified with a dynamic process simulator or else by repeating plant identification tests at low and high production rates. A method to scale higher order systems is to transform the linear time-invariant (LTI) model into discrete form. In discrete form, the sampling time is scaled by $(\bar{q}/q)$ and resampled to preserve the overall model sampling time. As an example of this time scaling approach, consider the 7th order system given by Equation 2 as a transfer function in terms of Laplace variable s .

$$G(s) = \frac{CV(s)}{MV(s)} = \frac{1.5}{(s^2 + 0.6s + 1)(0.5s + 1)^5} \quad (2)$$

Suppose that the dynamics of this system depend on the production rate and that the feed rate to the unit is reduced to half of the rate where the model is originally identified. When a time-scaling transformation of $q/\bar{q} = 2$ is applied, the new transfer function is also a 7th order system but with shifted dynamics. The steady state gain of the transfer function is preserved with this method of dynamic transformation. The resulting transfer function is Equation 3.

$$G(s) = \frac{CV(s)}{MV(s)} = \frac{1.5}{(4s^7 + 21.2s^6 + 47s^5 + 57s^4 + 42s^3 + 20s^2 + 6.2s + 1)} \quad (3)$$

The continuous transfer function is first converted to discrete form with a sufficiently small sampling time. For this case, a sampling time of 0.5 sec is chosen for the continuous to discrete transformation. The discrete model sampling time is set to $2 \times 0.5 \text{ sec} = 1.0 \text{ sec}$ based on the time-scaling factor

Figure 3: Time-scaling of a 7^{th} order system when the feed rate is reduced to half.

and then the model is resampled to 0.5 *sec* to be consistent with other unscaled MV/CV models. Continuous to discrete transformations and discrete model resampling for LTI models are standard methods [41] and are not repeated here for the sake of brevity. A graphical demonstration of this method is shown in Figure 3.

4. Scheduling and Control Formulation

An innovation of this work is to combine scheduling and control with linear models and quadratic objective functions for fast solution with Quadratic Programming (QP) [42] or Nonlinear Programming (NLP) solvers. There are multiple methods for formulating tiered price structures. The focus of this work is on creating mathematical expressions that have continuous first and second derivatives and fit within the QP or a QP with Quadratic Constraint (QPQC) framework. In contrast, most modern scheduling applications utilize integer variables, often as binary decision variables. Including integers requires MILP or MINLP solvers, which are significantly slower and more complex.

197 4.1. MPCC Steps for Product Pricing

198 The method uses a continuous formulation to logical decisions. It uses a
 199 Mathematical Programs with Complementarity Constraints (MPCC) formula-
 200 tion to avoid binary variables that would otherwise accommodate tiered pricing
 201 structures [43]. This formulation uses a step function MPCC, using constraints
 202 $v_0 y = 0$ and $v_1(1 - y) = 0$. v_0 and v_1 are positive slack variables. The com-
 203 plementarity constraints force variables to their bounds – resulting in y being a
 204 binary variable at its bounds $[0, 1]$.

205 This condition can be difficult for solvers to find a solution so the condition is
 206 typically either solved as an equivalent inequality ($v_0 y \leq 0$), a relaxed inequality
 207 ($v_0 y \leq \epsilon$), or included in the objective function ($\min v_0 y$) [44]. The step function
 208 MPCC that turns y from 0 to 1 at switching point x_p is shown in Equation 4a-4d.

$$\min_{v_0, v_1, y} v_0 y + v_1 (1 - y) \quad (4a)$$

$$x - x_p = v_1 - v_0 \quad (4b)$$

$$v_1, v_0 \geq 0 \quad (4c)$$

$$0 \leq y \leq 1 \quad (4d)$$

212
 213 To preserve the QP structure, the complementarity constraints are included
 214 in the objective function. If the complementarity constraints are included as
 215 inequalities a QPQC or NLP solver must be used. With sufficient weighting, the
 216 complementarity constraints in the objective function are zero at a final optimal
 217 solution but not necessarily along the search path to the solution. Being zero at
 218 the solution, the complementarity constraints do not influence other objective
 219 terms such as minimizing energy consumption or maximizing profit. The MPCC
 220 switching conditions are combined to create a tiered product pricing structure
 221 as shown in Figure 4.

222 Each product has a different value and potentially a different width of spec-
 223 ification limits. The positive and negative step functions at different switching

Figure 4: Individual MPCC step functions are combined to create a continuous differentiable expression of switching conditions.

224 points are combined with pricing information to create an objective function
 225 with multiple products. The individual steps are shown in the upper subplot of
 226 Figure 4 while the summation of all steps is shown in the lower subplot. Product
 227 *A* ranges from 0 to 1 and has a price of 1 per unit production. Product *B* ranges
 228 from 2 to 3 and has a price of 2 per unit production. Product *C* ranges from 2 to
 229 3 and has the highest price of 3 per unit production. The facility has a capacity
 230 of two units of production per hour and the minimum amount of production for
 231 each product over a 7 hour time window is 2 units of *A*, 5 units of *B*, and 3
 232 units of *C*. Because *C* is the most valuable product, any spare capacity should
 233 favor the production of *C*. In switching between products, a schedule should
 234 account for transition material between grades that does not have value. The
 235 speed of a transition is limited by the maximum move rate of the Manipulated
 236 Variable (*MV*) of 1.6 per hour and the dynamics of the process. The dynamics
 237 of the process are simply a linear first-order system as $\tau \frac{d(CV)}{dt} = -CV + MV$
 238 with a time constant τ of 1.0.

