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A mechanistic model supported by data-based classification models for batch hydrogen production with an immobilized photo-bacteria consortium

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ABSTRACT

A mechanistic model for batch hydrogen production through photo-fermentation with a consortium of purple non-sulfur bacteria is proposed and developed. Kinetic parameters were obtained from experimental photo-fermentations using fluorescent lamps as artificial light source. Three different light intensities (I) were tested in order to evaluate the influence of this process variable on growth rate and hydrogen production. Optimal conditions for state variables, such as I, pH and Temperature, were experimentally obtained and then used as parameters in the mechanistic model. Kinetics from either the proposed mechanistic model or the experimental photo-fermentations were compared, obtaining similar time trajectories for the process variables when operating at optimal conditions. However, this similarity decreased slightly at different light intensities, when the pH oscillated during the fermentations. Simulations under different initial conditions of substrate concentration, pH, and light intensity were run so as to generate data sets, used for constructing data-based classification models. A complete methodology, which entails a feature extraction step with Multi-way Principal Component Analysis technique and a proper classification stage using Support Vector Machines as algorithm, was proposed and addressed in order to develop such data models. These models were validated on both simulated and experimental data, which supported the robustness not only of the data-based models but also the developed mechanistic model. One-hundred percent classification performance was obtained after validating the data-based models, which envisages a further application of these models to other fields such as process monitoring, process control or fault diagnosis.

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Introduction

Biofuels have received remarkable attention since they are considered clean energy sources and hence a way to mitigate environmental pollution increase. Particularly, hydrogen has great potential as its combustion generates only water and it is characterized by a high heating value compared to other fuels [1,2].

Biohydrogen can be produced by several biological processes such as direct and indirect photolysis, dark fermentation and photo-fermentation [3–5]. This last alternative process is accomplished by purple non-sulfur (PNS) bacteria, which with the aid of light energy, convert organic matter i.e. volatile fatty acids (VFA) into CO_2 and H_2 at a higher theoretical yield under no O_2-evolving activity [4,6,7].

Until now, most of the research about hydrogen photo-fermentative production has been focused on using pure cultures [8–13], which can be expensive and impractical for degrading wastewaters or culture media with a mixture of different carbon sources [14]. Nevertheless, there are few studies using bacterial consortia that are reported in literature [15–18].

Many process variables affect hydrogen production by photo-fermentation, including light source and intensity, temperature, pH, carbon and nitrogen source, among others, which have to be of primary concern for an optimized fermentation [13,19,20]. Concerning to the optimal values reported in literature, Wang et al. (2010) found the best temperature range between 27.5 and 32.5 °C for *Rhodopseudomonas palustris* [21]. In addition, it has been documented 30 °C and pH = 7.0 as optimal values for several species of photo-bacteria [8,11,18,22–27].

It is worth mentioning that the optimal pH reported for the nitrogenase enzyme (reducing N_2 to ammonium and producing hydrogen simultaneously) is between 7.1 and 7.3 [28], which explains the pH values addressed in most investigations [11,18].

Besides, it is known that the bacterioclorophylls pigments, found in PNS bacteria, are responsible for capturing photons in the ATP synthesis, which is highly required by the nitrogenase enzyme [29]. In this context, some authors have demonstrated the use of artificial light sources from 522 to 860 nm wavelengths, covering the absorption spectrums of pigments [30,31], which is an important factor to consider for their selection.

According to the literature, immobilization of PNS bacteria helps them to be more resistant to inhibition by ammonium [32] and improves hydrogen production. Entrapment of pure cultures is mostly used because provides appropriate and stable conditions for cell growth [33,34].

On the other hand, bio-hydrogen production by photo-fermentation is a complex process to model. Nonetheless, different kinds of models have been developed and reported [22,35–41]. Most of them are mathematical or numerical models based on assumptions and restrictions, dealing only with some of the relevant process variables. Most of the research has been done with suspended pure cultures of PNS bacteria species, such as *Rhodobacter capsulatus* [10,12,22,35,41], *Rhodopseudomonas capsulata* [36], *Rhodobacter sphaeroides* [11,37,38], and *R. palustris* [8,13,40], using different carbon sources e.g. lactic acid [35,37,38], benzoate [36], acetic acid, malate, propionate and butyrate [37]. Particularly, it is important to highlight the contribution by Obeid et al. (2009), who report the influence of the light intensity over the specific growth rate and hydrogen production rate [35].

Just recently, Zhang et al. (2015) developed piece-wise models for hydrogen production with *R. palustris* in a batch suspended photo-bioreactor, in which two growth phases and the stationary phase are included [42].

Other authors have developed mathematical models for immobilized cultures of *R. palustris* growing on glucose as carbon source [23–27]. First, Liao et al. [23] delivered equations for the maximum growth rate (μ_{max}), maintenance coefficient (m) and the growth associated kinetic constant (α) as a function of pH, temperature (T) and light intensity (I) [23]. Later, Guo et al. [24] developed a similar model in which m, μ_{max}, and α, are only dependent on T and pH. For all the referenced studies, fermentations were carried out with LED lamps at 6000 lux.

Apart from these models, there is a lack of a mechanistic model for immobilized bacterial consortium that takes into account different light intensities and can be validated on both simulated and experimental data. In this context data-based models, used for classification and fault diagnosis [43], could be applied to validate mechanistic models.

This work addresses a mechanistic model for hydrogen production through batch photo-fermentation with an immobilized consortium of PNS bacteria, where *R. palustris* is the predominant species [34]. This model takes into account the influence of light intensity, temperature and pH on biomass, substrate and product concentration, and is used for creating data-based classification models, which are validated on both experimental and simulated data so as to confirm the reliability and robustness of either the mechanistic or the classification models. Multivariate Statistical Process Monitoring (MSPM) and Machine learning techniques [44,45], barely used for process monitoring, fault detection, and fault diagnosis [43,46], are exploited in this research.

Materials and methods

The whole methodology applied in this research involves several steps including the experimental procedure at laboratory, where all photo-fermentations were set up; the proposal and construction of the mechanistic model that fits experimental data; simulation runs with such mechanistic model; a feature extraction step performed by the application of a Multivariate Statistical technique; data-based classification models development through a Machine learning algorithm, and validation of these models onto experimental and simulated data. These steps will be explained in the following subsections.

Experimental procedure

A hydrogen-producing bacterial consortium, mainly composed by *R. palustris* and immobilized on luffa fiber, was used as biological source in all the experimental