Uncovering New Opportunities from Frequency Regulation Markets with Dynamic Optimization and Pyomo.DAE

Alexander W. Dowling[a*] and Bethany L. Nicholson[b]

[a]*Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, Indiana, 46556, USA*
[b]*Center for Computing Research, Sandia National Laboratories, Albuquerque, New Mexico, 87185, USA*
alex@dowlinglab.org

Abstract

Real-time energy pricing has caused a paradigm shift for process operations with flexibility becoming a critical driver of economics. As such, incorporating real-time pricing into planning and scheduling optimization formulations has received much attention over the past two decades (Zhang and Grossman, 2016). These formulations, however, focus on 1-hour or longer time discretizations and neglect process dynamics. Recent analysis of historical price data from the California electricity market (CAISO) reveals that a majority of economic opportunities come from fast market layers, i.e., real-time energy market and ancillary services (Dowling et al., 2017).

We present a dynamic optimization framework to quantify the revenue opportunities of chemical manufacturing systems providing frequency regulation (FR). Recent analysis of first order systems finds that slow process dynamics naturally dampen high frequency harmonics in FR signals (Dowling and Zavala, 2017). As a consequence, traditional chemical processes with long time constants may be able to provide fast flexibility without disrupting product quality, performance of downstream unit operations, etc. This study quantifies the ability of a distillation system to provide sufficient dynamic flexibility to adjust energy demands every 4 seconds in response to market signals. Using a detailed differential algebraic equation (DAE) model (Hahn and Edgar, 2002) and historic data from the Texas electricity market (ECROT), we estimate revenue opportunities for different column designs. We implement our model using the algebraic modeling language Pyomo (Hart et al., 2011) and its dynamic optimization extension Pyomo.DAE (Nicholson et al., 2017). These software packages enable rapid development of complex optimization models using high-level modelling constructs and provide flexible tools for initializing and discretizing DAE models.

Keywords: electricity markets, demand response, smart manufacturing, nonlinear programming, distillation

1. Introduction: Frequency Regulation Markets

Modern electricity infrastructures use complex hierarchical wholesale markets to coordinate generation, loads, and transmission networks. This results in temporal and spatial variations in prices set at multiple timescales (e.g., 1-hour prices in day-ahead markets, 5- to 15-minute prices in real-time markets) that directly impact large electricity producers/consumers including traditional utility companies, aggregators, and some

industrial sites. Dowling et al. (2017) and Zhang and Grossmann (2016) provide thorough background in electricity markets and emphasize emerging opportunities for industrial participants. Many recent studies focus on extending planning and scheduling formulations to account for time-sensitive energy prices.

Ancillary services, i.e., spinning/non-spinning reserves and frequency regulation capacity, are critical to provide contingency at fast timescales (minutes to seconds) and ensure grid reliability. Resources providing reserve capacity are compensated for making a commitment to either increase generation or shed load if dispatched. Often this dispatch occurs once a week or less and can provide new revenue opportunities for flexible industrial sites. Zhang et al. (2015) explore optimal scheduling strategies of reserve capacity under uncertainty for air separation units. Analysis of California market data shows that frequency regulation offers significantly greater revenue opportunities, but also requires more intimate integration with the grid (Dowling et al., 2017). Resources providing FR capacity must adjust their energy production/demands every 4 seconds in accordance with grid dispatch. As such, this market opportunity has received significantly less attention as it requires careful consideration of system dynamics. Dowling and Zavala (2017) formulated FR capacity allocation as a dynamic optimization problem,