239 The grade-specific objective function with a quadratic objective, linear equa-
 240 tion, and simple inequality constraints is added to the process model to opti-
 241 mize the timing of grade transition switches. A complete statement of the QP

242 optimization problem is shown in Appendix A. The series of three products
 243 demonstrates a simple combined control and scheduling problem as shown in
 244 Figures 5 and 6. The cases have different initial conditions and constraints but
 245 the same underlying model. The first case has an initial condition for CV of
 246 0.0 at the lower specification limit for product A while the second case starts at
 247 CV of 4.5.

Figure 5: The control and scheduling optimization are combined to determine optimal MV
 movement along with the optimal order and quantity of production for each grade.

248 The optimizer minimizes the amount of products A and B while meeting the
 249 minimum requirements before transitioning to the next grade. This allows the
 250 schedule to favor the production of C , the most profitable product. By minimiz-
 251 ing the amount of products A and B , the scheduler creates a plan that produces
 252 an extra unit of product C . The combined controller and scheduler anticipates
 253 grade transitions by shifting the production specification to the upper limit to
 254 minimize the transition time to the next grade. This is apparent at time 1.0 hr
 255 and 4.2 hr where the product is already transitioning to the new grade just
 256 as the minimum required amount for products A and B are produced. The
 257 combined scheduler and controller adjusts both the control actions as well as
 258 the order in which the products are produced. In the next example, the initial
 259 condition is shifted to a different starting location to demonstrate this feature

260 of the approach.

261 The computational time is an important factor for control problems where
262 the algorithm must return a solution within the cycle time necessary to rejected
263 disturbances and maintain process stability. The fully discretized combined
264 scheduling and control problem with 3 products and discrete time points has
265 2730 variables, 1820 equations, and 910 degrees of freedom. The problem is
266 solved on a Dell R815 server with an AMD Opteron 6276 Processor and 64
267 GB of RAM. The problem requires 8.6 s to converge with the APOPT solver
268 (version 1.0) or 4.0 s with the IPOPT solver (version 3.10). MPC commonly
269 uses a warm-start from a prior solution to improve efficiency. With a warm-start
270 from the prior time-step, the optimizer requires 0.5 s with APOPT and 3.0 s
271 with IPOPT. Active-set solvers (such as APOPT) and interior point solvers
272 (such as IPOPT) are both effective for large-scale MPC applications although
273 interior point solvers have better performance as degrees of freedom increase [7].

274 4.2. *Dynamic Cyclic Schedule*

275 A common method to optimize a schedule in current practice is to place
276 products on a fixed grade wheel where each product is visited sequentially in a
277 rotation. The cyclic schedule visits all grades in a forward and then a reverse
278 order to end up at the original grade and begin the cycle again. If there is a
279 sudden demand for a particular grade out of sequence, the product wheel is still
280 typically traversed in the grade wheel order but there may be a minimal amount
281 of the less desirable grades in favor of the desired grade production. In some
282 processes, such as polyolefin production, there are multiple versions of the grade
283 wheel. One version of the grade wheel may include only commodity products
284 while other wheels or sub-wheels may be a more complex cycles that include
285 less frequently produced products.

286 The contribution of this work is the discrete time, extended controller and
287 scheduler that is also able to produce a cyclic schedule. However, this cyclic
288 schedule is not fixed but adjusts the sequence of products automatically when
289 updated economic or constraint information is available. The schedule and

control action may update every controller cycle (e.g. every minute). Some constraints for scheduling are periodic boundary constraints where the final condition must be equal to the initial condition, contracted quantities that must be produced by a certain date or time, particular equipment limitation, or time-of-day transition constraints. An example of a time-of-day constraint is that certain grade transitions need start-up or shut-down of auxiliary equipment. A constraint may be that the grade transition should happen only during a weekday day-time shift where there is adequate operator support.

The prior example problem is augmented with intermediate production targets and a periodic constraint. The scheduler and controller, shown in Figure 6 produces an optimized schedule and control actions. It is a dynamic rather than a static grade wheel because the order of product production and quantity is re-optimized every cycle of the controller. The product order or quantity may change based on changing customer demand, price signals for electricity or feed costs, or disturbances that drive the system to a different state.

Figure 6: Optimized schedule with periodic condition, intermediate production targets, and final production targets. The schedule and control actions adjust to meet constraints and maximize profit (product C).

The optimized solution meets constraints as well as maximizes the production of product C , the highest value product. The intermediate constraints

307 originate from contracted delivery times and storage capacity of a particular
 308 product. In this case, the storage capacity of all products is less than 5 units
 309 of production. This requires two deliveries of product B that are scheduled at
 310 two equally spaced intervals of 5 hrs. The production of product C exceeds
 311 the required delivery amount because it is the highest value product. Although
 312 the initial condition is at product C , the controller immediately targets product
 313 B to meet the required delivery of 5 units of production at 5 hrs. Without
 314 the periodic constraint, production of product C would be maximized before
 315 transitioning because the scheduler evaluates the alternative that a transition
 316 back to product C results in lost profit potential. However, with the required
 317 transition back to product C , the scheduler puts excess production of product
 318 C at the end.

