# DISTRIBUTED CHEMICALS AND ELECTRICITY PRODUCTION WITH REGULATED ENERGY EXCHANGE

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*Abstract*

This paper explores the optimal operation of a distributed ammonia production facility which is coupled with local renewable energy generation. The coupling of stochastic renewables with this flexible chemical process enables exchange of energy with the utility in a highly regulated and benign manner. In particular, we analyze the ability of this facility to operate economically under a market structure which explicitly limits uncertainty and variability in energy exchanged with the macrogrid. A receding horizon control approach is formulated to optimally schedule local units and ensure that production targets and regulatory requirements are satisfied. The cost of regulating this energy exchange is shown to be minimal and the variability and uncertainty of energy exchange is shown to be significantly reduced. In addition, we show that a clear tradeoff emerges between the ability to sell excess power to the utility and the ability to meet previous power commitments when increasing renewables penetration.

*Keywords*

Process integration, Distributed energy systems, Microgrid, Distributed ammonia

## Introduction

Distributed production of fuels, chemicals, and electricity close to points of demand reduces transportation costs and losses, facilitates the incorporation of dispersed renewable feedstocks (e.g. wind and solar), and makes the infrastructure more resilient to catastrophic failures or extreme weather events. However, the variability and stochasticity introduced by renewables can be challenging to mitigate. In the context of renewable electricity, end users who employ local generation (a.k.a. prosumers) typically rely on a utility company to correct any imbalance between expected and realized renewables output. This increases uncertainty for utility companies, and may require a significant increase in the reserve margins and control effort for large power plants (Brouwer et al., 2015). These externalities decrease system-wide efficiency, increase electricity generation costs, and are counterproductive from an environmental perspective.

Previous authors have investigated a variety of ways to achieve utility-friendly operation of these distributed energy systems. The simplest way to achieve utility-friendly operation is to explicitly minimize, or entirely forbid, energy exchange between the distributed system and external utility (e.g. Teleke et al., 2010; Trifkovic et al., 2014). However, these stand-alone systems are significantly more expensive to own and operate since generation and/or storage units must be over-sized to mitigate stochasticity (Zachar et al., 2015; Alipour et al., 2015). Another approach is to have prosumers actively participate in the electricity market, e.g. via bidding in the wholesale market as in Liu et al. (2016) or via iterative negotiation with the utility as in Wang et al. (2015). These approaches reduce the uncertainty in energy exchange, as real-time purchases are discouraged, but they do not explicitly address the variability introduced by renewables. Moreover, market operations, e.g. market clearing which is formulated as a

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large-scale mixed integer problem, may scale poorly with the number of active participants. Other common approaches, such as introducing peak shaving constraints (Riffonneau et al., 2011) or applying demand charges (Zhang et al., 2013), partially address the challenges related to the variability and uncertainty in the energy exchange of these prosumers, but do not approach this problem in a holistic manner.

Motivated by this, we have proposed a market/regulatory framework for prosumers which seeks to address these issues and minimize the impact on the utility company (Zachar and Daoutidis, 2016). In particular, prosumers are obligated to explicitly limit the uncertainty and variability in their residual load (i.e. the load satisfied by the utility) by providing a day-ahead commitment. In this framework, tunable market parameters can be used to regulate the amount of stochasticity each party (i.e. the prosumer and the utility) must mitigate. In our preliminary examination of this market structure, we found that meeting commitments solely with typical microgrid units (i.e. microturbines and a battery) was very expensive for prosumers. In this work, we seek to modify our approach by considering a controllable load which can enable flexibility to meet energy exchange commitments at lower opportunity cost.

In this case, obvious parallels can be drawn to the field of demand-side management (DSM). In DSM, energy intensive customers (typically large industrial customers) are offered incentives to schedule their power consumption in a utility-friendly manner. Typical DSM activities include dynamic operation of a plant in response to time-varying electricity prices or demand charges (e.g. Pattison et al., 2016), offering interruptible load capacity to offset demand uncertainty (e.g. Zhang et al., 2016), and explicit load-shaping via direct negotiation between the utility and industrial customer (e.g. Nolde and Morari, 2010). An important difference in the case of prosumers is the presence of local generation, and, in particular, local renewables which increase stochasticity in the control and scheduling problems. Some further comparison of DSM and our approach are given in the Market Structure section.

