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# Combined scheduling and capacity planning of electricity-based ammonia production to integrate renewable energies

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ABSTRACT

Economic assessment of energy-related processes needs to adapt to the development of large-scale integration of renewable energies into the energy system. Flexible electrochemical processes, such as the electrolysis of water to produce hydrogen, are foreseen as cornerstones to renewable energy systems. These types of technologies require the current methods of energy storage scheduling and capacity planning to incorporate their distinct non-linear characteristics in order to be able to fully assess their economic impact. A combined scheduling and capacity planning model for an innovative, flexible electricity-to-hydrogen-to-ammonia plant is derived in this paper. A heuristic is presented, which is able to translate the depicted, non-convex and mixed-integer problem into a set of convex and continuous non-linear problems. These can be solved with commercially available solvers. The global optimum of the original problem is encircled by the heuristic, and, as the numerical illustration with German electricity market data of 2013 shows, can be narrowed down and approximated very well. The results show, that it is not only meaningfulness, but also feasible to solve a combined scheduling and capacity problem on a convex non-linear basis for this and similar new process concepts. Application to other hydrogen based concepts is straightforward and to other, non-linear chemical processes generally possible.

## 1. Introduction

Integrating intermittent electricity generation technologies requires new techniques and technologies, as well as the adaption of proven processes for emerging applications, to cope with the increased level of market flexibility and volatility. In addition, interdependencies between the electricity market and the markets of electricity consumers increase, such as between the electricity and the natural gas or the hydrogen market via electrolytic production of hydrogen (Marbán & Valdés-Solís, 2007; Barbir, 2009; Schüth, 2011; Azcarate, Blanco, Mallor, Garde, & Aguado, 2012).

R&D-needs range from technology issues to emerging markets and regulatory frameworks. Furthermore, the changing circumstances require currently used assessment techniques and evaluation approaches to adapt. An illustrative example for these new technology concepts can be observed at integrating hydrogen into the electricity market as electricity storage option (Rasmussen, Andresen, & Greiner, 2012) or as resource for the production of base chemicals such as methanol or ammonia (Benner, van Lieshout, & Croezen, 2012). The basic idea of these concepts is the use of volatile electricity production (identifiable through price signals or availability) for an intermittent production of hydrogen, and in a possible second step to hydrogen-rich chemicals. Capacity planning and scheduling methods for these processes need to consider the characteristics of the conversion of electricity to hydrogen, for example its load dependent efficiency.

In energy economics, scheduling problems are well known and widely used to analyze power plant scheduling with mixed-integer linear programming under volatile electricity prices. For an overview, see for example Gatzen (2008), Connolly, Lund, Mathiesen, and Leahy (2010) or Möst and Keles (2010). However, chemical processes usually feature distinct load-dependent (and therefore non-linear) consumption and efficiency characteristics, which need to be modeled in order to be able to assess the full potential of these technologies. This paper focuses on explicitly integrating the occurring non-linear operation characteristics into a combined scheduling and capacity planning model.

We will analyze the details of an exemplary hydrogen-based process, the production of ammonia from hydrogen produced in water electrolyzers. This is a new and innovative process concept, which intends to use cheap electricity to produce hydrogen in a first step, buffers hydrogen in a second step and produces ammonia in a third consecutive step (Schulte Beerbühl, Kolbe, Roosen, & Schultmann, 2014). Intermediate buffering decouples the price-signal driven scheduling decisions of individual subunits and

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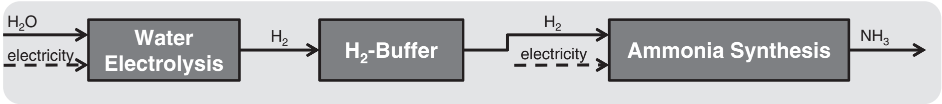

**Fig. 1.** Schematic overview of the considered electricity-to-hydrogen-to-ammonia plant.

introduces the choice of subunit capacity as a new degree of freedom. As both scheduling and subunit capacity planning are clearly linked, a combined approach—combined scheduling and capacity planning—is required.

The difference between this concept and the production of methane, methanol or other fuels and chemicals on the basis of hydrogen is solely at the last stage. The underlying challenge of non-linear, i. e. load dependent efficiencies remain. The general principle of ammonia production from electricity is well known and established for decades by using electricity from steadily operated hydro power plants (Grundt & Christiansen, 1982). The use of flexible water electrolyzers for absorbing solar- or wind-generated electricity is widely analyzed as well (Miland, Glöckner, Taylor, Jarle Aaberg, & Hagen, 2006; Clarke, Giddey, Ciacchi, Badwal, Paul, & Andrews, 2009; Millet, Dragoe, Grigoriev, Fateev, & Etievant, 2009). The combination of both, however, is new. Necessary technical adaptions to the ammonia production technology are described in Schulte Beerbühl et al. (2014), which enable the ammonia process to be flexible enough to follow an intermittently operated electrolysis, as it is foreseen in this paper.