319 While this method is capable of producing cyclic schedules, the optimizer
 320 should begin from current conditions rather than steady-state product condi-
 321 tions to fully integrate control and scheduling. Cyclic schedules combined with
 322 online control may lead back to off-spec conditions because of disturbances or
 323 because the controller is in a transition. Instead, this method is better suited
 324 to a different set of constraints – production amounts and due dates. These
 325 constraints give more freedom to the optimizer so the economic objective will
 326 improve or be equal to the solution with periodic constraints.

327 As with adding any constraint, there is potential to make the problem in-
 328 feasible. Multi-objective optimization statements, such as those used to refine
 329 a dynamic grade wheel sequence, can also be posed with a rank-ordered set of
 330 constraints with an explicit prioritization of objectives. The ℓ_1 -norm dead-band
 331 formulation is discussed in more detail in [7] and related to combined schedul-
 332 ing and control production targets in Section 4.3. Posing the constraints as
 333 multi-objective penalties versus hard constraints allows the problem to remain
 334 feasible yet still meet the most important objectives in order of priority.

335 4.3. Acceptable Range of Production Quantity

336 One drawback to the prior examples is that all spare production capacity is
 337 typically placed on the highest value product. Over-production of any product
 338 can have the effect of lowering the selling price because of supply and demand
 339 market forces. In scheduling, there is often a range of production quantity that
 340 is acceptable instead of just a single hard limit. To accommodate this, the
 341 scheduling and control algorithm can use an ℓ_1 -norm objective function to give
 342 a target region for the production quantity, rather than one specific hard limit.
 343 Equation 5 shows a generalized ℓ_1 -norm control formulation used in this work.

$$\begin{aligned}
 \min_{x, CV, MV} \quad & \Phi = w_{hi}^T e_{hi} + w_{lo}^T e_{lo} + x^T c_x + MV^T c_{MV} + \Delta MV^T c_{\Delta MV} \\
 \text{s.t.} \quad & 0 = f\left(\frac{dx}{dt}, x, \frac{dCV}{dt}, CV, MV\right) \\
 & e_{hi} \geq x - d_{hi} \\
 & e_{lo} \geq d_{lo} - x
 \end{aligned} \tag{5}$$

344 In this formulation, Φ is the objective function, x is the production quantity
 345 per grade. Parameters w_{lo} and w_{hi} are penalty matrices for solutions outside
 346 of the production target region. The slack variable e_{lo} and e_{hi} define the error
 347 of the dead-band low and high limits. Parameters c_x , c_{MV} , and $c_{\Delta MV}$ are cost
 348 vectors for the production quantity (positive values minimize production within
 349 region, negative values maximize production within region), the MVs (positive
 350 values minimize MV quantities such as energy use, negative values maximize
 351 MV quantity such as pump speed correlated to higher efficiency), and change
 352 of MVs, respectively. The function f is an open-equation set of equations as
 353 functions of x , CV , MV , and time derivatives of x and CV . The demand
 354 targets d_{lo} and d_{hi} define lower and upper target limits for production.

355 This range formulation is not used in this work but is presented to demon-
 356 strate one of many ways that this problem structure can be expanded to meet
 357 various scheduling needs.

358 5. Application: Continuously Stirred Tank Reactor

359 A continuously stirred tank reactor (CSTR) is a common benchmark used
360 in nonlinear model predictive control and scheduling applications [34, 3, 16].
361 This nonlinear application is used to demonstrate the strength of the approach
362 to time-scale based on throughput and combined scheduling & control.

363 The linear time-scaled model changes dynamics based on reactor flow rate,
364 allowing linear MPC to be used instead of nonlinear MPC. The multi-product
365 scheduling objective is used instead of a simple target tracking to combine the
366 scheduling and control into one application. Rapid convergence is ensured with a
367 linear model and quadratic objective because the problem is convex and because
368 QP solvers are efficient for large-scale systems.

369 The CSTR application is highly nonlinear because of an exothermic reaction
370 that has the potential to cause rapid reaction of stored reactant and thereby
371 cause a temperature run-away. The CSTR shares characteristics of many in-
372 dustrial processes such as polymer reactors or many refining processes but with
373 much simpler mathematics that are amenable to demonstrating a new approach
374 for control and scheduling. The liquid full reactor is used to convert compounds
375 $A \Rightarrow B$ with constant liquid density (ρ) and heat capacity (C_p) as shown in
376 Figure 7.

377 The reaction kinetics are first order and irreversible. Reaction of A to B is
378 exothermic with the potential for temperature run-away because of the exponen-
379 tial dependence of reaction rate on temperature, typical of an Arrhenius form
380 for reaction rates. The reactor is well-mixed with reactor concentration and
381 temperature equally distributed and also equal to the outlet measured values.
382 The reactor temperature is regulated with a cooling jacket liquid temperature,
383 T_c . The cooling jacket temperature is normally regulated by adjusting the rate
384 of cooling or the coolant flow rate but in this model the jacket temperature
385 is assumed to be controlled directly and the dynamics are approximated by a
386 maximum rate of change.

