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Modelling and control of an alkaline water electrolysis process

Marisol Cervantes-Bobadilla[1], Ricardo Fabricio Escobar Jiménez[2*], José Francisco Gómez Aguilar[3], Tomas Emmanuel Higareda Pliego[4] and Alberto Armando Alvares Gallegos[5]

[1]*Posgrado del Tecnológico Nacional de México / Centro Nacional de Investigación y Desarrollo Tecnológico. Int. Internado Palmira S/N, Palmira C.P.62490, Cuernavaca, Morelos, México.*

[2]*Tecnológico Nacional de México / Centro Nacional de Investigación y Desarrollo Tecnológico. Int. Internado Palmira S/N, Palmira C.P.62490, Cuernavaca, Morelos, México*

[3]*Conacyt-Tecnológico Nacional de México /Centro Nacional de Investigación y Desarrollo Tecnológico. Int. Internado Palmira S/N, Palmira C.P.62490, Cuernavaca, Morelos, México*

[4]*Tecnológico Nacional de México / Instituto Tecnológico de Zacatepec. Calzada Tecnológico No. 27, C.P. 62780, Zacatepec de Hidalgo, Morelos. A.P. 45, Morelos, México*

[5]*Universidad Autónoma del Estado de Morelos/Centro de Investigación en Ingeniería y Ciencias Aplicadas. Av. Universidad No. 1001, Col Chamilpa, C.P. 62209, Cuernavaca, Morelos, México*

Email: esjiri@cenidet.edu.mx

Abstract: In this research, an alkaline water electrolysis process is modelled. The electrochemical electrolysis is carried out in an electrolyzer composed of 12 series-connected steel cells with a solution 30% wt of potassium hydroxide. The electrolysis process model was developed using a nonlinear identification technique based on the Hammerstein structure. This structure consists of a nonlinear static block and a linear dynamic block. In this work, the nonlinear static function is modelled by a polynomial approximation equation, and the linear dynamic is modelled using the ARX structure. To control the current feed to the electrolyzer an unconstraint predictive controller was implemented, once the unconstrained MPC was simulated, some restrictions are proposed to design a constrained MPC (CMPC). The CMPC aim is to reduce the electrolyzer's energy consumption (power supply current). Simulation results showed the advantages of using the CMPC since the energy (current) overshoots are avoided.

Keywords: MPC, system identification, modelling.

1 Introduction

One of the hydrogen main advantages is that it is environmentally friendly since its combustion does not release CO_2. However, despite being the most abundant element on the planet, hydrogen is mixed with other gases, so to obtain pure hydrogen, it is necessary to perform separation process as alkaline water electrolysis to separate it from other elements. Currently, approximately 41 million tons of hydrogen are produced in the world, 96% is obtained from fossil raw materials, a process that is costly and is based mainly on the gasification of hydrocarbons combined with water vapor at high temperature and pressure. The remaining 4% of the hydrogen production comes from the dissociation of the water molecule by means of electrolysis, during which oxygen

is also obtained, making it a high-performance process able to take advantage of the raw material in its entirety.
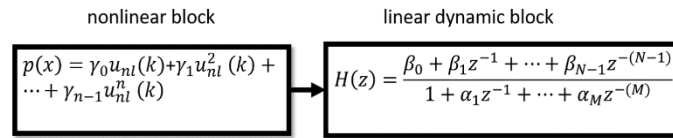
Nowadays, there are many efforts to improve the hydrogen production, these efforts have focused mainly on the developing new electrolyzers designs, the design of new materials for the electrodes and membrane, the analysis of the optimal space between the electrodes, the influence of a magnetic field in the hydrogen production, the electrolysis at high temperature and pressure, among others. [1-6]. However, there are very few works related to the electrolyzer dynamic modelling and the electrolyzer control [7]. In existing research, the electrolyzer is part of a larger system, and in most cases, the implemented control is of the on/off type, which depends on the other variables of the system. The aim of the present work is to propose both an electrolyzer model for control purposes and a control technique for the electrolyzer control.