In order to identify the challenges with this innovative technology and to present our approach to solve these, this paper is organized as follows: Section 2 introduces the new process concept and their modeling challenges. In Section 3 a general scheduling and capacity planning model with intermediate buffering is formulated, at which the modeling challenges as well as the literature approach to tackle these and similar challenges is discussed. Section 4 presents the electricity-to-hydrogen-to-ammonia model formulation on the basis of the general model. Herein, the process characteristics of the water electrolysis (Section 4.2), the intermediate buffer (Section 4.3) and the ammonia synthesis (Section 4.4) are derived in detail. However, as this section shows, load dependent characteristics will lead to a non-convex mixed-integer non-linear program, which is too big and too time-intensive to solve. Therefore, a heuristic procedure is developed in Section 5, which transforms the program into a set of convex and continuous non-linear programs. The described heuristic procedure is able to approach the global optimum of the original problem to a satisfying degree, as can be seen in the numerical example, which is presented in Section 6. Within this example, the effect of the heuristic is analyzed in detail (Section 6.2), as well as the importance of non-linear modeling (Sections 6.3 and 6.4). Conclusions with regard to the strengths, limitations and implications of this approach are drawn in Section 7.

## 2. Description of the process concept and its modeling challenges

### 2.1. General overview of the plant concept

The novel electricity-to-hydrogen-to-ammonia plant concept, which is subject of this paper, consists of three subunits, as depicted in Fig. 1:

- A water electrolysis, which splits water into its elements hydrogen and oxygen by applying an electrical current. Cooling water is needed for removing developed heat.
- An intermediate hydrogen buffer, which is realized as a gas buffer. Electricity and cooling water for compressor operation may be required at low buffer filling levels.

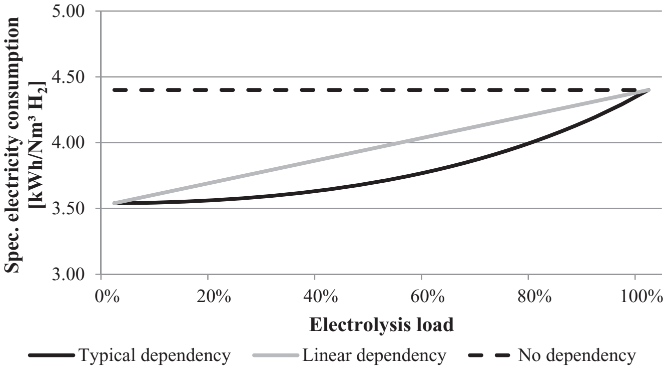

**Fig. 2.** Typical load-dependency of specific electrolyzer electricity consumption in comparison with a constant and a linearly dependent modeling approach.

- The ammonia synthesis, which converts hydrogen, together with nitrogen from air, into ammonia. Electricity and cooling water are required for process equipment operation.

Though both buffer and $NH_3$-synthesis require electricity for operations, the water electrolysis is the main consumer (approximate 95 percent; Schulte Beerbühl et al. 2014). Cooling water consumption implies further electricity demand for pumping and air fan operation in the cooling water cycle, usually between 0.005 kilowatt hour and 0.03 kilowatt hour electricity per kilowatt hour cooling water. Technical details of the plant concept have been published in Schulte Beerbühl et al. (2014). For the scope of this paper, load dependent transformation functions, i. e. yields and specific consumption functions will be determined in Section 4.

### 2.2. Modeling challenges

Electro- and thermochemical processes usually feature non-linear efficiency characteristics due to chemical and physical effects (Penkuhn, Spengler, Püchert, & Rentz, 1997). In most cases, load-dependency functions comprise quadratic or exponential components. For example, Abbaspour, Satkin, Mohammadi-Ivatloo, Hoseinzadeh Lotfi, and Noorollahi (2013) use a quadratic expression to model operating costs during partial load. In addition, plant minimum loads can be limited due to economical reasons, so that plant schedulers need to choose, whether to temporarily switch off or to operate between minimum and full load.

Water electrolysis is somewhat different to thermal power plants, as specific consumption rates do not increase but decrease in partial load mode, so that efficiency rises for lower loads (LeRoy, Bowen, & LeRoy, 1980; Hamann, Hamnett, & Vielstich, 2007). Current best available technology in water electrolysis features a design full load consumption of 4.40 kilowatt hours per newton cubic meter $H_2$ (efficiency of approximate 80 percent). As depicted in Fig. 2 (black line), specific consumption decreases with partial load toward the thermodynamic minimum of 3.54 kilowatt hours per newton cubic meter $H_2$, which is the higher heating value (HHV) and represents an energetic efficiency of 100 percent (Manabe, Kashiwase, Hashimoto, Hayashida, Kato, Hirao, Shimomura, & Nagashima, 2013; Marini et al., 2012; Smolinka, Günter, & Garche, 2010). Efficiency increases toward, but never reaches 100 percent. Reasons for this development are exponential correlations between voltage losses and area-specific output