

OPERATION OF A PTG PLANT UNDER POWER SCHEDULING

Savolainen, Jouni; Kannari Lotta; Pennanen Jari; Tähtinen Matti; Sihvonen Teemu; Pasonen Riku; Weiss Robert, VTT Technical Research Centre of Finland Ltd., P.O. Box 1000, FI-02044 VTT, Finland

Introduction

The purpose of this study was to investigate the behavior of a Power-to-Gas (P2G) plant when operated actively as a frequency control component of the electrical grid. In this context we present a simulator study of running the plant with optimized scheduling. The aim of the paper is to show that a P2G plant, producing synthetic natural gas (SNG), can act, not only as an energy storage / conversion plant, but also as an active player in electrical grid control.

On a *systemic level* energy storage and integration to renewable-energy system aspects of SNG have been studied for example by (Jürgensen et al., 2014; Minutillo and Perna, 2014; Moeller et al., 2014; Ma and Spataru, 2015). The fuel aspect of SNG has been also addressed by (Mohseni et al., 2013) with a techno-economical scope while (Vandewalle et al., 2015; Kötter et al., 2016) studied the interactions of P2G with the gas, electricity, heat and/or CO₂ markets. On *technological level*, reviews of recent decades' SNG production technologies have been provided by (Kopyscinski et al., 2010) and (Rönsch et al., 2015). The *chemistry* of SNG production from carbon monoxide (CO) and hydrogen has been known over 100 years, beginning from the work of Sabatier and Senderens (Sabatier and Senderens, 1902). Hydrogenation of carbon dioxide (CO₂), which is also sometimes referred to as the Sabatier process has received a lot of attention in recent years with recognition of CO₂'s key role of as a precursor chemical to SNG and other chemicals. For example, in addition to discussing SNG, Centi and Perathoner (Centi and Perathoner, 2009) have studied the reuse of CO₂ to produce fuels, e.g. methanol, di-methyl ether and hydrocarbons. Catalytic aspects of CO₂ conversion to olefins, syngas, formic acid, methanol, di-methyl ether, hydrocarbons and finally methane has been reported in (Wang et al., 2011; Centi et al., 2013; Koschany et al., 2016), among many others. Reaction mechanisms and kinetics have been reported for example by (Kopyscinski, 2010; Erbib and Bouallou, 2014; Kiewidt and Thöming, 2015). On the other hand, (Hoekman et al., 2010) studied in laboratory scale the use of flue gas CO₂ as source for SNG.

This paper aims to address the *operational level* of a P2G process. Especially noteworthy is that we study a multi-use P2G process. In other words the process acts a source of SNG but also at the same time actively participates in control of the electrical grid.

Methodology

The work presented here is a case-based, computational engineering research. In the following we present the case under study, the computational models and scheduling used in this study.

Case process and modelling principles

The structure of the process under study is depicted in the flowsheet of Figure 1.

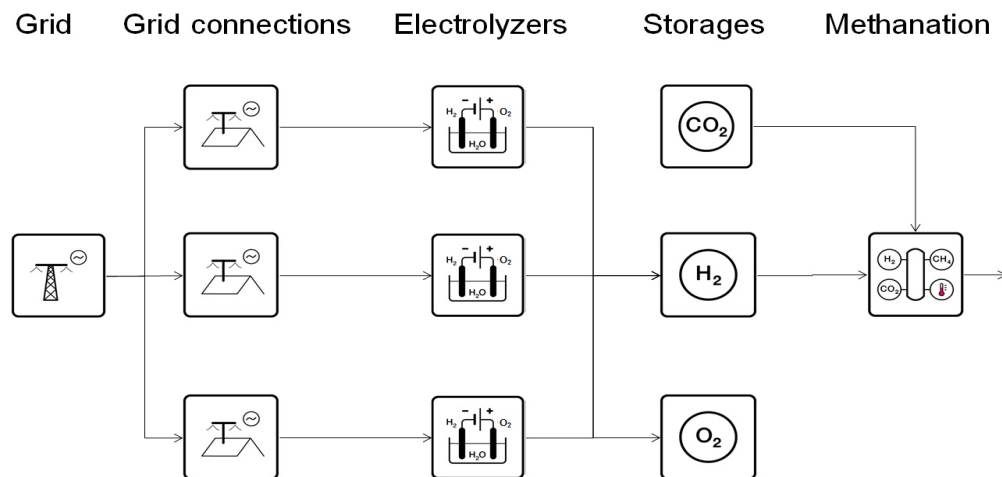


Figure 1 Flowsheet of the studied P2G process.

