A Demand-Responsive Green Ammonia Plant and its Impact on the Electricity Distribution System

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***Abstract*—Most large-scale ammonia production typically relies on natural gas or coal, which causes harmful carbon pollution to enter the atmosphere. The viability of a small-scale "green" ammonia plant is investigated where renewable electricity is used to provide hydrogen and nitrogen via electrolysis and air liquefaction, respectively, to a Haber-Bosch system to synthesize ammonia. A green ammonia plant can serve as a demand-responsive load to the electricity distribution system and provide long-term energy storage through chemical energy storage in ammonia. A coordinated operational model of an electricity distribution system and an electricity-run ammonia plant is proposed in this paper. Case studies are performed on a modified PG&E 69-node electricity distribution system coupled with a small-scale ammonia plant. Results indicate the ammonia plant can adequately serve as a demand response resource and positively impact the distribution locational marginal price (DLMP).**

***Index Terms*—renewable energy, distribution locational marginal price, green ammonia, food-energy-water nexus**

I. Introduction

This work aims to empower a more sustainable future in a rapidly changing world. For example, modern power distribution systems have seen significant growth in renewable energy (RE) resources connected to the grid to mitigate climate change. While this reduces harmful emissions from traditional power plants, an operational challenge of this increase in RE penetration is the generation and load mismatch due to the uncertain and variable generation output from RE sources. This mismatch is worsened with the rise in the unpredictability of customer demands due to increased penetration of distributed energy resources (DERs), such as small-scale wind and rooftop photovoltaic (PV) technologies. Solutions proposed in the literature for this challenge typically include increased energy storage resources, demand response techniques, or both [1].

A drawback to traditional storage options, particularly conventional battery energy storage, is that they face degradation of energy capacity over charging and discharging cycles, short storage times, and thermal runaway. Therefore, energy storage solutions lasting more than one day should be explored. Using the distribution locational marginal price (DLMP) as a price signal, green ammonia plants can offer a long-term storage solution through the chemical energy storage of ammonia and act as a demand-responsive load. The DLMP is the marginal cost to supply the next unit of power to a node in the distribution system. It's transmission counterpart, locational marginal price (LMP), is widely used in wholesale markets today. Compared to traditional battery storage, this work presents a new concept of grid integration of renewable energy.

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In the procedure modeled in this work, ammonia is produced by deriving hydrogen (H_2) from water, through the energy-intensive water electrolysis procedure, along with sourcing nitrogen (N_2) through an air separation unit. The N_2 and H_2 are then fed into the existing Haber-Bosch catalyst to create NH_3. The product is referred to as "green" ammonia if renewable energy is used to power this process. Fig. 1 outlines the procedure for ammonia synthesis considered in this work. This procedure is more sustainable than the current ammonia production process that relies on fossil fuels, which produces an estimated 670 million metric tons of fossil CO_2 emissions per year [2].

Under a similar concept to the research proposed in this paper, our previous work [3] considers flexibility and energy storage in drinking water pumps and elevated water tanks, respectively, when optimizing a day-ahead schedule in a distribution system. Authors in [4] investigate solar-powered intermittency mitigation using clean ammonia synthesis and direct ammonia fuel cells while evaluating the thermodynamic performance and energy efficiency of the process. A formulation to optimally schedule wind-powered ammonia generation with respect to least-cost annual operations is developed in [5]. A combined capacity planning and scheduling of green ammonia production is provided in [6]. Though these works investigate green ammonia as a storage medium for excess renewable generation and consider power balance constraints, physical grid constraints are not considered. Therefore, the impact of this procedure on the grid and DLMP appears to be a new area of research.

The novelty of this work resides in the quantitative con-

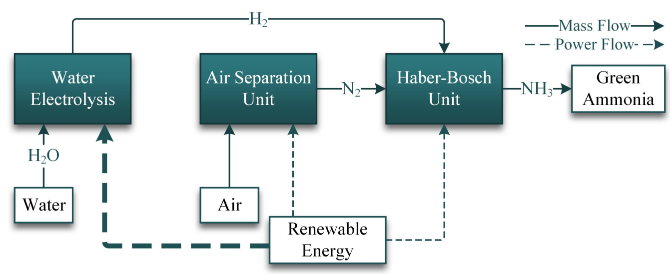

Fig. 1. Proposed green ammonia plant procedure. Dashed arrow width indicates relative size of energy transfer.

sideration of a combined electricity distribution system and ammonia production plant with constraints in a day-ahead or real-time scheduling problem. The impact of this coupling on the DLMP will be explored to realize the optimal operation of an ammonia plant and an electricity distribution system with renewable energy.