Chemical processes provide a power load which is controllable and typically contains some inherent flexibility. In particular, this work considers small scale, distributed ammonia production as the electrical load. Distributed ammonia production is an attractive process as the process features high flexibility in hydrogen and nitrogen production and the product features an inherently dispersed demand profile. In previous work, we analyzed the potential to incorporate distributed renewable-based ammonia plants into the existing supply chain, and showed that such plants can be economically competitive at a large scale depending on the market conditions and policy incentives (Allman and Daoutidis, 2016). We further concluded that to make smaller scale, distributed plants economically viable, further improvements to the economics, such as improving the operating cost through scheduling, were required. In this work, we focus on the operational aspects of such a renewable ammonia plant in concert with the proposed market structure for prosumers.

In what follows, we formally describe this proposed market structure. Then, we describe the system considered and formulate a receding horizon optimization problem for its dynamic scheduling. Next, we study the impact of the market structure on the process economics and evaluate the improvements in the residual load characteristics. Finally, we conclude with some important observations.

## Market Structure

The proposed market structure is an extension of a simple tariff structure where the rates for buying and selling power are known to the prosumer *a priori*. However, the prosumer is required to provide energy exchange commitments to the utility company for each 1-hour period over which energy exchange will be metered. These commitments must be relayed to the utility at least 24 hours before the start of the relevant time period.

During real-time operation, the utility is assumed to provide any needed balancing power, even if it results in a deviation from the established commitment. Prosumers are allowed some small deviation from the commitment value without penalty as governed by the *schedule elasticity* parameter:

$$p_v(t) = \max\big(0, p_c(t) - p_g(t) - \gamma\big) + \max\big(0, p_g(t) - p_c(t) - \gamma\big) \quad (1)$$

where $p_c$ is the commitment value, $p_g$ is the realized power exchange, $\gamma$ is the schedule elasticity, and $p_v$ is the commitment violation. Prosumers are economically penalized (i.e. fined) if this deviation is larger than the allowed schedule elasticity (i.e. if $p_v>0$).

In addition, adjacent commitments must be close in value to each other as governed by the *schedule adaptability* parameter:

$$p_c(t-1) - \delta \leq p_c(t) \leq p_c(t-1) + \delta \quad (2)$$

where $\delta$ is the schedule adaptability.

This problem is similar to industrial load shaping (e.g. Nolde and Morari, 2010). An important difference is that small deviations from the commitments are allowed (due to the difficulty of completely mitigating renewables on a local scale). Moreover, commitment values are unilaterally determined by the prosumer since direct negotiation between the utility company and a large number of prosumers is not scalable. Finally, unlike market mechanisms like demand charges, the proposed market structure places explicit limits on the uncertainty and variability in the energy exchange profile. Further discussion of this proposed market structure can be found in Zachar and Daoutidis (2016).

## Model Formulation

A distributed ammonia production facility is considered based on Reese et al. (2016). It consists of an air separation unit, electrolyzers, an ammonia generation unit (based on the Haber-Bosch process), and chemical inventory storage units. Power is generated locally by wind turbines. Any imbalance is rectified via power exchange with the

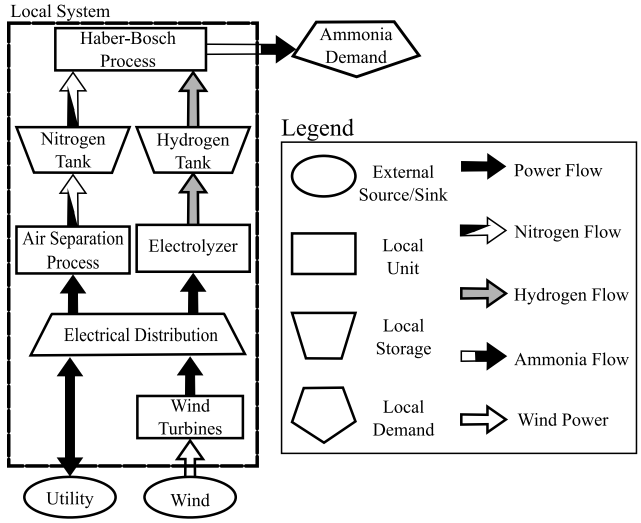


*Figure 1 - Mass and energy flow in the system.*

macrogrid. The flow of energy and materials in the system considered is shown Figure 1.