The process is driven by the frequency of the electrical grid. This grid frequency consists of actual grid frequency data from Finland during one 24 hour period in the summer of 2013. This grid frequency is fed to three identical grid connection blocks which are used to calculate the electrical power fed to the electrolyzers. The electrolyzers are all alkaline electrolyzers (AEC) and from each of these two flows are extracted, namely hydrogen (H₂) and oxygen (O₂). Both product gases are fed to their respective storages. Outlet flow from the hydrogen storage and an external source of carbon dioxide are mixed and fed to a chemical methanation reactor producing a flow of SNG.

Overview of the simulator environment

The process was modelled with the Apros[®] process simulator (“Apros,” 2010). For the fluid flow and pressure dynamics the simulator uses a combination of physical laws and empirical correlations. The physical laws are the conservation equations for mass, momentum and energy which are in this case written as partial differential equations with one spatial coordinate and time as the independent variables, see for example (Siikonen, 1987). Source terms of the equations are used to feed effects such as pressure increases/losses, heat flows etc. of equipment (pumps, valves, turbines etc.) into the equations. Also, the chemical reactions of methanation, described later, affect the equations through the source terms. Finally, the simulator provides a library automation function blocks some of which were used in this study to model stabilizing controls.

Grid connections

The grid connector block takes as its input the grid frequency (in Hz) and a value of its electrical power output at full operational, which in this study was set to 3MW_e for each of the grid connections. Although an electrolyzer cannot output power back to the grid, a bi-directional inverter model was built so that a possible storage system can be integrated with more ease later. The reason is to be able to use the model for simulate

electrolyzer active power control in frequency regulated reserve use. Reactive power capacity is also built to the model but this is not the focus of the study. The model here includes a control system so that reactive and active power commands can be given. Active power reference is generated using a droop curve from measurement of frequency like presented in Figure 2.

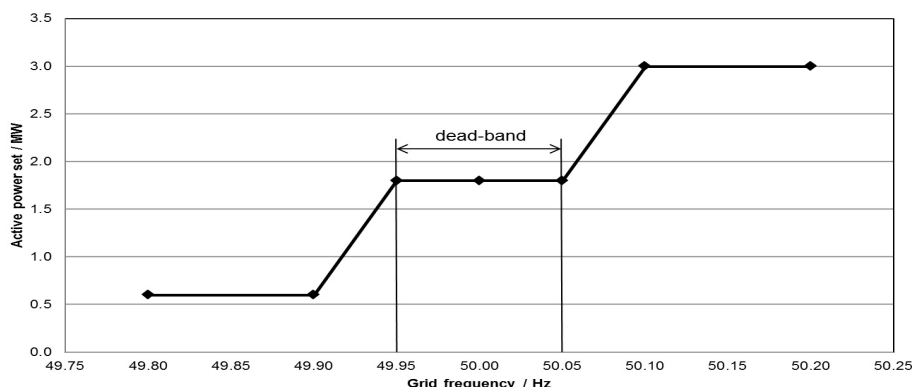


Figure 2 Droop curve of the grid connection.

The electrical power from the grid connection block to the electrolyzer is further limited by user definable ramps (e.g. $\pm 400\text{kW}/\text{min}$). These ramps are utilized when the grid frequency is outside the dead-band of Figure 2. When the frequency falls from outside the dead-band into it, no ramp limiting is used.

Electrolyzers

The electrolyzers in this study are 3MW_e maximum power, alkaline electrolyzers operating in atmospheric conditions with nominal temperature at 70°C . The overall structure of the electrolyzer is presented in Figure 3.

