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# Simulation of energy conversion in a plant of photocatalysts water splitting for hydrogen fuel

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Hydrogen is a kind of green fuel, and is considered as the substitute oil fuel for future. Although many of literature of photocatalyst water splitting have been presented, little of the literature focused on their energy conversions. Therefore, investigation of their energy conversions is carried out by simulation in this paper. Large energy is consumed in the plant for 1000 $m^3$ hydrogen fuels. In where, the efficiencies of hydrogen fuel generation are 29.9%, 15.6%, 10.5% and 7.95%, corresponding to the cases of one, two, three or four photons are needed to excite and generate one free electron by artificial light. While nature sunlight is utilized, the efficiencies are 48.4%, 25.2%, 17.8% and 13.6% corresponding to the four cases respectively; and the ratio between the combustion heat of generated hydrogen fuels and the total electric energy consumption is 319.0–333.0 %.



## 1. Introduction

Hydrogen is a kind of green fuel, which do not emit $CO_2$ and any other harmful substances when combustion. Hydrogen fuels are commonly generated via coal gasification, biomass gasification, water electrolysis, and water splitting by photo catalytic methods. Coal gasification for hydrogen fuels has been widely used in the fertilizer industry and IGCC (integrated gasification combined cycle). Zhang et al. (2013) obtained about 43.0–46.4 % energy efficiency with coalwater slurry gasification [1]. Parthasarathy and Narayanan (2014) carried out an experiment to generate hydrogen from steam gasification of biomass, obtained 63.0% of energy efficiency [2]. Nong et al. (2013) obtained 52.2–71.2 % of energy efficiency by black liquor gasification for biogas generation [3].

Hydrogen fuels can be achieved by water electrolysis. The electric energy consumption for hydrogen fuels is common exceeding 45.0 kWh per kilogram, and the energy efficiency is 92.0% for electrolysis on the wastewater containing anaerobic sludge [4]. Yilmaz et al. (2014) [5] perform energy analysis on a PEM (Proton Exchange Membrane) water electrolyzer driven by geothermal power for hydrogen production, obtained 62.2% of energy efficiency of PEM water electrolysis. Mbah J. et al. (2010) [6] report the ability to split $H_2O$ into hydrogen at a low working voltage by a special electrode, which was prepared via the ruthenium oxide ($RuO_2$) electrocatalyst deposited on silicon (Si) electrode. In the presence of $SO_2$, the theoretical equilibrium voltage requirement was only 0.19 V; thereby significantly reducing the energy consumption in hydrogen fuels generation by electrolysis.

Solar energy is the most abundant renewable energy resource available, thereby, generation of hydrogen fuels from water using solar energy is considered as a good ideal for energy source in future. Water electrolysis combined with PVC (photovoltaic cell) is a way of hydrogen fuels generation indirectly utilizing solar energy. Additionally, hydrogen fuels can be generated by photo catalytic water splitting directly utilizing solar energy. The practices of photocatalysts water splitting for hydrogen fuel have been carried out for 40 years. The practices were mainly catalyzed with catalysts of titanium dioxide, manganese compounds, tungsten oxide, nickel and silicon.

The basic $TiO_2$ photocatalysts water splitting reactor was carried out by Honda and Fujishima (1979). Which reactor successfully generated $H_2$ and $O_2$ at the surface of the Pt electrode and $TiO_2$ electrode, in the condition of photo irradiating on a $TiO_2$ electrode [7,8]. In order to enhance efficiency of photocatalyst water splitting, nano-scale particles of $TiO_2$ were used in the recent years. For example, Hiroshi Kominami et al. (2002) got 245 μmol/h of $H_2$ production rate catalyzed by nano-scale particles of $TiO_2$ [9].

Yoong et al. (2009) [10] developed a copper-doped $TiO_2$ photocatalyst for hydrogen production under visible light. Pérez-Larios et al. (2012) carried out a research on water splitting by $TiO_2$/ZnO

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catalyst, got 1300 μmol/h of $H_2$ production rate. Which research proved that $TiO_2$/ZnO mixed oxides photoconductors is more efficiency than only utilizing $TiO_2$ as photocatalysts [11]. Lee et al. (2013) carried out a research on water splitting by $TiO_2$/CuO catalyst, got 5000–7200 μmol/h of $H_2$ production rate [12]. Mixed $WO_3$ particle is considered as a desirable catalyst for enhanced electron conductivity, and Ho et al. (2011) obtained 3300 μmol/h of $H_2$ production rate by tungsten oxide/cesium carbonate as catalyst [13]. Abdi et al. (2013) achieved the energy efficiency of (hydrogen/solar) 4.90% by photo catalytic methods utilized sunlight, which is the highest efficiency of photo catalytic water splitting reported in literature [14].

Although many of literature of photocatalyst water splitting have been presented, little of the literature focused on their energy conversions. Therefore, investigation of their energy conversions is carried out by simulation in this paper.