2 Methodology

The electrolyzer model was developed using a nonlinear identification technique based on the Hammerstein structure which considers the system input and the output. The experimental data used to develop the model were obtained from an electrolyzer composed of 12 series-connected steel cells with a solution 30% wt of potassium hydroxide. After modelling the electrolyzer a control technique is proposed to ensure an optimal energy consumption. Simulation results of the electrolyzer control are presented.

3 Electrolyzer modelling using the Hammerstein identification technique

Because of lack of alkaline water electrolyzers models available to control the process. In this work, the Hammerstein identification technique is proposed, this technique consists of two stages or blocks Fig. 1, the first block contains non-linear static dynamics, and the second block contains linear dynamics.

nonlinear block   linear dynamic block

$$p(x) = \gamma_0 u_{nl}(k) + \gamma_1 u_{nl}^2(k) + \cdots + \gamma_{n-1} u_{nl}^n(k)$$ $$H(z) = \frac{\beta_0 + \beta_1 z^{-1} + \cdots + \beta_{N-1} z^{-(N-1)}}{1 + \alpha_1 z^{-1} + \cdots + \alpha_M z^{-(M)}}$$

Figure 1. Hammerstein structure.

The first block is modelled (identified) using the current feed (A) as the system input (Figs. 2) and the hydrogen flow as the system output (Figs. 3). To develop the model, different inputs signals were applied to the system to have more input and output data to reach higher model accuracy. This procedure is performed in open loop, the inputs currents were manipulated from 0 A to 47 A.
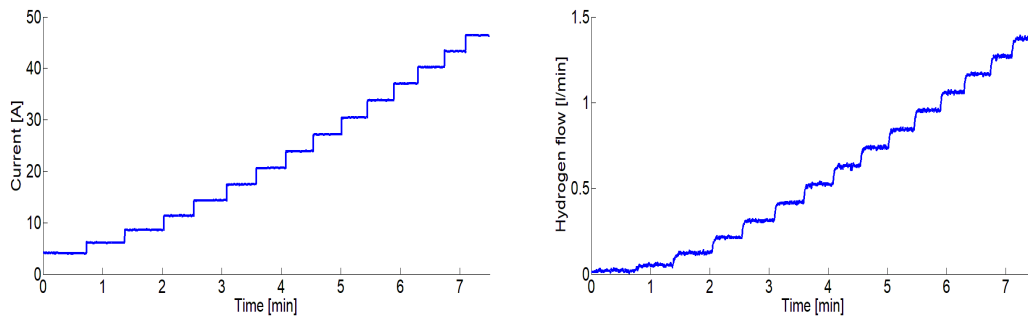
Figure 2. Current fed to the electrolyzer (A).   **Figure 3.** Hydrogen production (l/min)

Figs. 2-3 show the electrolyzer input and output experimental data used to identify the nonlinear static model.