387 The dynamics of the CSTR are dictated by a species and energy balance as

Figure 7: Diagram of the well-mixed and liquid-full CSTR. The $A \Rightarrow B$ reaction is exothermic and controlled by a cooling jacket fluid.

shown in Equations 6-7 and in Figure 8.

$$V \frac{dC_A}{dt} = q(C_{A0} - C_A) - k_0 V e^{\frac{-E_A}{RT}} C_A \quad (6)$$

$$\rho C_p V \frac{dT}{dt} = q\rho C_p(T_f - T) - k_0 V e^{\frac{-E_A}{RT}} C_A \Delta H_r - UA(T - T_c) \quad (7)$$

where V is the volume of the reactor, C_A is the concentration of reactant A , q is the volumetric flowrate, C_{A0} is the inlet concentration of reactant A . The energy balance includes terms UA as an overall heat transfer coefficient times the tank surface area, C_p as the reactor fluid heat capacity, ρ as the fluid density, T_f as the temperature of the feed stream, T as the temperature of reactor, and T_c as the temperature of cooling jacket fluid. Terms related to the reaction include ΔH_r as the heat of reaction, E_A as the activation energy, R as the universal gas constant, and k_0 as the pre-exponential factor. Table 1 lists the CSTR parameters and the associated values.

A regression is shown with varying orders for an Output Error (OE) time-series model in Figure 8. Second and third order models have nearly the same fit to the nonlinear regression while a first order model is insufficient in capturing

Table 1: Reactor Initial Conditions and Parameter Values

States	Description	Initial Condition
C_A	Concentration of reactant A	$0.1 \frac{mol}{L}$
C_B	Concentration of product B	$0.9 \frac{mol}{L}$
T	Reactor temperature	386.82 K
Manipulated Variables	Description	Initial Value
T_c	Cooling jacket temperature	300 K
Parameters	Description	Value
q	Volumetric flowrate	$12 \text{ m}^3/hr$
V	Tank volume	$40m^3$
C_{A0}	Feed concentration of reactant A	$1 \frac{mol}{L}$
UA	Overall heat transfer coefficient	$5000 \frac{W}{K}$
C_p	Heat capacity of reactor fluid	$0.239 \frac{J}{kg \text{ K}}$
ρ	Density of reactor fluid	$1000 \frac{kg}{m^3}$
T_f	Feed temperature	350 K
ΔH_r	Heat of reaction (exothermic)	$-11.95 \frac{MJ}{mol}$
k_0	Pre-exponential factor, rate constant	$1.8e10 \frac{1}{hr}$
E_A/R	Activation energy divided by R	$8750K$

the process dynamics. A second simulation is performed with the production rate reduced from $12 \text{ m}^3/hr$ to $6 \text{ m}^3/hr$.

The concentration response of the reactor at half production rate is shown in the bottom subplot of Figure 8 with the second order time-scaled model that originally fit with simulated data from the full production rate simulation. The time-scaled approach is effective at capturing the essential process dynamics without re-fitting a process model at low rates.

One reactor makes multiple products by varying the concentrations of A and B in the reactor. The cooling jacket temperature T_c is the manipulated variable in this optimization. The production rate of the reactor changes throughout a typical 24-hour period because of time-of-day pricing that necessitates a cut-

Figure 8: Step tests in the jacket cooling and linear model regression of the step response.

back of production during peak energy prices and when cooling capacity is limited. The production rate is modified by adjusting the total flow through the reactor (q) between half-rates at $6 \frac{m^3}{hr}$ and full-rates at $12 \frac{m^3}{hr}$.

There is demand for three products with quantities that must be met in the schedule over a 48-hour horizon. The product descriptions and quantities are shown in Table 2.

Table 2: Product Summary with Demand and Price

Product	C_A (mol/L)	Demand (m^3)	Price (\$/ m^3)
P_1	0.12 ± 0.01	120	9
P_2	0.25 ± 0.01	130	11
P_3	0.35 ± 0.01	150	6

The most valuable is product P_2 while the least valuable product is P_3 . Although P_3 has the lowest price, it also has the highest required quantity. Spare capacity in the production facility favors product P_2 . A potential drawback to always switching to P_2 at the end of a campaign is that there is lost material

423 during the transition back to P_2 . An improved strategy is to make excess P_2
 424 when the schedule requires it to meet a minimum target demand instead of
 425 transitioning back to P_2 near the end of the time period. The combined control
 426 and scheduling solution is shown in Figure 9 over a 48 hour time period with 6
 427 minute time intervals. The problem is discretized with orthogonal collocation
 428 on finite elements. Each 6 minute segment is integrated with Radau quadrature.
 429 The resulting QP or QPQC problem is solved with a nonlinear programming
 430 solver with a simultaneous solution of the objective and equations. If specific
 431 control action is needed at more frequent intervals, the first steps of the horizon
 432 could be adjusted to meet a required controller cycle time. This would develop
 433 a near-term move plan and simultaneously solve the scheduling optimization
 434 problem with one application. The feed flow rate is decreased to half each
 435 day between the hours of 08:00 and 18:00 as is done with some energy intensive
 436 processes that exploit time-of-day electricity pricing. The addition of production
 437 rate as a decision variable and the associated cooling constraints is outside the
 438 scope of this work because the model becomes nonlinear. The simultaneous
 439 control and scheduling of production rate and product grade sequence is the
 440 topic of a future publication (see [34] for preliminary results). The top sub-
 441 plot is the sequence of control moves to drive the system to produce on-spec
 442 products and transition between products. The middle sub-plot shows the grade
 443 specifications and the concentration in the reactor. The bottom sub-plot is the
 444 total production of each grade with the minimum required as indicated by the
 445 circle markers at hour 48. The production rate is non-zero during transition
 446 periods because the total rate includes production of off-spec as well as on-spec
 447 grade material.