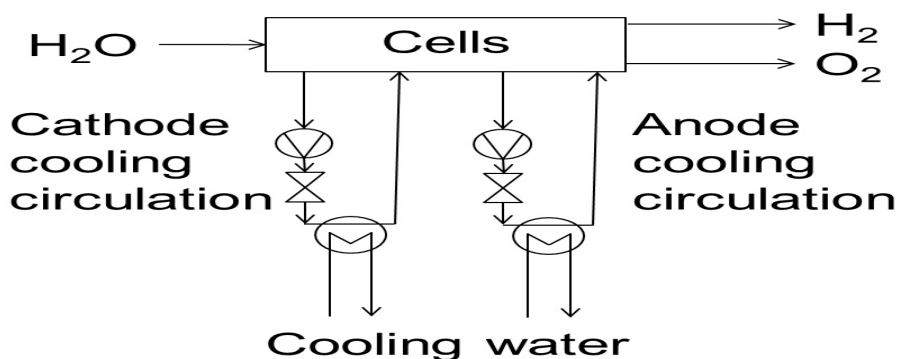


Figure 3 Overall structure of the alkaline electrolyzer model.

The modelling of the cells is based on their current-voltage curve or in other words the IV curve (Zhou and Francois, 2009). This is used to calculate molar flows of hydrogen and oxygen out of the electrolyzer as a function of electrical current. Furthermore, we simulate the heat released in the cells and the subsequent cooling circuits of the anode and cathode. The cooling is performed in heat exchangers dumping the heat to external water flows to which the heat exchange is calculated with the (ϵ, NTU) -model (Incropera and DeWitt, 1990). The heat dynamics of the model also include the metal and liquid masses present in the

device. This electrolyzer model has been validated with industrial scale data and in Figure 4 we show percentual errors of electrical current, voltage, electrolyzer cell temperature, hydrogen production and water consumption for five different time instants. The measurements were carried on three industrial scale electrolyzers over a five hour period under differing loads.

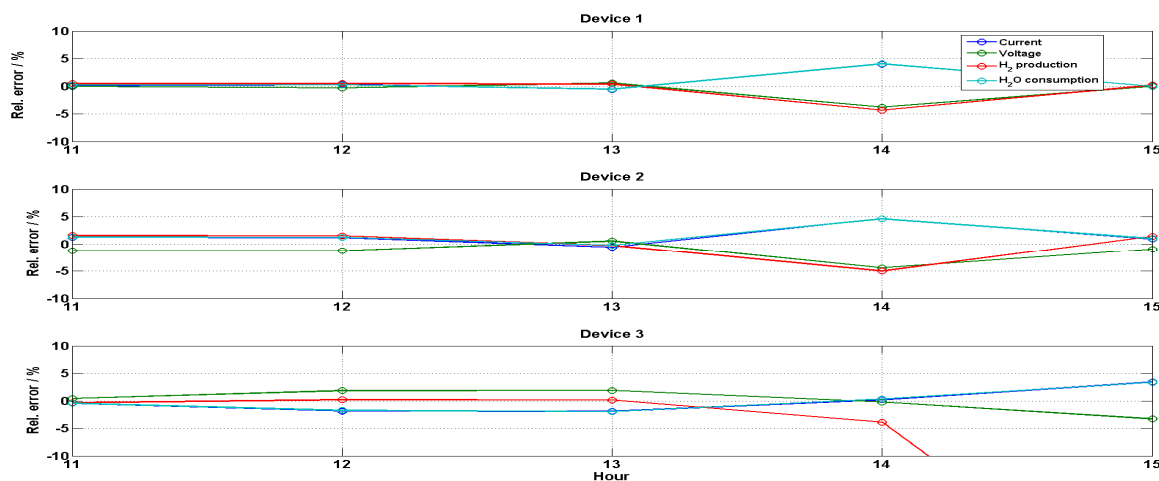


Figure 4 Percentual errors between electrolyzer model and measurements.

As can be seen relative errors are typically within $\pm 5\%$, the only exception being the H₂ production of device 3 at time 15 hours. The relative error there was nearly -40% . A closer examination of the measurement data set strongly suggested that this large error is due to measurement error. Thus we can quite safely conclude that the electrochemical model is valid.