The static non-linearity was identified using a polynomial function

$$p = -1.772 \times 10^{-8}x^5 + 2.567 \times 10^{-6}x^4 - 1.398 \times 10^{-4}x^3 + 3.518 \times 10^{-3}x^2 - 6.983 \times 10^{-3}x - 2.302 \times 10^{-4}$$
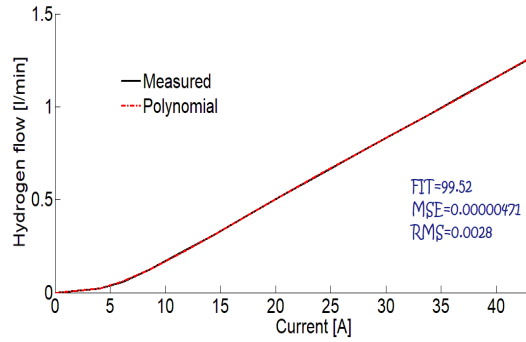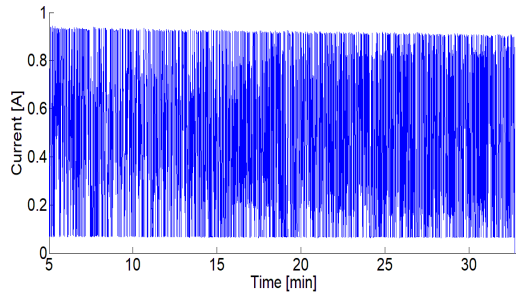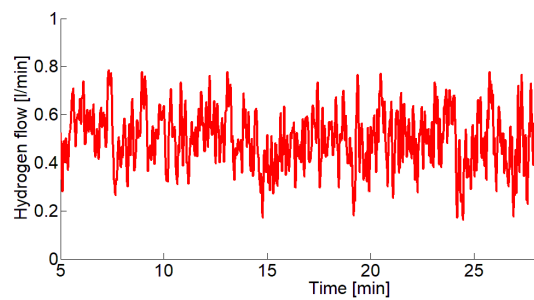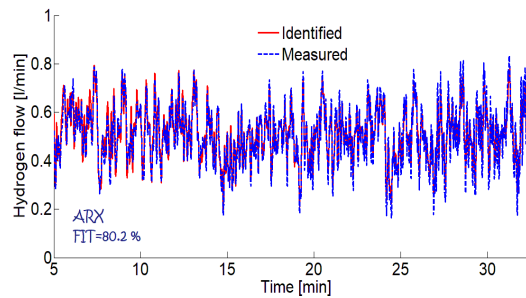

Figure 4. Static block validation.

Fig. 4 shows the result of the electrolyzer identification, the FIT value was 99.52%.

The second block contains the linear dynamics which are modelled for this particular case with an ARX structure [8] and the Pseudo-Random Binary Sequence (PRBS) (Fig. 5). Applying the PRBS to the hydrogen flow the resulting signal is shown in Fig. 6.

Figure 5. Input signal PRBS.   **Figure 6.** System response.

Once obtained the hydrogen flow signal with the PRBS signal, the following step is identifying the electrolyzer using the ARX structure.

Fig. 7 shows the comparison between the experimental data and the model approximation, the FIT value was 80.2%


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**Figure 7.** Dynamic block validation using
an ARX structure.

The model obtained using the ARX technique is:

$$H(z) = \frac{0.009672z^{-1} + 0.03917z^{-2} + 0.008136z^{-3}}{1 - 1.6730z^{-1} + 0.8806z^{-2} - 0.1507z^{-3}}$$

The cross method validation is used to validate the Hammerstein structure; the method consists of applying the same entering signal to the process and to the model. Fig 8 shows the current feed to the electrolyzer and to the model, to test the model in different operating points they were applied different current steps. Fig. 9 shows the model validation, the hydrogen flow values are represented by the green line and the model estimation is given by the red line, the model FIT value was 95.22 %. So, it is possible to conclude that the model is adequate to represent the electrolyzer dynamic.
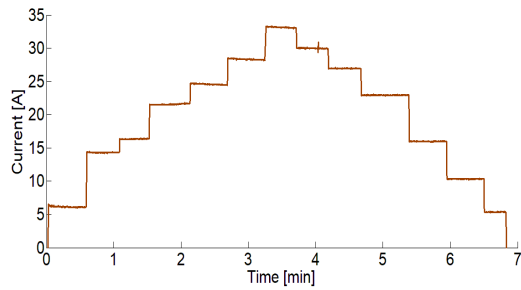
Figure 8. The input signal (Current (A)).
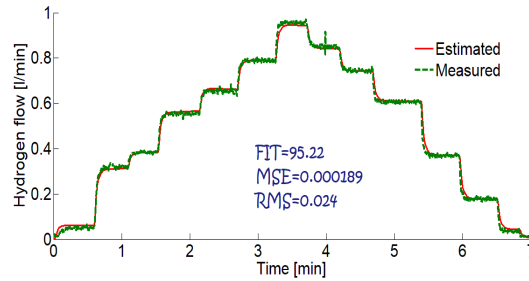
Figure 9. Model validation.

