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Dynamic Simulation of Hydrogen Generation from Renewable Energy Sources

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Electrolysers convert electrical energy to electrochemical energy and for this purpose it is shown as practical applications in energy storage systems, where the storage element in this case is the hydrogen which has highest energy density per mass. The main benefits of using a water electrolyser are the zero-emission of greenhouse gases, the use of water as source of hydrogen production and also, the high efficiency in energy conversion. In this paper, the work is based on mathematical modelling of a photovoltaic system for energy supply and hydrogen generation by an alkaline electrolyser according to the weather in Vienna during the whole year and the solar radiation data using TRNSYS 17. The goal of a dynamic modelling is to check how the system works against the load variations. A variation of hydrogen outflow rate and power with changing time are shown. The model scheme can be beneficial in the design and performance analysis of a complex hybrid-power plant system prior to practical realization.

1. Introduction

The consumption of fossil and nuclear fuels represents serious environmental threats such as natural sources exhaustion, pollutant gasses emission, waste generation, and climate change. As a result of the public awareness of these facts, an agreement has been reached in the sense that a novel, clean, sustainable and renewable resources-based energy system is needed (Darabnia et al., 2013). Among all renewable energies, global wind power capacity increased the most in 2010, by 38 GW, bringing the global total to 198 GW. The most important wind energy producers were the United States (40.3 GW), China (44.2 GW), Germany (27.2 GW), and Spain (20.8 GW). Global hydropower capacity reached an estimated 990 GW by the end of 2012 (reported by Renewable Energy Policy Network for the 21st Century Organization, 2010). An electric system based on renewable energies gives rise to new challenges concerning storing and utilization of the surplus energy, operation, distributed generation management, energy supply reliability, and future integration with an automotive sector based on the electric vehicle. Hydrogen is the simplest and lightest element of the periodic table. Its density as a gas (0.0899 kg/Nm^3) is 15 times lighter than of air. Hydrogen is a fuel with an inflammability range both in air, from 4 to 75 vol. %, and in oxygen, from 4 to 95 % Vol. It is also the fuel with the highest energy content per mass, being its higher heating value (HHV) 3.54 kWh/Nm^3 (39.42 kWh/kg), that is 2.5 and around three times more energetic than methane and gasoline (reported by L'Observatoire des énergies renouvelables, 2012).

Because of the increasing levels of greenhouse gas emissions and the rising universal energy demand new technologies for the generation of environmentally friendly power are needed. Renewable energy sources like solar and wind energy have undeniable potential, but their fluctuating and intermittent natures cause some challenges during usage. In electricity networks, renewable power sources with a low output can be balanced by a conventional power generator, however a higher percentage of renewable energy sources would need an improved energy storage system. Short-term storage of electricity like batteries, flywheels compressed air, or capacitors are adequate, but long-term storage could be realized with hydrogen. (Amyotte et al., 2013)

A hydrogen power system converts excess electricity from renewable energy in the system into hydrogen for chemical energy storage. This chemical energy can be re-electrified in the system during deficit energy supply from the renewable energy sources. The hydrogen subsystem, also called a hydrogen-loop, comprises an electrolyser for conversion of water and electricity to hydrogen, hydrogen storage unit.

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The present study is based on water electrolysis for producing hydrogen from water without the use of fossil fuels. Electrolysis is the most important method to obtain hydrogen from water. It is a mature technology based on the generation of hydrogen and oxygen by applying a direct electric current to water to dissociate it. The hydrogen is produced by electrolysis has a high purity that can reach 99.999 % Vol. once the produced hydrogen has been dried up and oxygen impurities have been removed. Since electrolytic hydrogen is suitable for being directly used in low-temperature fuel cells, such purity levels are of great advantage against both fossil fuels and biomass-based processes (Onda et al., 2004).