448 The control influences the scheduling solution and the scheduling solution
 449 gives the controller target values. The controller adjusts the jacket temperature
 450 (T_c) to minimize the transition time between grade specifications and remain
 451 within the grade limits. The controller response improves with knowledge of the
 452 scheduling targets because pro-active pre-transition movement shows that the
 453 product specification are pushed to an upper limit right before the transition

Figure 9: Combined control and schedule optimization results.

454 begins. One factor that affects the schedule is the speed of the transition from
 455 one product to another. The control dynamics are due to limitations in the
 456 manipulated variable movement and the process dynamics affecting the speed
 457 of attaining concentration range. The speed of the control response is factored
 458 into the schedule as lost production time when transition (off-spec) material is
 459 produced. Blending of transition material is one strategy to dilute the off-test
 460 material in prime products. This strategy is not considered in this approach
 461 but could be included as a constraint on the amount of reblend fraction that is
 462 allowed in the final product.

463 The scheduling profit function is an application and adaptation of Equations
 464 4a-4d. Figure 10 displays the slack and step function for each of the product
 465 limits along with the overall profit function.

466 The slack variables and complementarity conditions combine to create discrete
 467 steps with a function that has continuous first and second derivatives.
 468 For this problem, the complementarity constraints were included as constraints
 469 and in the objective function to assist the optimizer and ensure binary decision

Figure 10: Profit function and individual step functions for each product.

variables. The transition time to each product is not specified beforehand but is a result of the optimization solver finding a sequence of grade transitions that maximize overall profit. The individual steps of Figure 10 occur when one of the product grade limits is crossed. One of each of the slack variables for each step is non-zero before or after the step. The slack variables guide the solver with a continuous form of a discrete grade switching function. The overall solution is intuitive because the optimizer produces excess product P_2 (highest volumetric price) but meets only the minimum production quantities for the lower value products (P_1 and P_3).

A weakness of this method is that the CSTR is nonlinear but the solution is computed with a linearized model. Linearization neglects features of the process that may be optimized if a suitable process model more accurately represented

the physical process. A key contribution of this work is that the solution to the combined control and scheduling problem is relatively computationally inexpensive in comparison to a full nonlinear solution. In this case, the linearized model with time-scaling has a total of 22,048 variables and 16,640 equations and is solved on a Dell R815 with an AMD Opteron 6276 Processor and 64 GB of RAM. After initialization, the problem requires 23.7 s to converge with the IPOPT solver. This is representative of the cycle time of the application as it repeatedly solves to reject disturbances and as new objective information or demand constraint information is available. This speed, coupled with the inclusion of a process model sufficient for control, allows this formulation to be utilized for on-line control, on top of providing an advanced schedule. This is the epitome of combining scheduling and control – a fully unified optimization that can replace both layers.

A nonlinear version of this application is future work that will be reported in a subsequent publication. A key difference with the full nonlinear solution is that the solution in this work is several orders of magnitude faster because of the quadratic objective and linear time-scaled model. Although combined scheduling and control with linear models or feedback linearization does not always accurately predict a highly nonlinear system, the linearized solution is a valuable starting point to initialize a nonlinear solution. Also, many processes are not highly nonlinear and this approach is likely suitable for systems that are already controlled with linear MPC.

6. Conclusion

A combined scheduling and control application is enabled by an MPCC objective function, discrete-time, and linear time-scaling of process dynamics based on production rate changes. The objective of this work is to extend traditional linear MPC applications with a scheduling objective that allows for rapid convergence for real-time applications. One drawback of this work is that nonlinearities are not included in the application. These nonlinearities are the subject

of future work. The method is tested on a CSTR application that includes three grades over a 48 hour time horizon with 6 minute time intervals. The embedded controller simulates realistic transition times between each of the products. The scheduling objective determines the order and quantity of production at each grade even with half-rate reduction during peak electricity demand. The formulation is sufficiently fast enough, and includes enough process dynamics, to be utilized in on-line control. This presents a fully unified optimization that fulfills the roles of, and can replace, both control and scheduling for a comparable system. Although the method is demonstrated on the CSTR application, this formulation can be applied to other systems by replacing the model, pricing structure, and constraints of the scheduler.

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Appendix A. Combined Scheduling and Control Example

The following APMonitor model and Python script detail the variables, equations, and commands necessary to reproduce the combined scheduling and control presented in Section 4.1. The application uses two elements including the model file (schedule.apm) and a data file (schedule.csv). The data file is a list of times between 0 and 7 with time increment 0.1 and another column labeled *last* that is 0 everywhere except the end point as 1. The parameter *last* is to enforce the constraints that a certain amount of each product should be produced. All source files are available from <https://github.com/APMonitor>.

