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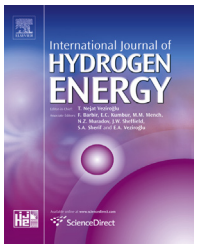

Simulation of transport phenomena in a photo-electrochemical reactor for solar hydrogen production

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ABSTRACT

A numerical simulation of transport phenomena in the photo-electrochemical (PEC) reactor is performed. The transport phenomena equations include the Navier–Stokes, the respective energy equation for electrolyte, and the radiative transfer equation (RTE). Two different designs, design A, and design B of photoelectrochemical reactors are suggested. The hydrogen production rate and solar-to-hydrogen efficiency are estimated for each design at different solar incident flux ranged from 500 to 2000 W/m^2 in increments of 500 W/m^2. Results have shown that the solar-to-hydrogen efficiency increases as solar flux increases for both designs. Its predicted values could reach 12.8% for design A, and 13.1% for design B. Moreover, by increasing the solar incident flux, the hydrogen volume production rate is increased as well. It is found to be 79 L/m^2·h for design A, and 85.4 L/m^2·h for design B. Comparison between currently predicted results and previous data indicates an enhancement of solar-to-hydrogen efficiency and hydrogen production that can be achieved with the suggested design.

Introduction

Hydrogen has the highest energy content per unit mass than any other fuel, making it especially valuable in many applications. It is considered the best candidate for replacing fossil fuels due to its cleanliness, availability and efficiency [1]. The increasing use of fossil fuels significantly increases the carbon dioxide concentration in the environment and consequently raises the global warming issue. Hydrogen can be produced using different renewable energy sources such as solar, geothermal, biomass, ocean, wind and hydro [2]. However, each method presents diverse advantages, as well as some challenges at the same time [3]. For instance, Hydrogen from biomass and fossil fuels can be produced using a Thermo chemical process. It includes various techniques such as Cu–Cl and Mg–Cl cycles [4]. This process has some advantages including the exploitation of waste heat, renewable energy and nuclear energy. Moreover, producing hydrogen from water using a natural energy source such as sunlight will

Abbreviations: PEC, Photoelectrochemical; QE, Quantum efficiency; FTO, Fluorine-doped tin oxide; TCO, Transparent conductive oxide.

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significantly contribute to the energy and environmental concern at a global level. In fact, different methods are used for solar hydrogen production that include the electrolysis of water using a photovoltaic cells, water splitting using photo-electrochemical cells, photo-biological and photo-degradation systems [5]. Some of the potential sources to produce hydrogen are electrical, thermal, biochemical, photonic, electro-thermal, photo-thermal, photo-electric, photo-biochemical, and thermal-biochemical [6]. The choice of the technology type depends on the source availability, costs, application of the usage and the maturity of this technology.

Hydrogen can also be produced by splitting water (electrolysis) [7,8]. Based on this method, the hydrogen can be obtained by photo-electrochemical (PEC) water splitting based on immobilized photo catalysts in thin films and by photo-catalytic (photochemical) water splitting based on powder photo catalysts in slurry system [9]. The photoelectrochemical (PEC) water splitting system for hydrogen production is one of the promising technologies that uses renewable energy such as sunlight. It produces non polluting fuels, the reactant and products of the reaction are environment friendly and solar energy is accessible to everyone. The PEC reactor contains two electrodes immersed in an aqueous electrolyte. There are several types of photoelectrodes such as n-type, p-type, coupling of n-type and p-type, hybrid, monolithic-bipolar and monolithic electrical connection as reported in Refs. [10,11]. As the semiconductor electrode (photoelectrode) is facing the illumination, it absorbs part of the light which has energy higher than the energy band gap (E_g). The short wavelength part generates electrons and electron holes. Those electron holes oxidize the water to get the oxygen and electrons which transport through an external circuit to reduce hydrogen ions which transport from anode to cathode in an aqueous electrolyte to generate the hydrogen. The long wavelength part is used to heat the electrolyte and consequently reduces the water splitting potential.