Hydrogen storage

The hydrogen storage process is a combination of three pressure vessels (low, middle and high pressure), compressors and intermediate water-driven coolers and safety valves to the ambient air. The structure of the storage process is shown in Figure 5. The incoming gas is firstly cooled and then fed to 6 m³ low pressure vessel (LP, 0.95 bar). From here it is transported with two compressors to a 50 m³ middle pressure (MP) vessel, operating around 16 bar. The rotation speed of these compressors is manipulated so that the LP vessel pressure is maintained at 0.95bar. The MP vessel is used to stabilize short term changes in hydrogen flow as from it the gas is taken out and fed towards the methanation. If the pressure of this vessel drops too low hydrogen from a 10 m³ high pressure (HP) vessel (300 bar) is used as makeup. The HP makeup control valve opens when hydrogen output flow drops below 98% of desired control value. There is also a 3-stage compressor train connecting the middle pressure vessel to the high pressure vessel. The rotational speed of this compressor train is controlled to keep the pressure in MP vessel at 16 bar. A safety valve in the MP vessel opens at 1.5 times higher pressure than this, leaving a safety margin to keep all hydrogen in the process. Flow of cold water to the intermediate coolers is manipulated in order to maintain a constant temperature before next compressor stage/pressure vessel. In addition to the process equipment the above described control logics are implemented into the model.

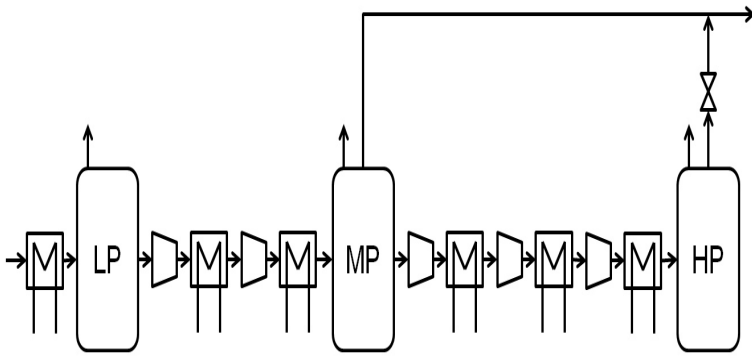


Figure 5 Structure of the hydrogen storage process.

The compression train is controlled so that the hydrogen storage system will produce a constant flow to methanation. Also, the temperature of methanation feed should stay relatively constant. The compression controls are separated before and after middle pressure vessel. This way the hydrogen storage system can handle variation of electrolysis without need to overuse compression and cooling power. Higher compression is used only if there is excess of hydrogen from electrolysis. Vessel sizing has been made such a way that hydrogen storage will fulfil need of methanation for 160 minutes without any hydrogen from electrolysis.

Oxygen storage

The oxygen storage model contains a similar structure as the hydrogen storage. The main difference is in the dimensioning of the equipment and in the fact that there is a 4-stage compression train connecting the LP and MP vessels and 2-stage compression train connecting MP and HP vessel. Pressure volumes and levels of the oxygen storage are: LP 1 m³ at 0.95 bar, MP 50 m³ at 10 bar and HP 20 m³ at 100 bar.

Methanation

The methanation process begins with mixing of reactant gases (H₂ and CO₂). The carbon dioxide comes as a constant pressure (12 bar) boundary condition to the model. Its flow rate is controlled using a PI-controller which strives to achieve a 4:1 H₂:CO₂ molar ratio to the methanation feed flow of approximately 1500 Nm³/h. The methanation reactor is a vessel (6m tall, 0.5m diameter). The reactor is discretized into ten equal sized calculation volumes. In each volume methanation reaction kinetics are calculated to obtain new concentrations and the heat released in that discretization volume. The kinetic equations from (Kopyscinski, 2010) are utilized. Heat conduction from the calculation volumes to a cooling water flow is calculated for each volume. The heat transfer takes into account the amount of metal separating the two flows and thus provides for the heat dynamics of the reactor.