# 4   Model predictive control design.

In this section two controls are proposed an unconstrained Model Predictive Control (MPC) and a Constrained Model Predictive Control (CMPC). For the MPC formulation [9] it is assumed that the electrolyzer model is linear time-invariant, the cost function is quadratic, and the constraints are given in linear inequalities form. For the control design, the identified transfer function was converted to state-space model; the prediction horizon and the control horizon were set at 6 and 3 respectively.

The constraints for the CMPC were set in ΔU and $u(k)$ as follows

$$14 \leq u(k) \leq 44$$

$$0.002 \leq \Delta U \leq 0.004$$

Fig. 10 shows the hydrogen production (controlled variable) using the MPC and CMPC, the blue line represents the production set-point, the red line represents the MPC's control action and the dashed black line represents the CMPC's control action. It is important to note that even when the CMPC has a slower response than the MPC, its signal converges to the reference before than the MPC signal, this is due to the constraints establishment.
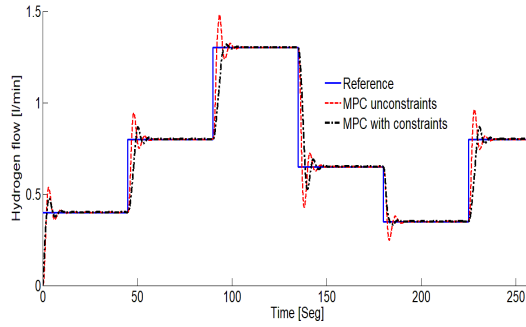
Figure 10. System response using a MPC
and CMPC (hydrogen production).

Fig. 11 shows the input Δu for the MPC and CMPC, the blue line represents the input Δu for the MPC and the red line represents the input Δu for the CMPC, for the CMPC case the constraints for the input were set at $0.002 \leq \Delta u \leq 0.004$, this avoids the overshoots on the feed current without compromising the controller performance as it was shown in Fig. 10. The restrictions over the input Δu caused that the power supply to the electrolyzer did not produce large overshoots in amplitude, this implies to have a better use of the current supplied to the electrolyzer, and an improved controller response, achieving better performance indices of the controller.

Fig. 12 shows the manipulated variable or input u (feed current), the blue line represents the input u calculated for the MPC and the red line represents the input u calculated for the CMPC. It is important to note that using the CMPC all overshoots are avoided, so it is possible to ensure that using the CMPC only the energy required to feed the electrolyzer will be applied without compromise the CMPC performance.
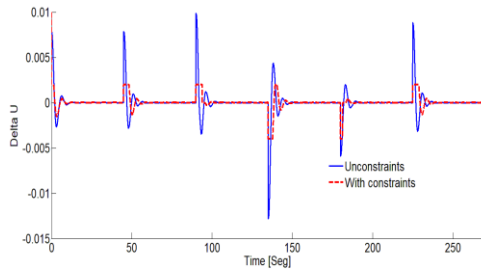
Figure 11. Increment in the future
input (Δu).
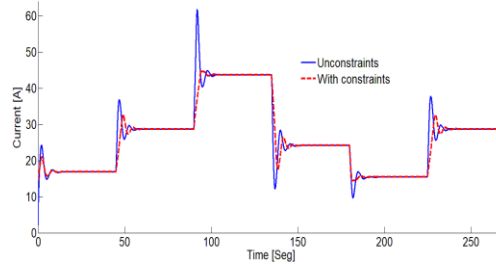
Figure 12. Process input (u).

5   Conclusion

In this work, alkaline water electrolysis process was modelled using the Hammerstein identification technique. The nonlinear identification FIT was 99.52, while the linear identification FIT was 80.2. Based on the electrolyzer model an unconstrained MPC and a constrained MPC were developed. Simulations results show that using the constrained MPC the overshoots on the feed current are avoided this means an optimal energy consumption. Furthermore, avoiding the feed current overshoots, the damage on the energy source is prevented.

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