Listing 1: Constants and Parameters

```

Constants
n = 3 % products
Parameters

```

```

539 % transition points for steps
540 b[1] = 0
541 b[2] = 1
542 b[3] = 2
543 b[4] = 3
544 b[5] = 4
545 b[6] = 5
546 % step up (+) or down (-)
547 sg[1] = 1
548 sg[2] = -1
549 sg[3] = 1
550 sg[4] = -1
551 sg[5] = 1
552 sg[6] = -1
553 % magnitude of step function
554 m[1] = 1
555 m[2] = 1
556 m[3] = 2
557 m[4] = 2
558 m[5] = 3
559 m[6] = 3
560 % demand for each product
561 d[1] = 2
562 d[2] = 5
563 d[3] = 3
564 % flowrate
565 q = 2
566 % manipulated variable
567 u = 0.0 >= 0.0 <= 8.0
568 % zero everywhere except last point
569 last = 0
570

```

Listing 2: Variables and Equations

```

571 Variables
572 x = 0.0
573 % individual step functions
574 w[1:2*n] >= 0 , <= 1
575 % slack variables
576 % should be positive when x - b is negative
577 s1[1:2*n] >= 0 , <= 1000
578 % should be positive when x - b is positive
579 s2[1:2*n] >= 0 , <= 1000
580 % profit function
581 pfcn = 0 >= 0 <= 3
582 % total profit at each time step
583 profit
584 % which is product is being produced
585 prod[1:n] = 0
586 % integral of product
587 iprod[1:n] = 0
588
589 Intermediates
590 % sum steps
591 z[0] = 0
592 z[1:2*n] = z[0:2*n-1] + sg[1:2*n] * m[1:2*n] * w[1:2*n]
593
594

```

```

595 Equations
596   pfcn = z[2*n]
597   profit = pfcn * q
598   d(x)/dt = -x + u
599   prod[1] = w[1] - w[2]
600   prod[2] = w[3] - w[4]
601   prod[3] = w[5] - w[6]
602   d(iprod[1:n])/dt = prod[1:n] * q
603   x - b[1:2*n] = s2[1:2*n] - s1[1:2*n]
604   last * (iprod[1:n] - d[1:n]) >= 0
605   % include as alternative to objective version
606   %s1[1:2*n]*(w[1:2*n]) <= 0
607   %s2[1:2*n]*(1-w[1:2*n]) <= 0
608   minimize 10000 * s1[1:2*n]*(w[1:2*n])
609   minimize 10000 * s2[1:2*n]*(1-w[1:2*n])
610   maximize profit
611

```

Python Script for Combined Control and Scheduling

```

612
613 from apm import *
614
615 s = 'http://byu.apmonitor.com'
616 a = 'products'
617 # set up problem
618 apm(s,a,'clear all')
619 apm_load(s,a,'schedule.apm')
620 csv_load(s,a,'schedule.csv')
621 # create manipulated variable
622 apm_info(s,a,'MV','u')
623 apm_option(s,a,'u.status',1)
624 apm_option(s,a,'u.dcost',1.0)
625 apm_option(s,a,'u.dmax',0.16)
626 apm_option(s,a,'u.upper',8.0)
627 apm_option(s,a,'u.lower',0.0)
628 # set options
629 apm_option(s,a,'nlp.imode',6)
630 apm_option(s,a,'nlp.max-iter',200)
631 apm_option(s,a,'nlp.solver',3)
632 apm_option(s,a,'nlp.nodes',2)
633 # solve combined scheduling and control
634 output = apm(s,a,'solve')
635 print(output)
636 # retrieve solution
637 sol = apm_sol(s,a)
638

```

References

- [1] S. J. Qin, T. A. Badgwell, A survey of industrial model predictive control technology, Control Engineering Practice 11 (7) (2003) 733–764.
- [2] Z. Y. Soderstrom, T.A., J. Hedengren, Advanced Process Control in Exxon-

- 643 Mobil Chemical Company: Successes and Challenges, in: CAST Division,
644 AICHE National Meeting, Salt Lake City, UT, 2010.
- 645 [3] M. Baldea, I. Harjunkski, Integrated production scheduling and process
646 control: A systematic review, *Computers & Chemical Engineering* 71
647 (2014) 377–390. doi:10.1016/j.compchemeng.2014.09.002.
- 648 [4] T. Backx, O. Bosgra, W. Marquardt, Integration of model predictive con-
649 trol and optimization of processes, in: IFAC Symposium: Advanced Con-
650 trol of Chemical Processes, Pisa, Italy, pp. 249–260.
- 651 [5] E. Capón-García, G. Guillén-Gosálbez, A. Espuña, Integrating pro-
652 cess dynamics within batch process scheduling via mixed-integer dy-
653 namic optimization, *Chemical Engineering Science* 102 (2013) 139–150.
654 doi:10.1016/j.ces.2013.07.039.
655 URL <http://dx.doi.org/10.1016/j.ces.2013.07.039>
- 656 [6] I. Harjunkski, R. Nyström, A. Horch, Integration of scheduling and
657 control-Theory or practice?, *Computers & Chemical Engineering* 33 (2009)
658 1909–1918. doi:10.1016/j.compchemeng.2009.06.016.
- 659 [7] J. D. Hedengren, R. A. Shishavan, K. M. Powell, T. F. Edgar, Nonlinear
660 modeling, estimation and predictive control in {APMonitor}, *Computers
661 & Chemical Engineering* 70 (2014) 133 – 148, manfred Morari Special
662 Issue. doi:10.1016/j.compchemeng.2014.04.013.
663 URL [http://www.sciencedirect.com/science/article/pii/
664 S0098135414001306](http://www.sciencedirect.com/science/article/pii/S0098135414001306)
- 665 [8] F. V. Lima, M. R. Rajamani, T. A. Soderstrom, J. B. Rawlings, Covariance
666 and State Estimation of Weakly Observable Systems: Application to Poly-
667 merization Processes, *IEEE Transactions on Control Systems Technology*
668 21 (4) (2013) 1249–1257. doi:10.1109/TCST.2012.2200296.
- 669 [9] W. Ma, G. Agrawal, An integer programming framework for optimizing