Operational scheduling

The model was controlled by an hour-by-hour operational schedule obtained from cost/income considerations. For each hour the process is either running with constant electricity consumption (“SPOT mode”) or participating in frequency control of the grid (“FCR mode”). The schedule was obtained from an

optimization algorithm (Weiss et al., 2016). The optimization gives to the simulation model the operating window in which it can be run. This operating window is characterized by upper and lower limits on the electrical power consumed by each electrolyzer. In the SPOT mode this upper and lower limits are the same but not necessarily zero and thus the system cannot participate in frequency control of the grid. In FCR mode the limits are not equal enabling the system to act in both up- and down-control of frequency. This kind of moving between FCR and SPOT modes can occur e.g. in a situation where the FCR price falls to zero i.e. there is no incentive to place an FCR bid. In this study one 24 hour period from the summer of 2013 in Finland was studied. The schedule is presented in Figure 6, which shows the upper and lower limits and indication of the SPOT and FCR modes.

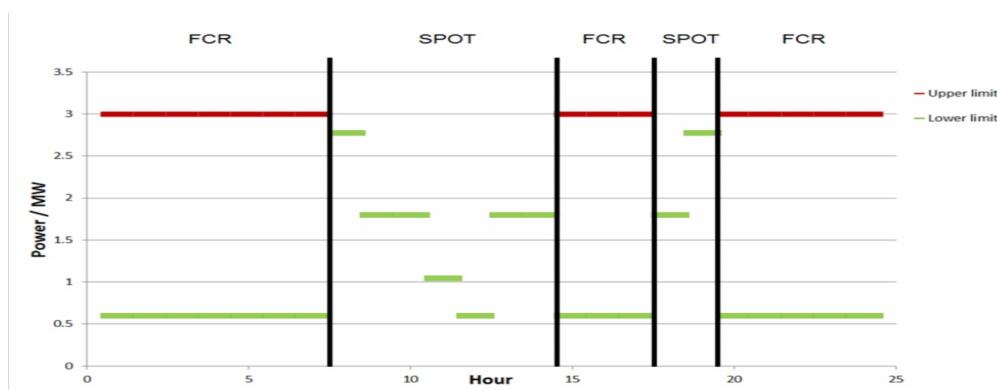


Figure 6 Schedule for a 24 hour period.

Results

The schedule of Figure 6 and the corresponding grid frequency data was fed into the simulator. The simulation output variables are depicted in the following figures. Figure 7 presents the actual power fed to one electrolyzer (bottom) along with the grid frequency (top). During the FCR mode the power varies with the grid frequency whereas in SPOT mode it is constant within each hour.