The remainder of this paper is organized as follows. We outline the mathematical model for the electricity distribution system and ammonia plant in Section II. Case studies utilizing anhydrous ammonia as a storage medium for excess renewable energy and its impact on the DLMP are provided in Section III. We conclude the work in Section IV.

II. Problem Formulation

An unbalanced three-phase electricity distribution system is considered. Modified DistFlow equations with losses are used. This three-phase model is adapted from our previous work in [9]. The substation node is indexed as 0 and the rest of the nodes are ordered from 1 to $\mathcal{N}$, where $\mathcal{N}$ is the total number of nodes/lines. Line i is the line connecting the upstream node, $u(i)$, and the set of downstream nodes, $d\{i\}$, to node i. All variables related to line i are subscripted by index $i \in \mathcal{N}$, for phase $\phi \in \Phi$, and time $t \in \mathcal{T}$.

A. Objective Function

The objective function, captured in C^E, is the least cost sum of operating the electrical distribution system (1).

$$C^E = \lambda_t^{p_0} \cdot p_{0,\phi,t} + \lambda_t^{q_0} \cdot q_{0,\phi,t} + \sum_{i,\phi,t} c_{i,\phi,t}^{G,P} \cdot p_{i,\phi,t}^{G} + \sum_{i,\phi,t} c_{i,\phi,t}^{G,Q} \cdot q_{i,\phi,t}^{G} + \sum_{i,\phi,t} \xi^R \cdot s_{i,\phi,t}^{R} \quad (1)$$

The real and reactive LMP prices at the substation node connected to the transmission system are represented by $\lambda_t^{p_0}$ and $\lambda_t^{q_0}$. The real and reactive net power injections at the substation node, which is assumed to be an infinite source, are represented by $p_{0,\phi,t}$ and $q_{0,\phi,t}$. Negative net power injections indicate the distribution system operator (DSO) is buying real or reactive power from the distribution system at the LMP of the substation node. Distributed generators (DGs) bid at $c_{i,\phi,t}^{G,p}$ for real power and $c_{i,\phi,t}^{G,q}$ for reactive power. The marginal cost of the generator is used as the bid of the DG in this work. The real and reactive power supplied by the generators are indicated by $p_{i,\phi,t}^G$ and $q_{i,\phi,t}^G$. The reactive power output of the DG must lie within a fraction, κ^G, of the real power output. The RE resources bid at \$0/MWh and are therefore not present in the objective function. Similarly, assuming the DSO owns these assets, the battery energy storage system (BESS) units do not bid into the market. Instead, this resource operates to best benefit the system. The final term in (1) penalizes RE curtailment ($s_{i,\phi,t}^R$) at a value of ξ^R to discourage inefficient utilization of the RE resources in the system. The RE generation is curtailed equally across all phases.

B. Electricity Model

Due to page restrictions, constraints for the electricity model are defined in [7] (and [8] for the BESS model) and leveraged in this work. Interested readers can refer to [7] for the development of the component-wise DLMP utilized in this work.

C. Ammonia Plant Model

Similar to the electricity system, indices $i \in \mathcal{N}$, $\phi \in \Phi$, $t \in \mathcal{T}$ are used. Here, i is the ammonia plant interconnection node. We consider a balanced, three-phase, real and reactive load for the green ammonia plant.