- shared memory use on gpus, in: 2010 International Conference on High Performance Computing, 2010, pp. 1–10. doi:10.1109/HIPC.2010.5713187.
- [10] M. Ellis, H. Durand, P. D. Christofides, A tutorial review of economic model predictive control methods, *Journal of Process Control* 24 (8) (2014) 1156–1178. doi:10.1016/j.jprocont.2014.03.010.
URL <http://dx.doi.org/10.1016/j.jprocont.2014.03.010>
- [11] D. Angeli, R. Amrit, J. B. Rawlings, On Average Performance and Stability of Economic Model Predictive Control, *IEEE Transactions on Automatic Control* 57 (7) (2012) 1615–1626. doi:10.1109/TAC.2011.2179349.
- [12] K. Subramanian, J. B. Rawlings, C. T. Maravelias, Economic model predictive control for inventory management in supply chains, *Computers & Chemical Engineering* 64 (2014) 71–80. doi:<http://dx.doi.org/10.1016/j.compchemeng.2014.01.003>.
URL <http://www.sciencedirect.com/science/article/pii/S0098135414000052>
- [13] K. V. Pontes, I. J. Wolf, M. Embiruçu, W. Marquardt, Dynamic Real-Time Optimization of Industrial Polymerization Processes with Fast Dynamics, *Industrial & Engineering Chemistry Research* 54 (47) (2015) 11881–11893. doi:10.1021/acs.iecr.5b00909.
URL <http://pubs.acs.org/doi/10.1021/acs.iecr.5b00909>
- [14] I. Harjunkski, C. T. Maravelias, P. Bongers, P. M. Castro, S. Engell, I. E. Grossmann, J. Hooker, C. Méndez, G. Sand, J. Wassick, Scope for industrial applications of production scheduling models and solution methods, *Computers & Chemical Engineering* 62 (2014) 161–193. doi:10.1016/j.compchemeng.2013.12.001.
URL <http://dx.doi.org/10.1016/j.compchemeng.2013.12.001>
- [15] L. Biegler, X. Yang, G. Fischer, Advances in sensitivity-based nonlinear model predictive control and dynamic real-time optimization, *Journal of*

- 698 Process Control 30 (2015) 104–116. doi:10.1016/j.jprocont.2015.02.001.
 699 URL [http://linkinghub.elsevier.com/retrieve/pii/](http://linkinghub.elsevier.com/retrieve/pii/S0959152415000281)
 700 [S0959152415000281](http://linkinghub.elsevier.com/retrieve/pii/S0959152415000281)
- 701 [16] J. Kelly, J. Hedengren, A steady-state detection (SSD) algorithm to detect
 702 non-stationary drifts in processes, *Journal of Process Control* 23 (3) (2013)
 703 326–331.
- 704 [17] A. Flores-Tlacuahuac, I. E. Grossmann, Simultaneous Cyclic Scheduling
 705 and Control of a Multiproduct CSTR, *Industrial & Engineering Chemistry*
 706 *Research* 45 (20) (2006) 6698–6712. doi:10.1021/ie051293d.
 707 URL <http://pubs.acs.org/doi/abs/10.1021/ie051293d>
- 708 [18] M. Baldea, J. Du, J. Park, I. Harjunkski, Integrated production schedul-
 709 ing and model predictive control of continuous processes, *AIChE Journal*
 710 61 (12) (2015) 4179–4190. doi:10.1002/aic.14951.
 711 URL <http://doi.wiley.com/10.1002/aic.14951>
- 712 [19] J. Du, J. Park, I. Harjunkski, M. Baldea, A time scale-
 713 bridging approach for integrating production scheduling and pro-
 714 cess control, *Computers & Chemical Engineering* 79 (2015) 59–69.
 715 doi:10.1016/j.compchemeng.2015.04.026.
 716 URL [http://linkinghub.elsevier.com/retrieve/pii/](http://linkinghub.elsevier.com/retrieve/pii/S0098135415001271)
 717 [S0098135415001271](http://linkinghub.elsevier.com/retrieve/pii/S0098135415001271)
- 718 [20] M. Baldea, C. R. Touretzky, J. Park, R. C. Pattison, Handling Input Dy-
 719 namics in Integrated Scheduling and Control, in: 2016 IEEE International
 720 Conference on Automation, Quality and Testing, Robotics (AQTR), 2016,
 721 pp. 1–6.
- 722 [21] J. Zhuge, M. G. Ierapetritou, Integration of Scheduling and Control with
 723 Closed Loop Implementation, *Industrial & Engineering Chemistry Re-*
 724 *search* 51 (25) (2012) 8550–8565. doi:10.1021/ie3002364.
 725 URL <http://dx.doi.org/10.1021/ie3002364>