$$\min \int_0^{t_f} \phi\big(z(t), u(t), d(t)\big) dt$$

$$\text{s.t.,} \quad \dot{z} = f(z(t), u(t), d(t))$$

$$g(z(t), y(t), d(t)) \leq 0 \tag{1}$$

$$y(t) = h(z(t))$$

$$d(t) = r_+ \beta_+(t) - r_- \beta_-(t)$$

$$0 \leq r_+, r_-$$

where $z(t)$ represents the states, $y(t)$ represents the observations, $u(t)$ represents the controls, and $d(t)$ represents the disturbances. The (non)linear functions $f(\cdot)$, $g(\cdot)$, and $h(\cdot)$ capture the system dynamics, operating restrictions, and transformation from states to observations, respectively. In this formulation, the dispatch signals coming from the grid for regulation up and down are encoded in $\beta_+(t)$ and $\beta_-(t)$, respectively, and are treated as disturbances. The economic objective is often $\phi = r_+ \pi_+ + r_- \pi_-$ where r_+ and r_- are the committed regulation up and down capacities during an hour and π_+ and π_- are the respective capacity prices. Thus, problem (1) seeks to maximize the revenue from frequency regulation capacity (i.e., maximizes the size of the disturbance) while determining a control strategy that maintains operational feasibility. This formulation is a generalization of Fares et al. (2014), which focuses exclusively on grid-scale redox flow batteries. Other emerging FR market participants include aluminium smelters (Zhang and Hug, 2014) and commercial HVAC systems (Lin et al., 2015).

2. Mathematical Models and Software Implementation

Many industrial sites have on-site utility plants that can directly participate in electricity markets. In this context, providing FR capacity requires either modulating electricity

demands of equipment such as pumps, arc furnaces, etc. (Zhang and Hug, 2014) or modulating steam production rates. Using the general formulation (1), Dowling and Zavala (2017) characterized revenue opportunities for a methanol-water distillation system providing FR by adjusting the energy input (reboiler steam flow rate). A key limitation of this analysis is that it relies on the simple two-input two-output transfer function model from Wood and Berry (1973) for a laboratory-scale system. Instead, the present work combines optimization formulation (1) with more detailed differential algebraic equation models. Thus, we seek to extend the results to industrial scale systems and explore how design decisions (e.g., holdup capacities) impact system dynamics and thus revenue opportunities. We start by considering the dynamic model from Hahn and Edgar (2002) adapted to a methanol-water separation with 8 trays:

Total condenser (tray 1): $\quad \frac{dx_1}{dt} = \frac{1}{A_{cond}} V(y_2 - x_1)$ $\hfill (2)$

Rectifying trays (i = 2, ..., 4): $\quad \frac{dx_i}{dt} = \frac{1}{A_{tray}} [L_r(x_{i-1} - x_i) - V(y_i - y_{i+1})]$ $\hfill (3)$

Feed tray (i = 5): $\quad \frac{dx_i}{dt} = \frac{1}{A_{tray}} [F x_f + L_r x_{i-1} - L_s x_i + V(y_i - y_{i+1})]$ $\hfill (4)$

Stripping trays (i = 6, ..., 9): $\quad \frac{dx_i}{dt} = \frac{1}{A_{tray}} [L_s(x_{i-1} - x_i) - V(y_i - y_{i+1})]$ $\hfill (5)$

Partial reboiler (tray 10): $\quad \frac{dx_i}{dt} = \frac{1}{A_{reb}} [L_s x_{i-1} - (F - D)x_i - V y_i]$ $\hfill (6)$

Condenser mass balance: $\quad V = L_r + D$ $\hfill (7)$

Saturated liquid feed quality: $\quad L_s = L_r + F$ $\hfill (8)$

Reflux ratio: $\quad R = \frac{L_r}{D}$ $\hfill (9)$

Constant relative volatility (i = 2, ..., 10): $\quad \alpha = \frac{y_i(1-x_i)}{(1-y_i)\,x_i}$ $\hfill (10)$

Reboiler energy balance: $\quad Q = \Delta H_{vap} V$ $\hfill (11)$

where index *i* indicates the tray, $x(t), y(t)$ are mole fractions of methanol, F and x_f are the constant feed flow rate and composition, $L_r(t)$ and $L_s(t)$ are the liquid flow rates in the rectifying and stripping sections, respectively, $V(t)$ is the vapor flow rate, $D(t)$ is the distillate product flow rate, $R(t)$ is the reflux ratio, $Q(t)$ is the reboiler duty, and ΔH_{vap} is the constant heat of vaporization (40 kJ/mol). This model assumes constant total molar holdups ($A_{cond} = 0.5$, $A_{tray} = 0.25$, $A_{reb} = 1.0$ moles), constant molar overflow, and constant relative volatility ($\alpha = 4.02$). Eqns (2) – (8) arise from mass balances, Eqn (9) is a definition, and Eqn (10) captures vapor-liquid equilibrium. Eqns (2) – (10) are from Hahn and Edgar (2002), whereas Eqn (11) was added to calculate the reboiler energy input. Similar to Dowling and Zavala (2017), we use the reboiler duty to track the regulation signal as follows:

$$Q(t) = \beta_+(t)\, r_+ - \beta_-(t)\, r_- + \bar{Q} \hfill (12)$$

where $Q(t)$ is the time-varying reboiler duty, $\beta_+(t)$ and $\beta_-(t)$ are the regulation tracking signals (input data), r_+ and r_- are the regulation capacity commitments (decision-variables) and $\bar{Q}$ is the reboiler duty offset (decision-variable). For most industrial sites, the distillation system would not be bidding by itself into the market, but instead the electricity generation of the onsite utility system would be modulated to track the FR signal. This would cause variations in the steam production flowrate, which would be

absorbed by the flexibility of several steam consumers. The present study focuses on the distillation system and does not consider dynamics of the utility plant. Thus Eqn (12) is a simplification and corresponds with an electrically heated reboiler. Using operational bounds on the distillate $0.92 \leq y_1(t) \leq 1.0$, bottoms $0.0 \leq x_{10}(t) \leq 0.02$, and reflux ratio $0.1 \leq R(t) \leq \rho$ and Eqns (2) – (12), we express the FR market participation problem in the form of (1). Unit conversions are omitted for brevity.

For each hour of data, we solve a nonlinear program (NLP) to determine the regulation capacity commitments, r_+, r_-, and optimal reflux ratio control profile, $R(t)$, that maximizes FR market revenue while satisfying path constraints (i.e., product quality bounds). Input data were obtained from the ERCOT website[1] and include the regulation capacity prices, π_+, π_-, which are set in 1-hour intervals and the regulation dispatch signals, $\beta_+(t), \beta_-(t)$, which are available in 4-second intervals. These models are implemented in Pyomo and Pyomo.DAE. Pyomo is an algebraic modeling language built on top of the Python programming language and Pyomo.DAE is an extension to Pyomo for representing and solving dynamic optimization problems. Moreover, Pyomo.DAE allows us to directly implement the derivatives and differential equations in Eqns (2) – (12), exploit DAE simulation tools for initialization, and automate the transformation of the continuous-time model into a discrete approximation. For this particular problem, we choose a backwards Euler discretization (although several other discretization schemes, including collocation over finite elements, are also natively supported in Pyomo.DAE) with a 4-second time step to match the resolution of $\beta_+(t), \beta_-(t)$. A 1-hour horizon resulted in a NLP with approximately 32,000 variables (with bounds) and equality constraints. IPOPT (Wächter and Biegler, 2006) was used to solve these problems, requiring up to 5 minutes per instance.

3. Results and Discussion

The previously described NLP was solved for each hour of March 1st, 2016 using historical market data $\pi_+, \pi_-, \beta_+(t), \beta_-(t)$ as input parameters. Figure 1 shows the time-evolution of the bottoms composition, distillate composition, and reflux ratio. For the bottoms composition and the reflux ratio, the upper bounds are active during the first 1-hour horizon.
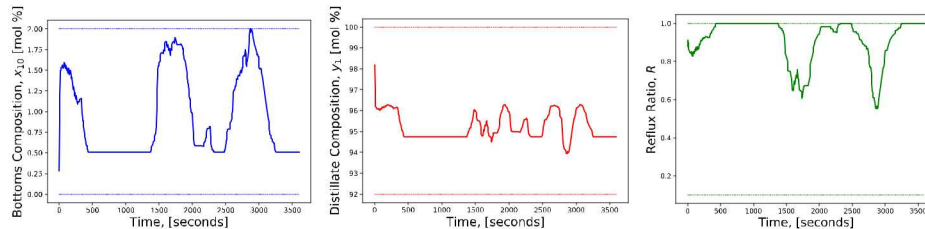

Figure 1. Composition of the bottoms (left), composition of the distillate (center), and reflux ratio (right) as a function of time with $\rho = 1$. Dashed lines indicate operational bounds.