The electricity demand and production tracking of an ammonia plant are modeled by constraints (2)–(17). The total electrical load ($p_{i,\phi,t}^{D,A}$) for the ammonia production process is comprised of loads from the water electrolysis, air separation, and Haber-Bosch units. The chemical process used for ammonia production in this work is formulated as $6H_2O + 2N_2 \rightarrow 4NH_3 + 3O_2$. Hydrogen sourcing through water electrolysis requires the most significant portion of energy to operate. Assumed at a power consumption rate of 41.79 MWh/ton of H_2, this process requires 17.6% of the tons of ammonia produced in H_2. The nitrogen production assumes a rate of 0.243 MWh/ton of N_2 while requiring 82.4% of the tons of ammonia produced in N_2 [2]. The Haber-Bosch unit requires 0.144 MWh/ton of energy to operate. In total, the energy demand per metric ton rate ($p^{D,AR}$) for this process is 7.7 MWh/ton [10] and is defined in (2).

The power demand of the ammonia plant depends on the operational mode of the plant and is captured in (2). The total power demand is divided by three and equally assigned to each phase as we consider the load equivalent across all three phases of the distribution feeder. The total demand must be less than the total renewable power in the system at a given time, $\sum_{i,\phi} p_{i,\phi,t}^R$, as in (3), to ensure the ammonia produced is categorized as "green" ammonia.

Binary indicators $\mathbb{I}_{i,\phi,t}^A$ and $\mathbb{I}_{i,\phi,t}^P$ allow for 'on', 'off', and 'warming' modes. If the plant is 'on' ($\mathbb{I}_{i,\phi,t}^A = 1$) and producing ammonia ($\mathbb{I}_{i,\phi,t}^P = 1$), the power demand is modeled as a linear relationship between the production rate and the amount of ammonia produced in metric tons in that timeslot, $A_{i,t}^P$. A 'warming' mode allows for a reduced plant energy consumption at desired times. The Haber-Bosch reactor can be kept hot at a significantly lower power demand than when producing ammonia, due to the high energy demand of water electrolysis. Considering maintaining British thermal units, the warming state minimizes shut down and start-up operations. If the plant is 'on' ($\mathbb{I}_{i,\phi,t}^A = 1$), but not producing ammonia ($\mathbb{I}_{i,\phi,t}^P = 0$), it is in the 'warming' mode and the power demand is a constant based on the energy necessary for warming the reactor, $p^{D,W}$. Finally, there is no power demand if the ammonia plant is 'off' ($\mathbb{I}_{i,\phi,t}^A = 0$). Shutting off the ammonia plant is rare but is included in this model for completeness. Note, as enforced in (4), the plant is not allowed to be 'off' ($\mathbb{I}_{i,\phi,t}^A = 0$) and producing ammonia ($\mathbb{I}_{i,\phi,t}^P = 1$) at the same time. The power demand for the 'off' mode is also reflected in (2) when $\mathbb{I}_{i,\phi,t}^A$ and $\mathbb{I}_{i,\phi,t}^P$ both equal '0' and there is no ammonia produced when $\mathbb{I}_{i,\phi,t}^A$ is '0', as enforced in (5).

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We consider the ammonia plant a demand response system that produces $A^P_{i,t}$ tons of ammonia in an hour. The amount of ammonia produced in a timeslot must fall between the minimum ($\underline{A}^P$) and maximum ($\overline{A}^P$) amount of ammonia capable of being produced in that time frame (5). At the end of the time frame ($\mathcal{T}$), the summed amount of ammonia produced in a timeslot ($A^P_{i,t}$), must sum to at least $\underline{A^S_i}$ metric tons per day (TPD), as determined by the ammonia plant owner (6). In the case of excess renewables, the ammonia plant can produce more ammonia to assist the utility in reducing voltage violations, line congestion, or both. The excess renewable energy is stored as chemical energy in ammonia. This commodity can then be used as locally-produced fertilizer, sold to the expanding ammonia market, or consumed to produce electricity using a fuel cell.