During operation, the goal is to minimize the cost of meeting local ammonia demand, avoid violation of previously established energy exchange commitments, and optimally make new commitments. Operating cost is minimized over a 48 hour receding horizon, optimized repeatedly every hour over the course of a year:

$$Op = \sum_{t=1}^{48} \Big( \zeta_b p_b(t) - \zeta_s p_s(t) + \zeta_{el} \dot{m}_{H_2}(t) + \zeta_{psa} \dot{m}_{N_2}(t) + \zeta_{su} n_{su}(t) + \zeta_{up} \left( \tau - \dot{m}_{NH_3}(t) \right) + \zeta_v p_v \Big) + \zeta_N (m_{N_2}(0) - m_{N_2}(48)) + \zeta_H (m_{H_2}(0) - m_{H_2}(48)) \tag{3}$$

Equation (3) shows the objective function, which is the sum of the cost of buying (or selling back) power, operating costs for the electrolyzer and pressure swing adsorption (PSA) units, costs for starting up electrolyzers, penalty costs for underproducing ammonia, penalty costs for violating previously made power commitments, and penalty costs for using hydrogen or nitrogen from storage. Symbol nomenclature is shown in Table 1. Realized costs are calculated based on the implemented decisions determined by the first time period results in each iteration, excluding the penalties related to using gas from storage and underproducing ammonia.

During operation, the set point of the ammonia generation process is changed only every 12 hours. At the end of each day, the target ammonia production level is adjusted based on the amount of realized production over the previous day. Production below this target value is penalized. The rate of ammonia generation can vary between 75% and 110% of the nominal production rate.

All other units are dispatched on an hourly basis. An integer number of 2 MW electrolyzers are used which must operate between 30% and 100% capacity when turned on. The PSA unit can vary between 0% and 100% of its nominal production rate. Hydrogen and nitrogen can be pressurized

*Table 1 - List of objective function symbols and definitions*

| Symbol | Definition |
|---|---|
| $\boldsymbol{p_b, p_s}$ | Power bought or sold from macrogrid |
| $\boldsymbol{p_v}$ | Magnitude of violation of power commitment |
| $\boldsymbol{\dot{m}_i}$ | Mass flowrate of component *i* |
| $\boldsymbol{m_i}$ | Amount of component *i* in storage |
| $\boldsymbol{n_{su}}$ | Number of electrolyzers starting up |
| $\boldsymbol{\tau}$ | Target ammonia production rate |
| $\boldsymbol{\zeta_j}$ | Cost parameter for *j* |

and stored. The nominal output rates from storage to the ammonia process for $N_2$ and $H_2$ are defined with respect to the nominal $NH_3$ production rate by the reaction stoichiometry.

A nominal power balance is used to relate the power consumption from the ammonia generation system, the expected wind power, and the expected energy exchange with the utility:

$$\mu(t) = p_s(t) - p_b(t) + \rho_H \dot{m}_{H_2}(t) + \rho_N \dot{m}_{N_2}(t) + \rho_A \dot{m}_{NH_3}(t) \tag{4}$$

In Eq. (4), $\mu$ is the forecasted wind power and $\rho_i$ is the conversion factor between power and mass of component *i*. Forecasted wind power is determined adding white noise to the TMY3 wind speeds for Morris, MN, extrapolated to a hub height of 80m using a 1/7 power law expression. The standard deviation of the noise increases as times further into the 48-hour horizon are considered.

In addition, we define upper and lower bounds on hydrogen and nitrogen generation. This process flexibility is obtained by varying the production schedule of $H_2$ and $N_2$ without changing the total production. The ability to shift $H_2$ and $N_2$ production is bounded by the ability to make up production in different hours while still meeting the 12-hour ammonia production schedule, the maximum (and minimum) production rates and maximum (and minimum) storage capacities:

$$\dot{m}_{lo,H_2}(t) \geq \sum_{\substack{h=1 \\ h \neq t}}^{12} \left( \dot{m}_{H_2}(h) - \frac{n_{on}(h) p_{el,max}}{\rho_H} \right) + \dot{m}_{H_2}(t) \tag{5}$$

$$\dot{m}_{lo,H_2}(t) \geq \dot{m}_{H_2}(t) - m_{H_2}(t) + m_{min,H_2} \tag{6}$$

$$\dot{m}_{lo,H_2}(t) \geq \frac{n_{on}(t) p_{el,min}}{\rho_H} \tag{7}$$

Equations (5-7) show the inequalities used for the lower bound of hydrogen production, where $n_{on}$ is the number of electrolyzers on, $p_{el,i}$ is the maximum or minimum capacity of a single electrolyzer, and $m_{min,H2}$ is the minimum storage level of hydrogen. In these equations, hydrogen production at time *t* is bounded below by the amount of hydrogen that would still need to be produced if electrolyzers were running at maximum capacity for all other 47 hours, the minimum storage capacity of hydrogen, and the minimum power that can be given to the electrolyzers. Analogous equations are used for upper bounds of hydrogen production and for flexible nitrogen production. These upper and lower bound values are used in the following power balance inequalities:

$$p_c(t) + \gamma + p_v(t) - \rho_H \dot{m}_{lo,H_2}(t) - \rho_N \dot{m}_{lo,N_2}(t) - \rho_A \dot{m}_{NH_3}(t) \geq -\mu(t) + 1.96\sigma(t) \quad (8)$$

$$p_c(t) - \gamma - p_v(t) - \rho_H \dot{m}_{hi,H_2}(t) - \rho_N \dot{m}_{hi,N_2}(t) - \rho_A \dot{m}_{NH_3}(t) \geq -\mu(t) - 1.96\sigma(t) \quad (9)$$

Equations (8-9) ensure that sufficient process flexibility is available to utilize all available wind power with at least a 95% confidence level, where $\sigma$ are the forecasted wind power and standard deviation, respectively.

The resulting scheduling problem is formulated as a mixed integer linear program in the GAMS programming environment and solved via the CPLEX solver. Integer decisions include the number of electrolyzers turned on, and if an electrolyzer should be turned on or off at a given time period.

**Case Study**

*Market Participation*

The capacity to leverage process flexibility to effectively participate in the proposed market structure is explored by varying the market parameters (i.e. schedule elasticity and adaptability) with fixed unit sizes. For this case, the nominal $NH_3$ production rate is taken to be 1000 kg/h (resulting in a total nominal power consumption of 13.34 MW). This gives an annual production of 8760 t/y, which is on the scale of ammonia demand for 1-2 counties in the upper Midwest, or 160,000 acres of corn farms. The maximum $N_2$ and $H_2$ storage levels are 4522 kg and 808 kg, equivalent to 20 m$^3$ and 50 m$^3$ of storage, respectively, at 200 bar. The minimum storage level is taken as 1 bar of storage. Up to 7 electrolyzers are available for $H_2$ generation, and a 1.8 MW PSA unit is included for $N_2$ generation The wind power capacity is taken to be 15 MW, where this size was chosen to offset ~27% of the annual power consumption. Fixed electricity pricing was considered where power can be bought from or sold to the utility at 7.917 ¢/kWh and 3.565 ¢/kWh, respectively. A base case in which no regulatory/market constraints (i.e. schedule elasticity and adaptability = ∞) is used for comparison.

*Optimal Sizing*

Synergies between the renewable power generation and chemical synthesis, as well as the tradeoffs that occur when varying power or storage capacity, are explored by varying the number and sizes of the process units at fixed market parameters. Wind turbine capacity is analyzed with a schedule elasticity and adaptability of 1000 kWh, while electrolyzer capacity is analyzed with a schedule elasticity and adaptability of 500 kWh.

**Results and Discussion**

*Market Participation*

The regulatory requirements imposed by the market structure have little impact on the cost. The annual cost is typically within 1% of the base case value, and the cost is only 2.1% higher when the schedule elasticity and adaptability are both set as low as 500 kWh. Thus, unlike the microgrid-only case considered in Zachar and Daoutidis (2016), the system considered here is able to effectively regulate energy exchange with the utility at practically no opportunity cost.

The proposed market structure is effective at reducing uncertainty in the residual load. Figure 2 shows the cumulative annual magnitude of commitment violations. In all cases, these are small relative to the cumulative annual residual load which is ~85000 MWh.

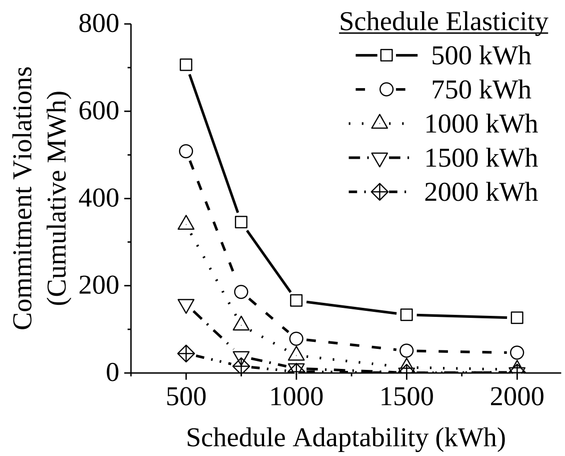


*Figure 2. Cumulative commitment violations.*

The proposed market structure also reduces the short-term volatility in the power load, quantified here in terms of load variability and load curvature:

$$\text{Load Variability} = \frac{\sum_{t=1}^{8759} \left| P_g(t+1) - P_g(t) \right|}{8759} \quad (10)$$

$$\text{Load Curvature} = \sqrt{\frac{\sum_{t=1}^{8758} \left( P_g(t) - 2P_g(t+1) + P_g(t+2) \right)^2}{8758}} \quad (11)$$

where $p_g$ is the residual load served by the utility. When these parameters are lower, it implies that the utility needs to do less ramping of its power to be able to balance the load, leading to more efficient operation.

Figures 3 and 4 show the case study results for these metrics. These values are well below the base case values shown on the figures. Long term variations in the residual load are analyzed in terms of the load factor and range:

$$\text{Load Factor} = \frac{\sum_{t=1}^{8760} P_g(t)}{8760 \cdot \max_t \left( P_g(t) \right)} \quad (12)$$

$$\text{Load Range} = \max_t \left( P_g(t) \right) - \min_t \left( P_g(t) \right) \quad (13)$$

However, the results for these values are not significantly different from the base case values of 0.55 and 24,800 kW for load factor and range, respectively.

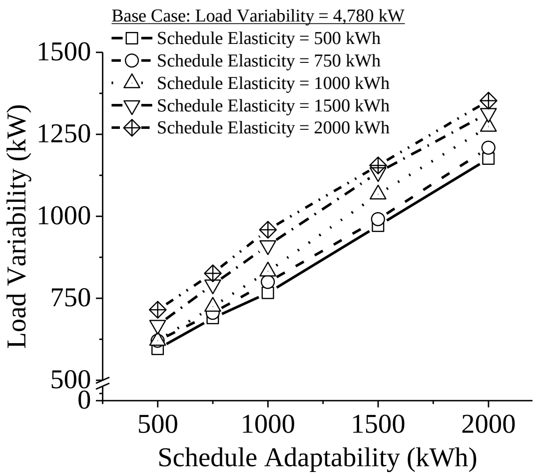


*Figure 3. Residual load variability.*

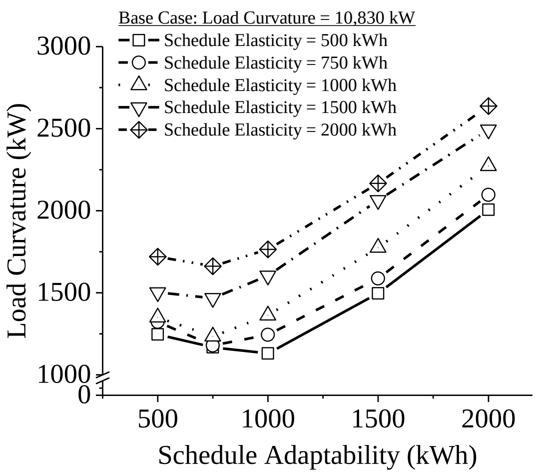


*Figure 4. Residual load curvature.*

Therefore, the utility's capacity requirements and annual utilization factor for power plants would remain unaffected by this market structure, but short-term ramping and reserve margins could be significantly reduced.

*Optimal Sizing*

To examine the effect of unit sizing, wind turbine capacity is varied while keeping all other system and market parameters the same. When examining the effect of wind capacity on the realized operating cost, a clear tradeoff emerges. Additional wind capacity allows for more selling of power back to the utility, a benefit for the system, but also incurs larger and more frequent commitment violations. This is an additional system cost resulting directly from the stochasticity of the wind resource. This tradeoff causes the realized cost to reach a minimum value at 22.5MW of wind capacity built. Note that this cost figure only includes operation cost, and not the annualized capital cost required to build the wind capacity or partner with existing wind capacity. Figure 5 shows the realized cost and cumulative violations vs. wind capacity.