- [22] Y. Chu, F. You, Integration of production scheduling and dynamic optimization for multi-product CSTRs: Generalized Benders decomposition coupled with global mixed-integer fractional programming, *Computers & Chemical Engineering* 58 (2013) 315–333. doi:10.1016/j.compchemeng.2013.08.003.
- [23] Y. Chu, F. You, Integration of scheduling and control with online closed-loop implementation: Fast computational strategy and large-scale global optimization algorithm, *Computers & Chemical Engineering* 47 (2012) 248–268. doi:10.1016/j.compchemeng.2012.06.035.
URL <http://dx.doi.org/10.1016/j.compchemeng.2012.06.035>
- [24] Y. Nie, L. T. Biegler, J. M. Wassick, Integrated scheduling and dynamic optimization of batch processes using state equipment networks, *AIChE Journal* 58 (11) (2012) 3416–3432. doi:10.1002/aic.13738.
URL <http://doi.wiley.com/10.1002/aic.13738>
- [25] A. Prata, J. Oldenburg, A. Kroll, W. Marquardt, Integrated scheduling and dynamic optimization of grade transitions for a continuous polymerization reactor, *Computers & Chemical Engineering* 32 (3) (2008) 463–476. doi:10.1016/j.compchemeng.2007.03.009.
- [26] A. Flores-Tlacuahuac, I. E. Grossmann, Simultaneous scheduling and control of multiproduct continuous parallel lines, *Industrial and Engineering Chemistry Research* 49 (17) (2010) 7909–7921. doi:10.1021/ie100024p.
- [27] H. Farhangi, The Path of the Smart Grid 18, *IEEE Power & Energy Mag.*, (2010) 1828.
- [28] U S Department of Energy, Benefits of Demand Response in Electricity Markets and Recommendations for Achieving Them, Tech. Rep. February, US DOE (2006). doi:citeulike-article-id:10043893.
- [29] S. M. Safdarnejad, J. D. Hedengren, L. L. Baxter, Dynamic optimization of

- a hybrid system of energy-storing cryogenic carbon capture and a baseline power generation unit, *Applied Energy* 172 (2016) 66–79.
- [30] S. M. Safdarnejad, J. D. Hedengren, L. L. Baxter, Plant-level dynamic optimization of cryogenic carbon capture with conventional and renewable power sources, *Applied Energy* 149 (2015) 354 – 366. doi:10.1016/j.apenergy.2015.03.100.
URL <http://www.sciencedirect.com/science/article/pii/S030626191500402X>
- [31] S. Safdarnejad, L. Kennington, L. Baxter, J. Hedengren, Investigating the impact of cryogenic carbon capture on power plant performance, in: *Proceedings of the American Control Conference (ACC)*, Chicago, Illinois, 2015, pp. 5016–5021. doi:10.1109/ACC.2015.7172120.
- [32] R. Deng, Z. Yang, M.-Y. Chow, J. Chen, A Survey on Demand Response in Smart Grids: Mathematical Models and Approaches, *IEEE Transactions on Industrial Informatics* 11 (3) (2015) 1–1. doi:10.1109/TII.2015.2414719.
- [33] J. Y. Feng, A. Brown, D. O’Brien, D. J. Chmielewski, Smart grid coordination of a chemical processing plant, *Chemical Engineering Science* 136 (2015) 168–176. doi:10.1016/j.ces.2015.03.042.
- [34] L. Beal, J. Clark, M. Anderson, S. Warnick, J. Hedengren, Combined scheduling and control with diurnal constraints and costs using a discrete time formulation, in: *FOCAPO / CPC 2017, Foundations of Computer Aided Process Operations*, Chemical Process Control, 2017.
- [35] D. I. Mendoza-Serrano, D. J. Chmielewski, Demand Response for Chemical Manufacturing using Economic MPC, *Proceedings of 2013 American Control Conference (ACC)* (2013) 6655–6660.
- [36] R. Huang, E. Harinath, L. T. Biegler, Lyapunov stability of economically oriented NMPC for cyclic processes, *Journal of Process Control* 21 (4) (2011) 501–509. doi:10.1016/j.jprocont.2011.01.012.

- [37] J. D. Hedengren, A. N. Eaton, Overview of estimation methods for industrial dynamic systems, *Optimization and Engineering* 18 (1) (2017) 155–178. doi:10.1007/s11081-015-9295-9.
- [38] Y. Zhang, D. S. Naidu, H. M. Nguyen, C. Cai, Y. Zou, Time scale analysis and synthesis for model predictive control under stochastic environments, in: 2014 7th International Symposium on Resilient Control Systems (IS-RCS), 2014, pp. 1–6. doi:10.1109/ISRCS.2014.6900085.
- [39] L. Ji, J. B. Rawlings, Application of MHE to large-scale nonlinear processes with delayed lab measurements, *Computers & Chemical Engineering* 80 (2015) 63 – 72. doi:10.1016/j.compchemeng.2015.04.015.
- [40] D. Srinivasagupta, H. Schättler, B. Joseph, Time-stamped model predictive control: an algorithm for control of processes with random delays, *Computers & Chemical Engineering* 28 (8) (2004) 1337 – 1346. doi:10.1016/j.compchemeng.2003.09.027.
- [41] D. E. Seborg, D. A. Mellichamp, T. F. Edgar, F. J. Doyle III, *Process dynamics and control*, John Wiley & Sons, 2010.
- [42] Y. Wang, S. Boyd, Fast model predictive control using online optimization, *IEEE Transactions on Control Systems Technology* 18 (2) (2010) 267–278.
- [43] K. M. Powell, A. N. Eaton, J. D. Hedengren, T. F. Edgar, A continuous formulation for logical decisions in differential algebraic systems using mathematical programs with complementarity constraints, *Processes* 4 (1) (2016) 7.
- [44] B. Baumrucker, J. Renfro, L. T. Biegler, Mpec problem formulations and solution strategies with chemical engineering applications, *Computers & Chemical Engineering* 32 (12) (2008) 2903–2913.