The feedstock of ammonia ($A^S_{i,t}$) is tracked in (7), and must not exceed the maximum amount of ammonia capable of being stored on-site, $\overline{A^S_i}$. Here, $A^S_{i,t-1}$ is the initial value of the amount of ammonia stored on-site.

$$p^{D,A}_{i,\phi,t} = \frac{p^{D,W}}{3} \cdot (\mathbb{I}^A_{i,\phi,t} - \mathbb{I}^P_{i,\phi,t}) + \frac{p^{D,AR}}{3} \cdot A^P_{i,t} \tag{2}$$

$$\sum_{i,\phi} p^{D,A}_{i,\phi,t} \leq \sum_{i,\phi} p^R_{i,\phi,t} \tag{3}$$

$$\mathbb{I}^P_{i,\phi,t} \leq \mathbb{I}^A_{i,\phi,t} \tag{4}$$

$$\underline{A}^P \cdot \mathbb{I}^P_{i,\phi,t} \leq A^P_{i,t} \leq \overline{A}^P \cdot \mathbb{I}^P_{i,\phi,t} \tag{5}$$

$$A^S_{i,\mathcal{T}} \geq A^S_{i,0} + \underline{A^S_i} \tag{6}$$

$$A^S_{i,t} = A^S_{i,t-1} + A^P_{i,t} \leq \overline{A^S_i} \tag{7}$$

We consider the ammonia plant to remain 'on' for a minimum of UT_i hours and 'off' for a maximum of DT_i hours for best performance. The 'on' ($T^{on}_{i,\phi,t}$) and 'off' ($T^{off}_{i,\phi,t}$) time counters are positive and should not exceed the scheduling horizon limit ($\mathcal{T}$), as modeled in (8) and (11). The respective time counter is increased by one if the unit remains 'on' or 'off', as modeled in (9) and (12), respectively. Equations (10) and (13) constrain the minimum number of consecutive hours 'on' and the maximum number of consecutive hours 'off'. This is achieved with the use of binary 'on' and 'off' indicators ($\mathbb{I}^{on}_{i,\phi,t}$) and ($\mathbb{I}^{off}_{i,\phi,t}$), which are '1' in the timeslot the plant turns 'on' or 'off', and '0' otherwise. Equation (14) enforces these indicators to not both be activated in the same timeslot. If there is a change in the plant's 'on'/'off' status within two timeslots, the respective indicator will capture this change (15).

$$0 \leq T^{on}_{i,\phi,t} \leq \mathcal{T} \cdot \mathbb{I}^A_{i,\phi,t} \tag{8}$$

$$(\mathcal{T}+1) \cdot \mathbb{I}^A_{i,\phi,t} - \mathcal{T} \leq T^{on}_{i,\phi,t} - T^{on}_{i,\phi,t-1} \leq 1 \tag{9}$$

$$T^{on}_{i,\phi,t} \geq UT_i \cdot \mathbb{I}^{off}_{i,\phi,t+1} \tag{10}$$

$$0 \leq T^{off}_{i,\phi,t} \leq \mathcal{T} \cdot (1 - \mathbb{I}^A_{i,\phi,t}) \tag{11}$$

$$1 - (\mathcal{T}+1) \cdot \mathbb{I}^A_{i,\phi,t} \leq T^{off}_{i,\phi,t} - T^{off}_{i,\phi,t-1} \leq 1 \tag{12}$$

$$T^{off}_{i,\phi,t} \geq DT_i \cdot (1 - \mathbb{I}^{on}_{i,\phi,t+1}) \tag{13}$$

$$\mathbb{I}^{on}_{i,\phi,t} + \mathbb{I}^{off}_{i,\phi,t} \leq 1 \tag{14}$$

$$\mathbb{I}^{on}_{i,\phi,t} - \mathbb{I}^{off}_{i,\phi,t} = \mathbb{I}^A_{i,\phi,t} - \mathbb{I}^A_{i,\phi,t-1} \tag{15}$$

The ammonia plant can be turned 'on' and 'off' on the order of minutes. Therefore, the on and off time lags can be ignored in the model within an hour timeslot. Further, the ammonia plant ramps up at RU_i MW/h (16) and ramps down at RD_i MW/h (17) as the ammonia plant is not able to instantaneously change its power consumption.