A key advantage of model Eqn (2) – (12) and formulation (1) is the ability to explicitly connect design decisions with revenue opportunities from FR markets. Interestingly, we find that increasing the reboiler holdup A_{reb} from 1.0 moles to 10.0 moles only increases revenues by 3%. This trend makes sense as larger holdups give rise to slower system

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[1] http://www.ercot.com/mktrules/pilots/frrs

dynamics which further increases the ability to reject fast market signals. We also find that revenues are extremely sensitivity to the maximum reflux ratio ρ as shown in Figure 2. Furthermore, realizing the revenues for $\rho = 10$ require dramatic changes in the reflux ratio, which may not be acceptable to operators. This is because of the constant holdup and constant molar overflow assumptions in the system model. The vapor flow rate V and thus reboiler duty Q are tightly coupled with the reflux ratio R, and thus ρ acts as an implicit bound on Q and thus regulation capacity. Furthermore, the chosen composition operating bounds are such that the upper bound on R limits the FR capacity and not the system dynamics. Again, this explains why revenue weakly depends on A_{reb}. These insights are not available from the transfer function model previously analysed.
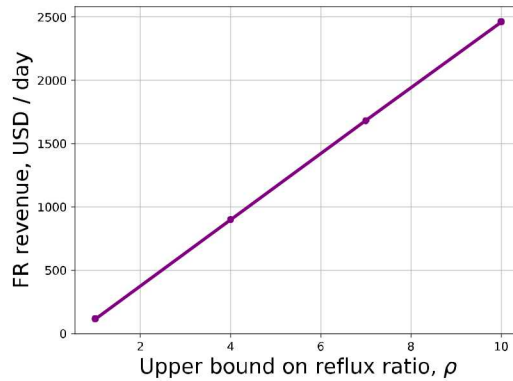

Figure 2. Sensitivity analysis of revenue with respect to the upper bound for reflux ratio (ρ). Revenue is scaled for nominal reboiler duty of 1 MW.

4. Conclusions and Future Directions

Opportunities in FR markets are emerging for chemical industrial systems. Their inherently slow dynamics filter out high-frequency disturbances from market signals. This paper expands upon a dynamic optimization framework that explicitly calculates revenue opportunities from historic market data and dynamic process models. We believe that the presented modelling and optimization tools are an essential first step to understanding and exploiting revenue opportunities ranging from $100 to $2,500 / day for a 1 MW (nominal) system. In the presented distillation case study, sensitivity analysis is used to understand how design decisions impact system dynamics and market revenues. In particular, we find that column diameter (which limits reflux ratio) is much more important than reboiler holdup capacity. Pyomo and Pyomo.DAE facilitate rapid model development, debugging, initialization, and automation of data-driven analysis, which has historically been difficult for dynamic optimization with algebraic modelling languages such as GAMS, AMPL, AIMMS, etc.

As future work, we plan to consider more detailed dynamic models with variable material holdups, such as those from López-Negrete et al (2013). We hypothesize that the current case study underestimates the flexibility and thus revenue opportunities of distillation systems because holdup capacities are fixed. We anticipate that it is possible to further increase the range of feasible energy inputs by strategically controlling holdups levels. An industrial FR capacity provider would likely exploit flexibility from several sources. We plan to investigate other equipment (e.g., pumps) as well as plant-wide coordination

schemes. Moreover, the present analysis assumes perfect information and may overestimate realistic market revenues. As future work, we plan to characterize the impact of market uncertainty on chemical manufacturing systems, and anticipate PySP, a separate Pyomo extension for stochastic programming, will be especially helpful (Watson et al, 2012). Finally, we plan to expand the case study to balance new market revenue against operating costs from more dynamic operation such as equipment wear-and-tear.

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