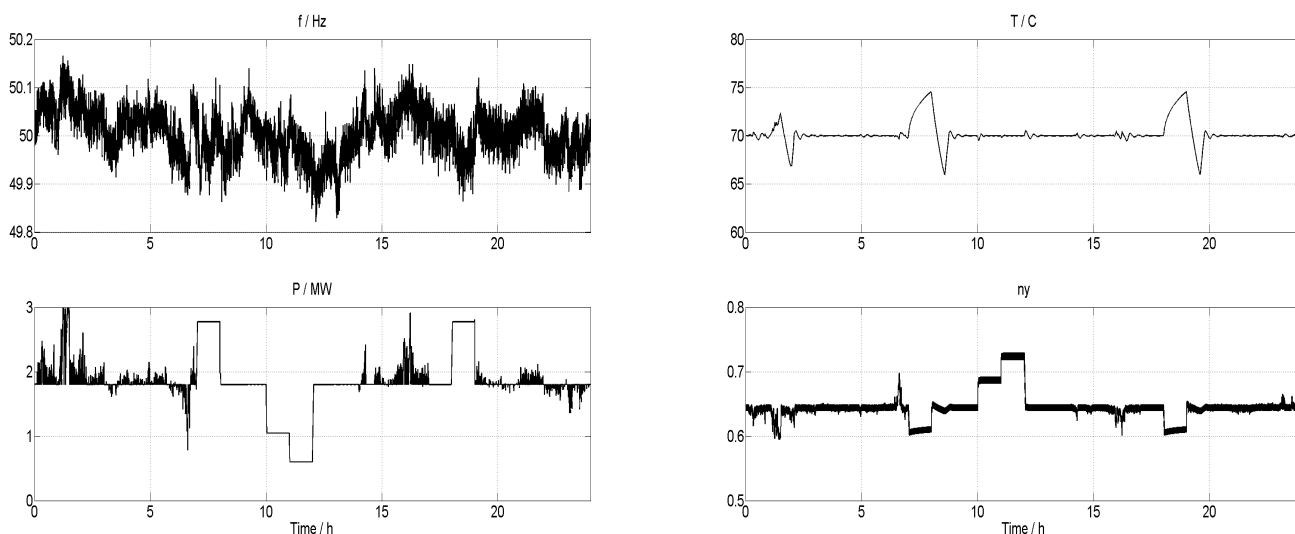


Figure 7 Actual power fed to one electrolyzer (left), electrolyzer temperature and efficiency (right).

The effect of this on one electrolyzer is depicted on the right in Figure 7. We see that changing input power affects the temperature of the electrolyzer, top curve and that the cooling control of the electrolyzer is able to keep the temperature within 5°C of set point value, 70°C. The electrolyzer efficiency (defined as $\eta = \frac{\dot{m}_{H_2} LHV_{H_2}}{P}$ with one minute averaging, shown on the bottom) follows the power feed in a mirror-like fashion.

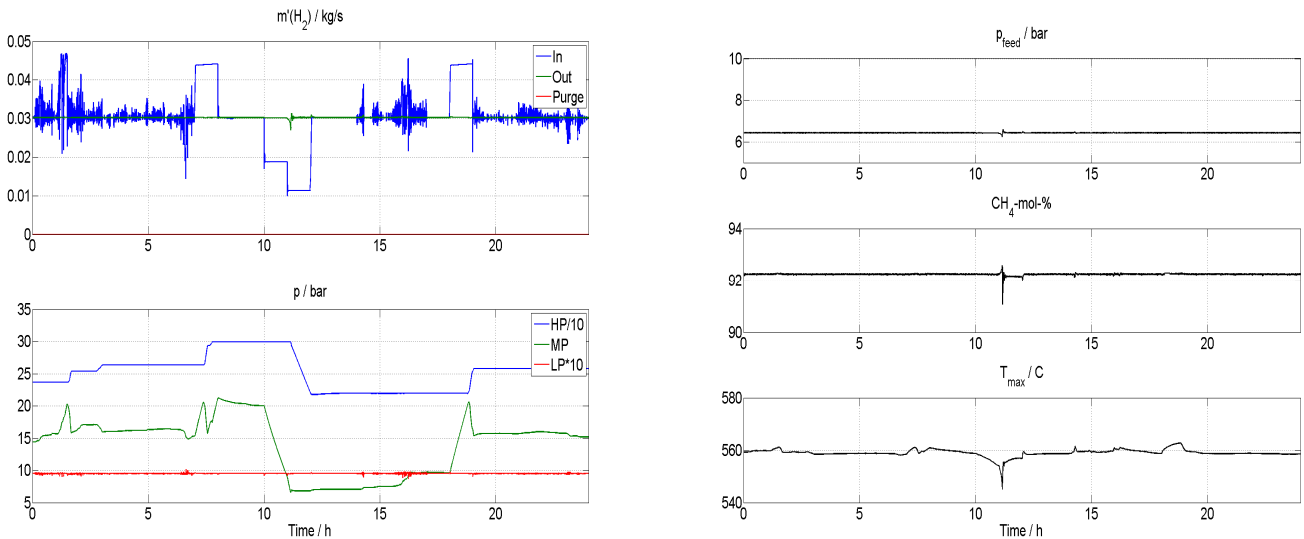


Figure 8 Effect of the scheduling and grid frequency on hydrogen storage (left) and the methanation reactor (right).