$$p^{D,A}_{i,\phi,t} - p^{D,A}_{i,\phi,t-1} \leq RU_i \tag{16}$$

$$p^{D,A}_{i,\phi,t-1} - p^{D,A}_{i,\phi,t} \leq RD_i \tag{17}$$

D. Coupled System Model

Optimization problem, $\mathbf{P_1}$, captures the linear coupled electricity and ammonia plant model. We consider the ammonia plant a controllable demand response system in this model. Therefore, ammonia production is not optimized for the most profit, but all constraints must be met, including the minimum required metric tons per day. The total power demand at a node is the combination of the non-ammonia electrical demand and the optimized ammonia demand, $p^{D,A}_{i,\phi,t}$, associated with its respective node i. A similar coupling is made for reactive power demand. We define the coupled optimal power flow and ammonia production problem, $\mathbf{P_1}$, as:

$\mathbf{P_1}$: min(1)
  subject to: (2)-(17), and electricity grid constraints

III. Numerical Results

To validate our proposed model and investigate its impact on the DLMP, we consider a modified, unbalanced three-phase electricity distribution system based on the PG&E 69-node distribution system connected to a small-scale, electricity-run ammonia plant. Fig. 2 shows a oneline diagram of the system. We consider renewable generation units at Nodes 21, 22, 42, 44, 48, 49, and 61. Three single-phase 0.5 MWh BESS units are on each phase at Node 2. The balanced, three-phase energy demands of the green ammonia plant are included in the hourly electrical demands for Node 7. A balanced, three-phase 4.5MW distributed generator is located at Node 62. This DG bids into the market at \$61.69/MWh per phase. The substation LMP ranges from \$16.56/MWh to \$42.14/MWh. Historical data from the Western Wind and Solar Integration Study [11] is modified and used for hourly samples of wind and PV generation. The green ammonia plant, at minimum, must produce a desired 5 TPD of ammonia. Table I shows the green ammonia plant parameters considered in this study.

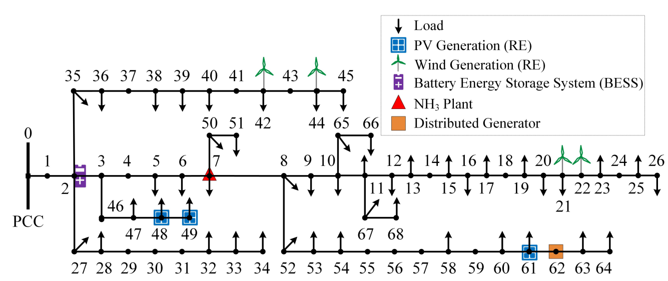

Fig. 2. An electricity distribution system based on a modified three-phase PG&E 69-node distribution system with diverse distributed energy resources coupled with an electricity-run ammonia production plant.

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GAMS/CPLEX [12] was used to solve the proposed MILP, $\mathbf{P_1}$. We create the following two cases:

Case 1: Consider decoupled electricity and ammonia models. The ammonia plant operates without knowledge of the grid conditions. The ammonia demand is fixed and must be met in the electricity model. The output of ammonia is exactly $\underline{A_i^S}$ tons.

Case 2: Consider coupled electricity and ammonia models. The electric utility operates the demand-responsive ammonia plant to best serve the electricity grid. The output of ammonia must be at least $\underline{A_i^S}$ tons.

TABLE I
GREEN AMMONIA PLANT PARAMETERS USED IN CASE STUDY.

UT_i	2 h	DT_i	6 h
RU_i	1 MW	RD_i	2 MW
$\underline{A_i^S}$	5 tons	$\overline{A_i^S}$	200 tons
$\underline{A^P}$	0.05 tons	$\overline{A^P}$	5 tons
$p^{D,AR}$	7.7 MWh/ton	$p^{D,W}$	0.002 MW

A. Impact on DLMP

The coupling of the green ammonia plant and the electricity system has an evident impact on the three-phase DLMP, as shown in Fig. 3. In decoupled Case 1, the ammonia plant runs at a constant load to produce the desired tons of ammonia by the end of the day. Case 1 sees voltage violations and line congestion occurrences throughout the day, as shown with voltage and congestion DLMP components in the left-hand side of Fig. 3, which are scaled-down to better understand the visualization. Also, power loss is unavoidable, and the system sees loss DLMP components at every timeslot, though not all are visible due to their small size. Negative DLMP components indicate that the system incentivizes higher demands at particular nodes to relieve operational issues. For example, many timeslots see negative voltage DLMP components due to the maximum voltage limit being met. In these timeslots, the system benefits from more energy demand at appropriate nodes due to the reduction in the nodal voltage.