2. Water electrolysis

Water splitting into hydrogen and oxygen can be performed by passing an electric current between two electrodes separated by an aqueous electrolyte with proper ionic conductivity. Into this a molecule of hydrogen is generated in the cathode by decomposition of two molecules of water. Furthermore a molecule of oxygen is generated in an anode and at the same time one molecule of water is regenerated. Eqs(1) to (3) are presented to describe this procedure;

$$H_2O_{(l)} + 237.2\ kj\ mol^{-1}(electricity) + 48.6\ kj\ mol^{-1}(heat) \rightarrow H_2 + O_2 \quad (1)$$

$$Anode: 2OH^{-1}(aq) \rightarrow \frac{1}{2}O_2(g) + H_2O(l) + 2e^- \quad (2)$$

$$Cathode: 2H_2O(l) + 2e^- \rightarrow H_2(g) + 2OH^-(aq) \quad (3)$$

In an alkaline electrolyser the main components of the cell are the anode, cathode and diaphragm. The electrodes must have good electric conductivity and they must be resistant to corrosion. The diaphragm should have low electrical resistance. At standard conditions (25 ºC and 1 atm) the reaction Eq(1) is a non-spontaneous reaction, which means that the change in the Gibbs energy is positive.

$$\Delta G = \Delta H + T_{el}\Delta S \quad (4)$$

LeRoy et. al. (1980) described the thermodynamics of water electrolysis. The enthalpy of water splitting is expressed as follows:

$$\Delta H_{t,p} - \Delta H_t^0 = \left[\Delta H_{t,p} - \Delta H_t^0\right]_{H_2} + 0.5\left[\Delta H_{t,p} - \Delta H_t^0\right]_{O_2} - \left[\Delta H_{t,p} - \Delta H_t^0\right]_{H_2O} \quad (5)$$

The decomposition reaction of water by electrolysis is an endothermic reaction where energy corresponding to ΔG must be supplied in the form of electricity. Faraday's law relates the electrical energy (emf) needed to split water to the chemical conversion rate in molar quantities (Eq 6).

$$U_{rev} = \frac{\Delta G}{nF} \quad (6)$$

Where n is number of moles of electrons transferred per mole of water, and F is Faraday constant (F=96485 $Cmol^{-1}$) .The theoretical voltage (U_{tn}) is defined by Eq(7);

$$U_{tn} = \frac{\Delta H}{nF} \quad (7)$$

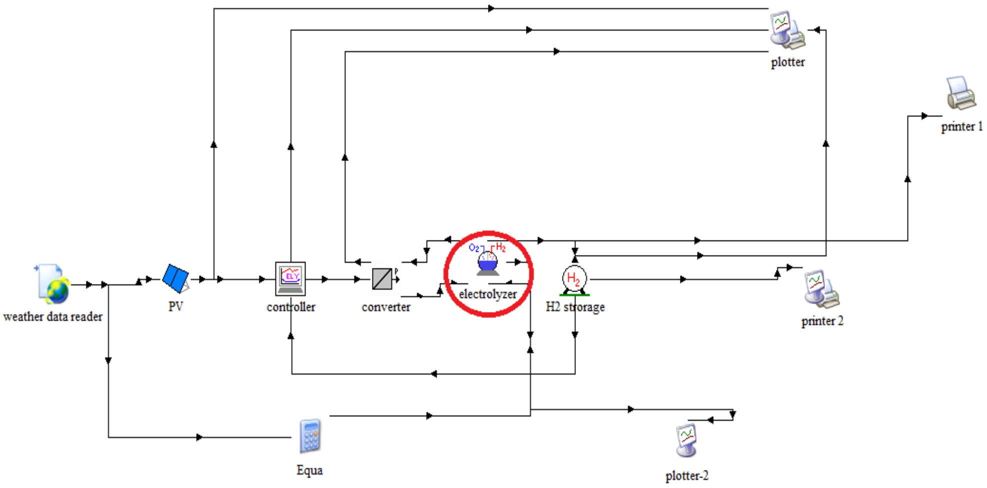


Figure 1: Schematic of hydrogen production system by water electrolyser using TRNSYS

3. Modelling

In this research, TRNSYS is implemented as one the best tools for dynamic simulations especially in renewable energy systems. TRNSYS has a modular structure. It contains a variety of individual subroutines and the components, representing the mathematical model description of real physical devices. The modular nature of TRNSYS facilitates the modelling number of different system configurations.

The weather data is provided by Meteonorm Co which is data sets of hourly values of solar radiation and meteorological elements for a 1 y period. In the TRNSYS library, there various choices of components particularly for photovoltaic, therefore Type 94 is used for this study, as one the most popular kinds (Jürgen, 1990). This component characterizes the electrical performance of a photovoltaic array. Type 94 may be applied in transient simulations involving electrical storage batteries, utility grid connections, and direct load coupling which are based on calculation method expressed by Soto et al. (2006). The model specifies power and current of the photovoltaic array at a determined voltage.