Since H_2 production is directly linked to the electrical power fed to the electrolyzers, the H_2 storage has to react to the varying H_2 flow as shown on the left side of Figure 8. Here, the top part shows in blue the combined hydrogen mass flow from all three the electrolyzers to the hydrogen storage. The inflow of hydrogen directly follows the electrical power fed to the electrolyzers. Also, the flows of hydrogen out of the storage to the methanation and to then natural gas grid (“purge”) are shown, in green and red, respectively. The H_2 flow to methanation is controlled by a flow control loop which attempts to hold a constant flow. As can be seen, the inflow of hydrogen oscillates considerably during the FCR mode whereas the output flow oscillates clearly less than the feed. In fact, the only major disturbances occur when the system is run at a fairly low load, around time 11-12 hours. At this time the inflow of hydrogen is so low that the system has to resort to the HP tank for makeup, which can be seen as a drop in the blue pressure curve of the HP-tank on the bottom part of the figure. Prior to this the MP tank pressure, shown in green, has already decreased due to the drop in hydrogen production at time 10 hours. The HP and MP tank pressures start to recover around time 16 hours when the electrolyzers are run again at higher powers. They finally reach their initial levels after the SPOT mode operation around 18 hours.

The effect on the methanation reactor is shown on the right hand side of Figure 8. From the topmost curve we see, that the feed flow pressure stays very nearly constant. This leads to a fairly constant methane molar percent in the product gas. The only noticeable disturbance occurs at time of low electrical load of electrolyzers. This is the same effect as seen earlier in right hand of Figure 8 when the H_2 storage control

switches the source from MP to HP tank. The bottom curve of Figure 8's right hand side shows the maximum temperature of the reactor. It too exhibits a dip around time 11 hours, but otherwise is quite flat. The very steady operation of the methanation reactor is due to the control strategy of the H₂ storage process: trying to keep a constant flow of H₂ to the reactor. On the other extreme is a control strategy in which the flow of H₂ out of the storage is following closely the inflow of H₂ to the storage, but this kind of control hardly seems realistic because it entirely nullifies the storage's ability to dampen incoming variations and it was not investigated further.

Discussion

The aim of the paper was to investigate whether a P2G plant can also act as a multi-use process: on one hand acting as an electrical grid control element and on the other hand being an energy conversion plant. In the currently presented case this was seen to be possible since different operational modes and transitions between them did not have a major disturbing effect neither on the H₂ storages nor on the methanation reactor. It must be noted though that some recent studies have suggested that, in fact, the methanation is quite resilient to load changes (Götz et al., 2015). Furthermore, the system studied did not exhibit unwanted behaviour such as unnecessary gas purges to the sky. Naturally, all this is dependent on the sizing of the process, most critically the H₂ storages, an aspect that has been investigated by Tähtinen et al. (Tähtinen and Sihvonen, 2016). Also, a critical factor on how well the process is able to handle the schedule given to it is its lower level controls and their tuning. This is an area well suited for the dynamic simulation tools utilized here. The validity of the results is also dependent on the validity of the models used. Even though this paper presented a "generic P2G plant", with no real-life counterpart we remain confident that the results have validity and are useful. This is due to the fact that all the models have been constructed from validated unit operation models and the whole system dimensioned with the use of generic process engineering know-how. Thus it stands to reason, that the presented approach is generalizable to other P2G processes as well.

Conclusions

This paper presented an operation study of a Power-to-Gas process under varying operational schedule. The research was conducted as a simulation case study. The main conclusion to be drawn from the results is that even though the electrical power fed to the system varied considerably both in level (from 0.6 MW to 3MW) and in variability (from fast variations in frequency control to step-wise variations in SPOT mode), the system exhibited enough dampening capacity to produce a steady quality of SNG. Thus a P2G plant can be used as multi-use plant performing the duties of a frequency control element in the electrical grid as well and SNG producer.

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Authors and their degrees with corresponding author indicated

Savolainen, Jouni¹, M.Sc. (Tech.), jouni.savolainen@vtt.fi, corresponding author

Kannari Lotta¹, M.Sc. (Tech.)

Pennanen Jari¹, M.Sc. (Theor. Phys.)

Tähtinen Matti¹, M.Sc. (Tech.)

Sihvonen Teemu¹, M.Sc. (Tech.)

Pasonen Riku¹, M.Sc. (Tech.)

Weiss Robert¹, Lic. Tech.

¹VTT Technical Research Centre of Finland Ltd., P.O. Box 1000, FI-02044 VTT, Finland

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