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A virtual lab as a complement to traditional hands-on labs: Characterization of an alkaline electrolyzer for hydrogen production

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ABSTRACT

Laboratories are commonly included as part of university courses as a way to relate theoretical lectures with experimental processes. In this sense, an excellent tool widely employed in academic teaching is the use of simulation software as a link between theory and traditional hands-on practice. This work is focused on the use of a virtual lab, i.e., a simulation, to study the electrolysis of water for hydrogen production, as a complement to traditional hands-on labs to help students comprehend the basics of this industrial process. At Complutense University of Madrid, students perform this laboratory as part of an engineering course included in the program of the chemical engineering bachelor's degree during their junior year. First, in this work, the hands-on lab is described as one of the cases proposed. Three more cases involving the virtual lab are also included as part of the laboratory experience. The last proposed case is focused on the theoretical background that students should have acquired during the hands-on and virtual lab sessions: three questions have to be addressed by the students. This work also includes a section where the opinions of students, their feedback after performing the labs, and the opinions of their professors (the authors) are incorporated to finally report some ideas for future work and conclusions about the ongoing teaching experience. A peculiarity of the use of virtual labs is that, in this case, they are performed after the hands-on labs, and therefore, they do not aim to prepare students for the laboratory by presenting the necessary theory for the experiment. The motivation of this virtual lab is to provide students with knowledge of the physical/chemical phenomena that govern the electrolysis process through the use of a theoretical model in order to reduce the limitations of the hands-on labs, such as the operating conditions, i.e., time, temperature, and number of cells, and to provide them with values for the parameters of a real Q4 system that can help with a critical discussion of the measured results.

1. Introduction

Currently, Information and Communications Technology (ICT) facilitates the development of new learning processes, particularly for university instruction. The use of these tools as part of the laboratories that are included in many of the offered courses as a method of improving teaching is becoming quite common (Gautam et al., 2016). In the field of chemical engineering, there are many teaching experiences in which simulations are used as part of new teaching training (Calvo and Prieto, 2016; Golman, 2016; Komulainen et al., 2012; Ruiz-Ramos et al., 2017) in the development of virtual laboratories (Domingues et al., 2010; Iborra et al., 2014; Rasteiro et al., 2009). Although simulations are a fundamental tool for the future chemical engineer (Dahm et al., 2002), there is still some skepticism as to the extent of the usefulness of these tools, in particular, their use as a replacement of the traditional hands-on laboratory experiences (Hawkins and Phelps, 2013). For this reason, virtual labs are usually implemented prior to hands-on labs. The effectiveness and relevance of this pre-laboratory training have been tested for its use as a tool that enhances the laboratory experience of the students (Gautam et al., 2016) whenever the difficulty and the goals have been stated previously (Hawkins and Phelps, 2013). Q5

The motivation of this study arose when checking the deficiencies and difficulties that students showed in understanding the process of the electrolysis of water while performing a traditional hands-on lab. The solution to this problem was found in the opportunities offered by the new ICT, specifically the development of

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Nomenclature

A (m^2) Area of the electrode
C_t ($J\,K^{-1}$) Overall thermal capacity of the electrolyzer
C_{pw} ($J\,g^{-1}\,K^{-1}$) Specific heat of water
HHV ($J\,mol^{-1}$) Higher heating value
HPCE ($kWh\,Nm^{-3}$) Hydrogen production energy consumption
HPE (%) Hydrogen production efficiency
I (A) Current
J ($mA\,cm^{-2}$) Current density
$\dot{m}_w$ ($g\,s^{-1}$) Water flow rate
n_c Number of cells of the electrolyzer
$\dot{Q}_{H_2}$ ($Nm^3\,h^{-1}$) Volumetric flow-rate of hydrogen
$\dot{Q}_{gen}$ (W) Generated heat transfer rate
$\dot{Q}_{loss}$ (W) Loss heat transfer rate
$\dot{Q}_{cool}$ (W) Cooling heat transfer rate
R_{cell} (Ω) Resistance of a cell
R_t ($K\,W^{-1}$) Overall thermal resistance of the electrolyzer
R_{total} (Ω) Resistance of the electrolyzer
T (K) Temperature
T_a (K) Ambient temperature
$T_{cw,o}$ (K) Outlet temperature of the cooling water
$T_{cw,i}$ (K) Inlet temperature of the cooling water
t (h) Time
U (V) Voltage
U_0 (V) Minimum voltage required
$U_{over.cell}$ (V) Overvoltage per cell
$U_{overvoltage}$ (V) Overvoltage of the system
U_{rev} (V) Reversible cell voltage
U_{tn} (V) Thermoneutral cell voltage
ε (%) Efficiency of an electrochemical cell
η_e (%)s Energy efficiency
η_{far} (%) Faraday efficiency