A part from the quantity in Figure 2, the monthly power generated by PV is presented. Because of the high solar radiation rate in summer the maximum power can be produced according to Vienna's annual weather information. An electrolyser controller implements a set of control functions for an electrolyser of an integrated mini-grid connected system (e.g. RE source, electrolyser, hydrogen storage, fuel cell). The electrolyser can operate in two power modes (constant or variable power). The next unit is power conditioner which is a device that can invert DC power to AC power, and/or vice versa, or they function as DC/DC converters.

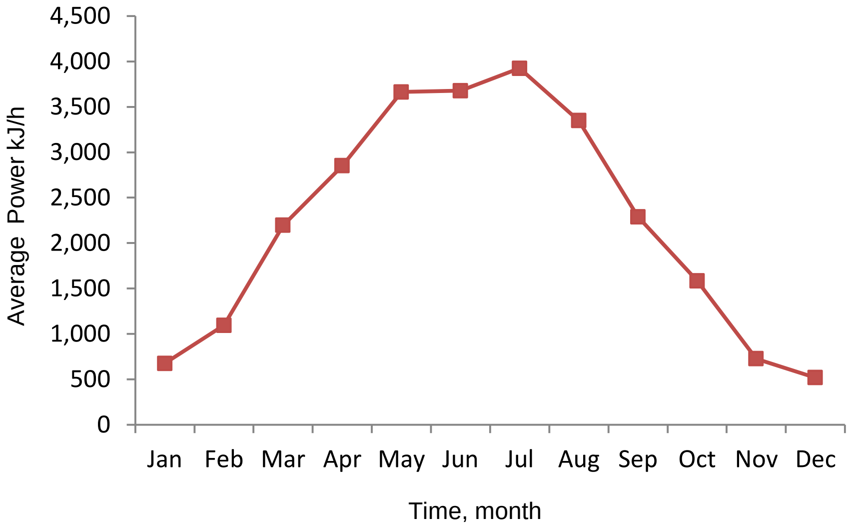


Figure 2: Power generated during the whole year by PV in Vienna, Austria

After power generator electrolyser plays important role among operational units (Figure 1). An actual alkaline water electrolyser consists of several electrolyser cells connected in series. The electrolyser model implemented here is based on the characteristics of individual cells. The calculations of the required operation voltage, mass flow production rate of hydrogen and oxygen, and internal heat generation are all carried out per cell basis, while the corresponding values for the whole electrolyser unit are simply found by multiplying by the number of cells in series. A temperature dependent current-voltage curve for a given pressure and a Faraday efficiency relation independent of temperature and pressure form the basis of the electrochemical model. The electrolysers and fuel cells are characterized by semi-empirical temperature dependent current-voltage models based on the laws of electrochemistry and thermodynamics. For the electrolyser, the following IU-model applies (Vanhanen, 1996):

$$U_{el} = N_S \left\{ U_{rev} + (A + B \times lnI) + C \times ln(1 - \frac{I}{I_l}) + R_{\Omega} \times I \right\} \quad (8)$$

Where N_S is the number of cells connected in series; A, B, C, R_{Ω} and I_l are parameters of which temperature dependencies are described by the mathematical functions which correlate with the empirical data. Equation (8) can be modified into a more detailed IU-model (Ulleberg, 1998).

$$U = U_{rev} + \frac{r_1 + r_2}{A} I + S \times log \left[\frac{t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}}{A} I + 1 \right] \tag{9}$$

Where , S and t are parameters for overvoltage on electrodes and r, for resistance of electrolyte. T, is electrolyte temperature (ºC) and A, is electrode area (m²).