The decoupled green ammonia plant in Case 1 cannot respond to the needs of the electricity system reflected in the DLMPs. Therefore, we consider a coupled green ammonia plant and electricity system in Case 2. The ammonia plant acts as a demand-responsive load to the electricity distribution system. It, therefore, improves the DLMP of the system by reducing voltage violations, line congestion, and RE curtailment while staying within the physical limits of the ammonia plant. As shown in the right-hand side of Fig. 3, when the DLMPs are lower, the ammonia plant demand is higher and lower when the DLMP is high. For example, in peak load Timeslots 12-18, the ammonia plant is in the ‘warming’ or ‘off’ state for Case 2 due to the high DLMPs at this time.

Additionally, the large, negative congestion DLMP components on Phase B in Timeslots 9 and 10 in the decoupled case are completely removed in the coupled system. Note that the ammonia plant consumes balanced three-phase power, which must be considered when serving the electricity system. For example, Timeslot 4 sees congestion in the system on Phase A but a negative voltage component on Phase B. Considering the overall DLMP and all other constraints, the ammonia plant best serves the system by operating at a greater capacity during this timeslot.

B. Impact of Demand-Responsive Green Ammonia Plant

In addition to the improvements on the DLMP, the green ammonia plant also reduced the amount of RE curtailed in the system, as shown in Fig. 4. The RE curtailment is lower in the coupled case in all timeslots. In some instances, Timeslots 8 and 20, for example, RE curtailment is completely removed by allowing the green ammonia plant to consume the excess RE generation in the coupled system. A constant demand is required in the decoupled case, and thus, the base, non-ammonia plant demand is equally raised throughout the day. The total demand in the system is increased in the coupled case by storing excess RE in ammonia. The base demand in some timeslots completely utilizes the renewable energy. For example, the ammonia plant is in the ‘warming’ state in Timeslots 12-16 and in the ‘off’ state in Timeslots 17-18 to not further increase the load and require more expensive energy from the substation node or the distributed generator. The demand-responsive green ammonia plant operates with means to level out the electricity demand throughout the day.

Notice, even in the coupled case, that the RE is still curtailed in most timeslots. Congested lines, nodal voltage limits met in the system, or a combination of the two cause RE curtailment. The activated voltage and congestion DLMP components in Fig. 3 graphically depict these limits being reached. This sustained curtailment indicates the importance of smart DER planning and grid upgrades to handle large amounts of distributed renewable energy resources expected in future distribution systems. Additionally, in both cases, the renewable energy is sold to the substation node at LMP until a constraint is met and the excess energy can no longer be sold. The flexible demand from the ammonia plant allows some of the curtailed RE in the previous case to be consumed by the ammonia plant. Still, physical constraints of both systems can limit this impact. Due to the incentive in the objective function for selling excess energy to the substation node at LMP, the system will attempt this option first and then store excess RE as ammonia to avoid the penalty for RE curtailment. The ammonia produced and the utilization of renewable energy in the system for each case is outlined in Table II. Case 2 shows an improvement in renewable energy utilization over Case 1 while producing over three times the ammonia by the end of the day.

TABLE II
CASE STUDY RESULTS COMPARISON.