## 2. Methods

### 2.1. The structure of the photocatalyst water splitting plant

Based on the investigation of the basic researches mentioned ahead, it is obvious that the production rates of catalyzed by titanium oxide combined with ZnO and CuO are higher than others. They are regarded as the promising methods for industrial applications. In order to investigate their energy consumption and the efficiency of hydrogen fuels generation, a model of hydrogen fuels manufacture plant is composed as Fig. 1.

The manufacture plant mainly consists of water splitting chamber, a compressor and a $H_2$ separation unit. The water splitting chamber is installed with numbers of lamps and stirrers, and the reaction water is 3796 $m^3$ played in deep about100 cm. The separation unit is a membrane separation unit, which can separate gases by their different permeation rates in organic polymer menbrance [15], metal menbrance [16] or cermet membrance [17], under certain pressure. The membrane separation technology has been successfully applied in separation $H_2$ from the exhaust gas in Yulin energy chemical co., Ltd. and Yankuang Group Co., Ltd, China. The parameters of membrane separation are: Operating temperature, 65 °C; enter pressure, 7.45 MPa; outer pressure, 5.45 MPa [18].

### 2.2. Investigation of the least electron consumption for light irradiation

Shown in Fig. 2 is the mechanism of photocatalyst water splitting [7]. In where the electric energy converses to light energy at first, then the light energy irradiates the catalyst powder to activate the electrons from the basic orbital to the active orbital of the molecules or crystals, generating free electrons and holes. Finally, the free electrons are donated to the hydrogen ion in the water, generating hydrogen gas, and the holes accept electrons from the hydroxide ions in the water, generating oxygen gas. The mechanism of photocatalyst water splitting can be described as Equations (1)–(3)

$$hv + TiO_2 \rightarrow TiO_2 + e^- + h^+ \quad (1)$$

$$4^-OH + 4\,h^+ \rightarrow O_2 + 2H_2O \quad (2)$$

$$4H^+ + 4e^- \rightarrow 2H_2 \quad (3)$$

The light energy exists in the form of photons; at least one of those photons is consumed to generate one free electron in the electrons activated process. And two free electrons are consumed to generate one $H_2$ molecule. Thereby, the least number of photons is two times of the numbers of $H_2$ molecules. Provided the conversion is a% from electric energy to photons, the least electric energy consumption for light irradiation can be calculated by Equation (4).

$$E_{ir.least} = \text{Light energy}/a\% \quad (4)$$

where, a% = 0.58 for the common incandescent lamp, in which the electric energy converses to 42.0% of heat, 22.0% of sensible light and 36.0% of infrared light. The light energy is the numbers of photon by the energy of each photon, the numbers of photons is two times of the numbers of $H_2$ molecules, and the energy of each photon is their average value of 4.2 × $10^{-19}$ J. Thereby, the least

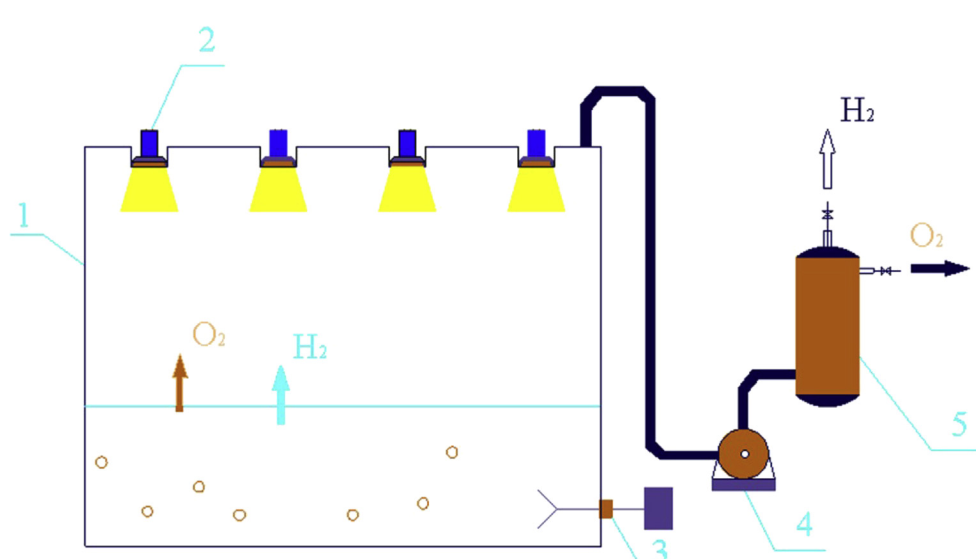


**Fig. 1.** The model of hydrogen fuels manufacture plant .1: water splitting chamber; 2: lamp; 3: stirrer; 4: compressor; 5: $H_2$ separation unit.