Unit sizing also has a small impact on the variability of the residual load profile. As expected, long term variability increases with increased wind capacity, evidenced by

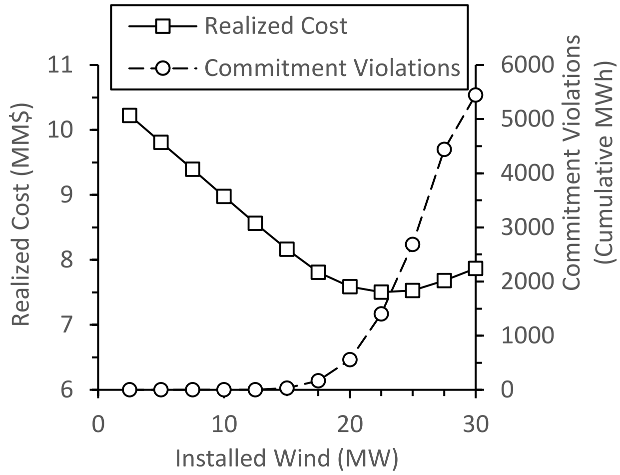


*Figure 5. Realized cost and commitment violations vs. installed wind capacity.*

increasing load ranges and decreasing load factors. Figure 6 shows that the short-term variability also increases with increasing wind capacity; however, no definitive trend is seen with the load curvature. Note that the low curvature and high variability seen for high wind capacity cases suggest a more linear load profile, indicating that the market structure is limiting the system's ability to take full advantage of the differences in wind power. Instead, the load profile varies at the maximum value allowed by the schedule adapatability for many time points. Conversely, the high curvature and low variability seen at low wind capacities indicates that the system can adjust its residual load more freely, without the constraint from the schedule adaptability parameter limiting these variations. These trends make sense due to the fact that increased wind capacity increases the magnitude of stochasticity in the system.

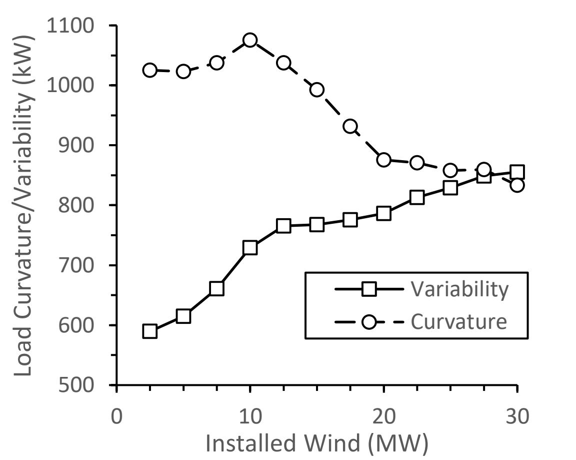


*Figure 6. Load variability and curvature vs. installed wind capacity.*

The effects of electrolyzer capacity are also analyzed by varying number of installed electrolyzers while holding all other parameters constant. Installing additional electrolyzers imparts a higher capital cost but gives the system additional flexibility to use more wind energy to produce hydrogen. A minimum of 6 electrolyzers are needed to supply a nominal ammonia capacity of 1000 kg/h.

As shown in Figure 7, when the number of electrolyzers increases, the commitment violations and realized cost decrease. However, there are diminishing returns to continuing to add electrolyzers, as storage constraints can play a part in limiting the effect of additional electrolyzers. In practice, the reduced operating costs would need to be balanced with the additional capital costs incurred.

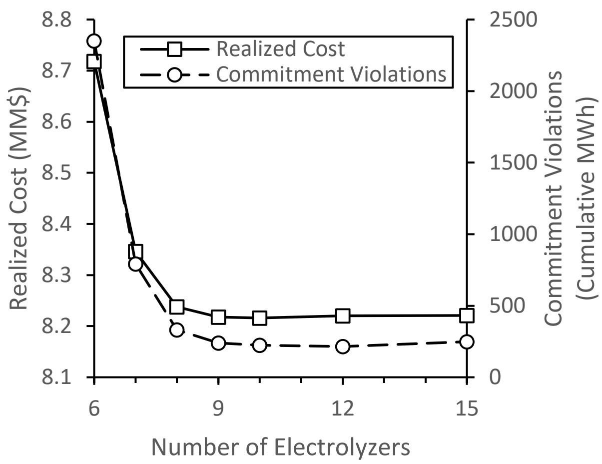


*Figure 7. Realized cost and commitment violations vs. number of electrolyzers.*

## Conclusions

In this paper, a market structure was proposed that required prosumers to limit the uncertainty and variability in their residual loads serviced by the utility. We applied this market structure to the distributed ammonia generation process and demonstrated that the market structure can be very effective at reducing uncertainty in the residual load at little additional cost of operation. We further explored the effects of wind turbine size for a given plant size and presented data displaying the clear tradeoff between ability to sell extra power and additional uncertainty of power generation. As future work, we intend to compare this market structure with others used for demand side management.

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