virtual labs. Typically, these virtual labs have been programmed as pre-laboratory training that could offer a viable solution to usual challenges, providing the students with a background of the theory behind the hands-on experience and some practical information mostly about the procedure of the labs, providing them with a holistic picture. However, since the difficulties faced by the students were detected mainly in the treatment and discussion of the experimental results and not during the performance of the hands-on lab experience which, for this experiment, is even simpler than for the rest of the experiments carried out during this course, a schedule different from the conventional one was chosen. Following the conclusions of Chini et al. (2012), who recommended the ad hoc design of the sequence of hand-on/virtual labs depending on the concept to be learn, the virtual lab was scheduled after the traditional hands-on lab. Therefore, the usual advantages of the pre-laboratory virtual experience mentioned before were offered in this case as a solution to the difficulties already encountered by the students and not as a preparative training. Some of the advantages of virtual labs that can be better exploited using this sequence (hands-on/virtual) are: the virtual lab provides errors-free data to the students that could help the students in the detections of measurement errors obtained in the hands-on lab (Pyatt and Sims, 2012); the students can modify variables, time scale, for instance, that could help in the interpretation and discussion of phenomena occurred during the experience (Trundle and Bell, 2010); due to the less setup time required for the virtual lab (Zacharia et al., 2008), students can perform more experiments/simulations and they gather more information to obtain a holistic picture of the practice. Finally, students can be critic with the setup of the hands-on labs, carried out in the previous session, and even propose improvements/changes based on their findings during the virtual lab (De Jong et al., 2010). Previous experiences on this schedule revealed better results for young students; the students obtained higher scores under this sequence than when the virtual laboratory was performed previously to the physical lab (Chini et al., 2012).

This work summarizes our experience in the implementation of a post-hands-on virtual lab. The main objective of this experience was to study the utility of a virtual lab carried out after the traditional hands-on labs for teaching the water electrolysis process. In this way, the specific goals of the post-hands-on virtual lab were not stated in the usual way that is done for pre-laboratory training experiences. Specifically, these objectives were as follows: 1) deepening the knowledge acquired during the hands-on laboratory session since the students could study and analyze the process of water electrolysis in more detail, performing simulations under operating conditions unavailable in our traditional laboratories; 2) utilizing “real” results (at least within the actual ranges of operational variables and parameters, given the good predictions of the selected research model) to improve the discussion of the experimental results obtained previously; 3) comprehending a theoretical model that describes the process; and 4) improving the use of scientific literature. In this work, the theoretical model used is that proposed by Ulleberg (2003). This model was chosen because it was developed for advanced alkaline electrolyzers (similar operating conditions to the conditions used during the hands-on labs) based on a combination of thermodynamics, heat transfer theory, and empirical electrochemical relationships, and the model can be employed under steady and transient system simulations.

2. Laboratory methods: hands-on and virtual labs

The laboratory experience presented in this work is carried out in two sessions: one in a testing laboratory (hands-on lab) and the other on a computer (virtual lab). The sequence followed in the experience is as follows: the experimental determination of the different parameters of the alkaline electrolyzer in the laboratory, followed by the virtual lab the next day. The materials and methods used in each of the two work sessions are described below.

2.1. Hands-on lab: equipment and procedure

The electrolysis of water is carried out in an alkaline electrolyzer, as shown in Fig. 1, consisting of 6 cells connected in series that can be used independently, i.e., the electrolyzer can use from 1 to 6 cells. The experimental installation includes a voltmeter and an ammeter to control the electric current (I) and voltage (U) applied to the system. In addition, the volumetric flow rate of oxygen is measured by a flow meter. The hydrogen produced is discharged into the atmosphere due to the high risk of explosion if accumulated in the lab, especially taking into account that some other lab experiences are carried out simultaneously. However, the hydrogen flow rates are calculated from the oxygen flow rates by the stoichiometry (twice the molar flow rate of oxygen).

The main goals of the hands-on lab are the characterization of the efficiency of the alkaline electrolyzer under different operating conditions (electric current and voltage), which are quite similar to those used industrially, and a comparison of its behavior working with a different number of connected cells (for instance, half capacity, 3 cells, and full capacity, 6 cells). The procedure followed Q6 during the lab experiment is described in Section 2.1.1.

Traditionally, alkaline water electrolyzers employ an aqueous potassium hydroxide solution with a concentration in the range of

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