Fujishima and Honda [12] illustrated the capability of electrolysis of water without electric power using a photo anode covered with n-type TiO_2. Consequently, many research studies have been extended to split water into hydrogen and oxygen more effectively. The decomposition of water occurs according to the following equations:

$$\text{Excitation of photo anode by light}: TiO_2 + 2h\nu \rightarrow 2e^- + 2p^+ \quad (1)$$

$$\text{At photo anode}: 2p^+ + H_2O \rightarrow \frac{1}{2}O_2 + 2H^+ \quad (2)$$

$$\text{At metal cathode}: 2e^- + 2H^+ \rightarrow H_2 \quad (3)$$

$$\text{The overall reaction is}: H_2O + 2h\nu \rightarrow \frac{1}{2}O_2 + H_2 \quad (4)$$

Most of the previous research studies were aimed to improve the materials of photoanode to enhance the solar-to-hydrogen efficiency and improve the hydrogen production rate [13–16]. Licht [17] suggested a new model, which explained the restriction of the energy band gap to improve the efficiency for the first time. His objective was to raise the temperature of the electrolyte in order to lower the water splitting potential to enhance solar-to-hydrogen efficiency. Latter Licht [18] confirmed his previous goal using a molten Sodium hydroxide (NaOH) as an aqueous electrolyte that will never boil. He supposed that saturated NaOH is useful medium for water electrolysis at a very high temperature. By using Silicon (Si) which has a small band – gap, an improved of the solar-to-hydrogen efficiency can be achieved.

Boudjemaa et al. [19] used hematite Fe_2O_3 as a photo-cathode to obtain 6 ml/((g catalyst) min.) rate evolution experimentally. They concluded that the best activity was occurred in solution of sulfite ion (SO_3^{2-}) consisting of 0.5 M with 13.8 pH. Kudo [20] reported that the highest activity for the hydrogen production can be occur using Pt-loaded (photocatalyst) $AgInZn_7S_9$ (2.3 eV) immersed in an aqueous electrolyte consisting of potassium sulfite 0.5 M K_2SO_3. This resulted in hydrogen production rate 944 μmol/h for 33 cm^2 effective areas at 20% quantum efficiency at 420 nm using 300 W Xe lamp. An interesting investigation was conducted by Carver et al. [21]. They developed a two PEC reactor designs to study the effect of the sheet resistance of fluorine-doped tin oxide (FTO) electrode on the potential, and current density distributions at which the oxygen bubble formation at the photoanode. They concluded that the saturation of the electrolyte close to the photoanode surface with oxygen was occurred at current densities as low as (2–3 Am^{-2}). Furthermore, the oxygen saturation ratios could be decrease by increasing the electrolyte flow rate through the reactor. Lopes et al. [22] presented an innovative PEC cell and tested a three different photoelectrodes: WO_3 applied on metal and on Transparent Conductive Oxide glass (TCO-glass) substrate and undoped hematite deposited on TCO-glass substrate. They obtained the highest photocurrent density of 0.90 mA cm^{-2} with photoelectrode of WO_3-Metal at 1.45V_{RHE}, and the hydrogen evolution rate of 0.27 mmol H_2 s^{-1} and a STH efficiency of 1.28%. For WO_3 and undoped-Fe_2O_3, the Photocurrent was: 0.30 mA cm^{-2} and 0.40 mA cm^{-2}. They proposed a Teflon diaphragm in the new PEC cell, they found that when transparent WO_3 photoelectrode was used, a 47% photocurrent density enhancement was achieved.

Hernández et al. [23] developed new designed transparent, conductive and porous electrodes of photo-electrochemical water splitting for a compact laboratory. They reported that the new electrodes are considered as the ideal for testing new anodic and cathodic photoactive materials working in tandem configuration for solar fuels production by water photoelectrolysis. Choi et al. [24] analyzed solid polymer electrolyte (SPE) based on Butler–Volmer kinetics for electrodes and transport resistance in the polymer electrolyte. They studied the relation between applied terminal voltage of the electrolysis cell and current density of Nernst potential equation, exchange current densities, and conductivity of polymer electrolyte. They reported that the conductivity of the solid polymer electrolyte inversely proportional to the overpotential where the high anode overpotential is the restrictive cause for the whole process and responsible for the energy needed for the cell. Hernández et al. [25] prepared the photoanode by depositing a thick film of TiO_2 nanoparticles on the FTO-side of the drilled electrode, by the doctor blade method. They reported that it can be used to reduce the overpotential due to the distance between anode and cathode. Hernández et al. [26] studied the effect of the bubbles formation and