	Case 1	**Case 2**
Tons of Ammonia	5	17.27
RE Utilization	81.02%	84.56%

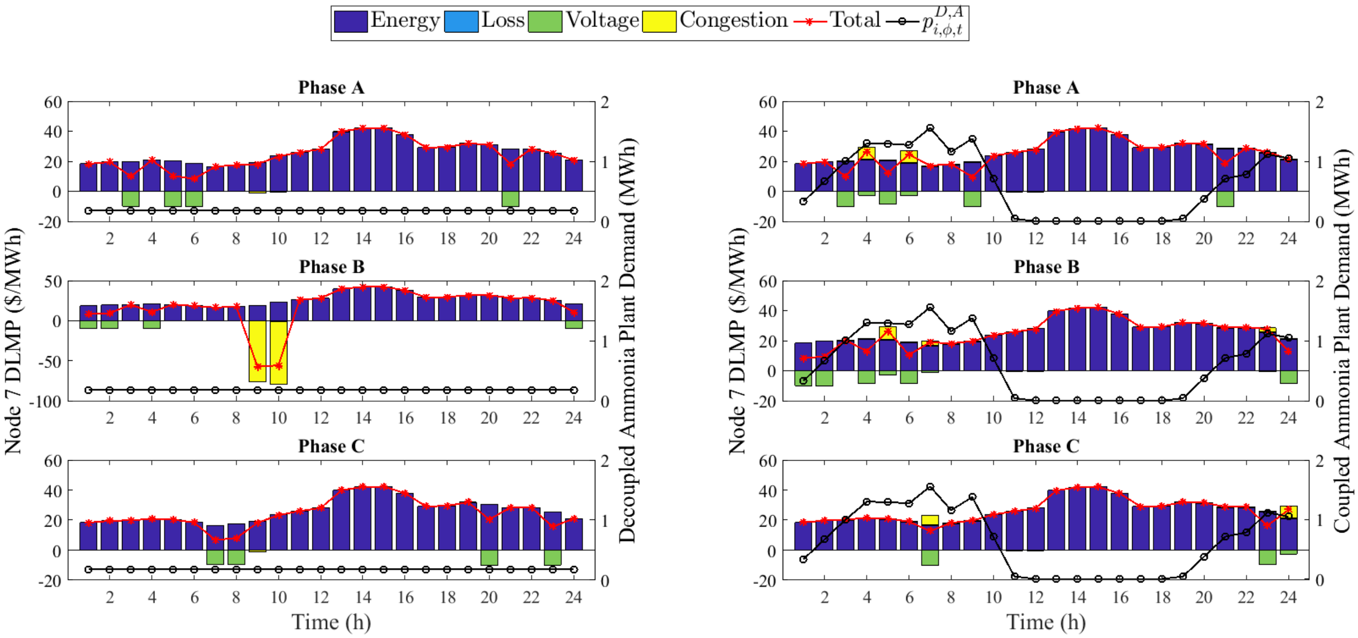

Fig. 3. Node 7 three-phase component-wise DLMP comparison for decoupled and coupled electricity system and green ammonia plant models (Cases 1 and 2). The flexible green ammonia plant operates to ease operational burdens in the grid in the coupled case.

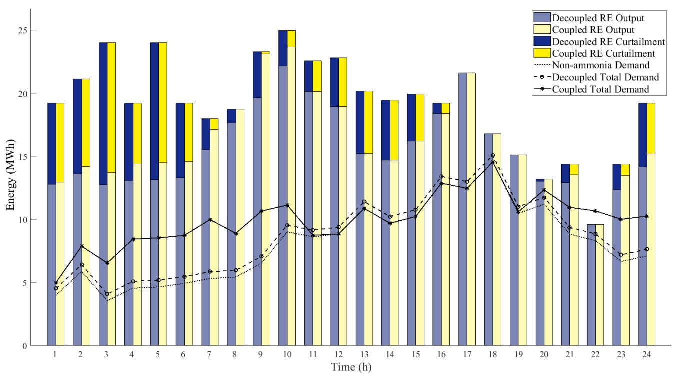

Fig. 4. Comparison of decoupled and coupled electricity system and green ammonia plant (Cases 1 and 2). Renewable energy curtailment reduces in the coupled case as the flexible demand from the green ammonia plant increases.

IV. Conclusion

A novel coordinated electricity and green ammonia plant model was formulated and validated on an electricity distribution system based on the PG&E 69-node distribution system coupled with a small-scale green ammonia plant. The impact on the DLMP of coupling the electricity system and the green ammonia plant was shown for the first time. This cooperation could strengthen future electricity distribution markets that consider DLMP. Further, the proposed model and method can offer utilities a unique tool in managing high renewable energy scenarios by coupling electricity distribution systems and green ammonia plants for storage and demand response techniques. Our future work includes the impact of power-to-ammonia-to-power applications using a direct ammonia fuel cell to sell energy back to the grid.

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