The Faraday efficiency is defined as the ratio between the actual and theatrical maximum amount of hydrogen produced in the electrolyser. Since the Faraday efficiency is caused by parasitic current losses along the gas duct, it is often called the current efficiency (Klein S.A et al., 2006).

$$\eta_f = \left[\frac{(I/A)^2}{a_1 + (I/A)^2} \right] \times a_2 \tag{10}$$

Where η_f, is Faraday efficiency, a_i are empirical parameters, an electrode area and I is current A. According to Faraday's law, the production rate of hydrogen in an electrolyser cell is directly proportional to the transfer rate of electrons at the electrodes, which in turn is equivalent to the electrical current in the external circuit. Hence, the total hydrogen production rate in an electrolyser, which consists of several cells connected in series, can be expressed in Equation (11):

$$\dot{n}_{H_2} = \frac{NI}{2F} \eta_f \tag{11}$$

Where, N is number of cells in series. The water consumption and oxygen production rates are simply found from stoichiometry.

$$\dot{n}_{H_2} = \dot{n}_{H_2O} = 2\dot{n}_{O_2} \tag{12}$$

Table 1: Parameters in equations 9-10 obtained from U-I curve (Ulleberg, 1989)

r_1	8.05e-5 Ωm²	t_2	8.424 ºCm² /A
r_2	-2.5e-7 Ωm²/ºC	t_3	247.3 ºC²m² /A
S	0.185 V	a_1	250 mA²/cm⁴
t_1	-1.002 m² /A	a_2	0.98

The electrolyser can operate in two power modes (constant or variable power).The controller unit has two modes, the difference between them occurs when the electrolyser works (switch ON). Both of them have a set point power P_{idle} (minimum power), when the electrolyser is ON mode 1 sends maximum power between PV generated and set point to the next component, so using auxiliary power is necessary but mode 2 always sends PV power when the electrolyser is ON. This means that in constant power mode, the controller will allow the electrolyser to operate at a power below the set limit for idling. Figure 3 is presented .to show the system performance with auxiliary power (5,000 W) or without auxiliary power.

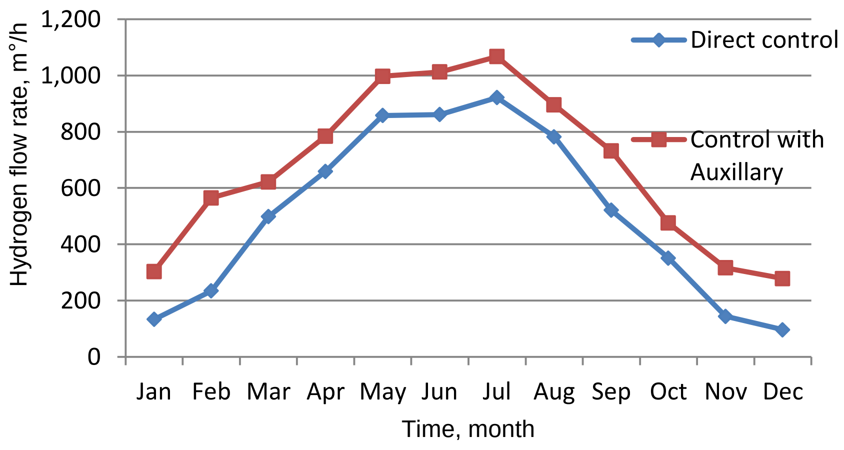
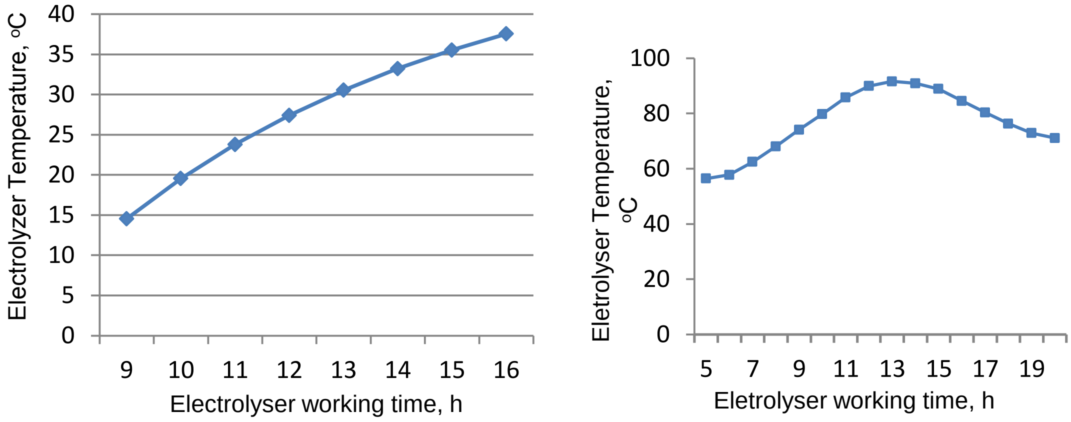


Figure 3: Predicted hydrogen production with and without auxiliary power

The temperature of the electrolyser can be defined using simple or complex thermal models, depending on the need for accuracy. A method to calculate the electrolyser's temperature is to assume a constant heat generation rate and heat transfer rates for a given time interval. If the time steps are chosen sufficiently small, the result is a quasi-steady-state thermal model (TRNSYS documentation part 4).



(a) (b)

Figure 4: Electrolyser temperature changes versus time, (a) Vienna, July 1st (b) Vienna, January 1st

$$C_t \frac{dT}{dt} = Q_{gen} - Q_{loss} - Q_{cool} \tag{13}$$

$$Q_{gen} = n_c (U - U_{tn}) I \tag{14}$$

$$Q_{loss} = \frac{1}{R_t}(T - T_a) \tag{15}$$

$$Q_{cool} = C_{w(}T_{wi} - T_{wo}) \tag{16}$$

$$T = T_{initial} + \frac{\Delta t}{C_t}(Q_{gen} - Q_{cool} - Q_{loss}) \tag{17}$$

Where, n_c cell numbers in series, T_a ambient temperature (°C), R_t thermal resistance (KW^{-1}), C_w heat capacity of cooling water (JK^{-1}), C_t electrolyte heat capacity (JK^{-1}), T_{wi} and T_{wo} temperature of cooling water in inlet and outlet (°C) are parameter of Eqs(13) to (17).

Table2: Main characteristics of PV electrolyser system

Photovoltaic	2 modules in series	12 modules in parallel	Modules current at the maximum power:35 A	Module area: 10 m²	Type 94	Slope of surface 45°
Electrolyzer	Electrode area 0.25 cm²	Number of stacks in parallel per unit: 1	Number of cells in series per stack: 20	Maximum temperature 90 °C	Type 160	Maximum allowable current density per stack: 300 mA/cm²

4. Conclusion

The hydrogen production based on a seasonal energy storage system has been described mathematically to identify possibilities according to the given Vienna weather data. Because of many renewable energy sources in Austria, saving is a big issue. In the present work, a transient model of a photovoltaic hydrogen system has been implemented in the mathematical simulation environment and utilized to predict its operational behaviours through numerical simulation. In this paper, TRNSYS is implemented as a tool to show the differences in hydrogen generation rate and power for whole year. As the seasonal energy storage system is quite sophisticated, it usually needs a separate control system for controlling hydrogen production in the electrolyser and the storage tank which it determines if the electrolyser operates in a minimum set point power entry (Figure 3). Figure 4 shows electrolyser's temperature changing in different working time. Generally all mathematical modelling are based on the local weather data which are provided by Meteonorm Co. Obviously from March to the end of October, there is much solar radiation and it would be enough for the electrolyser to work by PV power directly and without any auxiliary power supplement. All these mathematical simulations are repeated by MATLAB to valid the results obtained with TRNSYS. Figure 5 presents these two tool's performances on July 1st in Vienna and it shows that they have a good agreement.

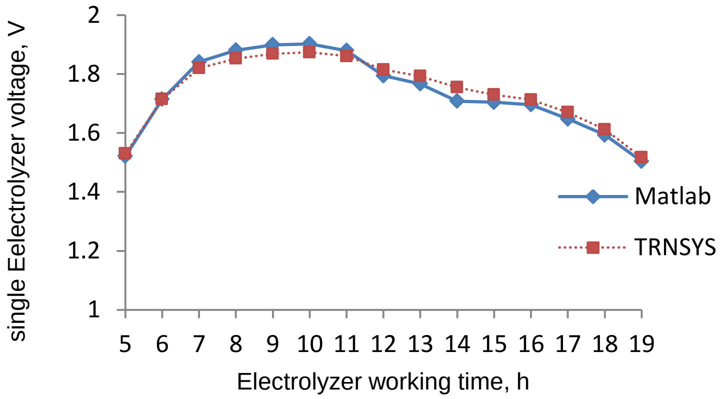


Figure 5: Single electrolyser voltage changes versus working time, July 1st, Vienna

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