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Modelling the Steady State Characteristic of pH Neutralization Process: a Neuro-Fuzzy Approach

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Abstract

In this paper it is presented a neuro-fuzzy approach on modelling the highly nonlinear steady state characteristic of pH neutralization process. The hybrid neuro-fuzzy technique is applied to model the titration curve from a weak acid with a strong base. Depending on the starting point of the solution that needs to be neutralized there can be determined the set of titration curves. Usually the titration curve has three major parts that describe the system behaviour: above the equivalence point, near equivalence point and under equivalence point. In order to control the process it is very important to determine process gain that in the pH case has an important variation due to its high nonlinearity. The hybrid neuro-fuzzy method provides a suitable solution in modelling this nonlinear titration curve. The resulted model can be used to control the pH neutralization process.

Key words: *advanced modelling, ANFIS, pH neutralization*

Introduction

The pH neutralization process has a highly nonlinear behaviour. The Adaptive Network based Fuzzy Inference System (ANFIS) method is used to model highly nonlinear systems, with a behaviour that can be described by rules. Nie et al. [1] proposed a simplified fuzzy model based on the identified rule-base derived using three network-based self-organizing algorithms: unsupervised self-organizing counter-propagation network, supervised self-organizing counter-propagation network, and self-growing adaptive vector quantization. Saoud et al. [5] present a dynamic modelling of pH neutralization process using Fuzzy Dynamic Neural approach. The proposed architecture is specific to pH chemical reactor and the simulation results proved also realistic dynamic nonlinear modelling. The main goal of pH neutralization process modelling is to ensure the best control algorithm. Inverse modelling can be used to find the more suitable control algorithm. Such controller is presented in [4], tested through simulations and experimental studies. Pishvaie and Shahrokhi [3] propose two control algorithms using a new approach of fuzzy modelling of titration curves. The efficacy of proposed approach is demonstrated via simulation and experimental study. In [6] Zanil et al. propose a hybrid model to identify the on-line pH characteristic of a neutralization plant.

In this paper it is presented a neuro-fuzzy approach for modelling the titration curve in the case of weak acid with strong base. The resulted model can be used with inverse modelling to build the pH controller.

The ANFIS Approach to Model the Titration Curve

The ANFIS method is extensively presented in Oprea et al. [2]. Model validation is obtained using Neuro-fuzzy editor from MATLAB [8]. The ANFIS editor presented in figure 1 comprises four sections for:

1. Loading, generating the plot, and erasing data.
2. Generating or loading a FIS (Fuzzy Inference System) structure.
3. Training the hybrid FIS structure.
4. Validating the trained hybrid FIS structure.

In Figure 1 is presented the training data set corresponding to a weak acid with strong base titration curve. The selected method for generating the FIS structure is Grid Partition. The MATLAB ANFIS editor uses an input/output data set. Usually the FIS structure generated or loaded is based on Sugeno architecture (figure 2). Using an input/output data set, the ANFIS generates a fuzzy inference system with adjustable parameters of the membership functions. Back propagation algorithm is used or in combination with a least square error method. This adjustment of system parameters is made so that the FIS structure fit the proposed data. For our titration curve the acid volume is kept constant and the volume of the strong base *Vb* is modified. The output data represents the pH of the resulted solution.

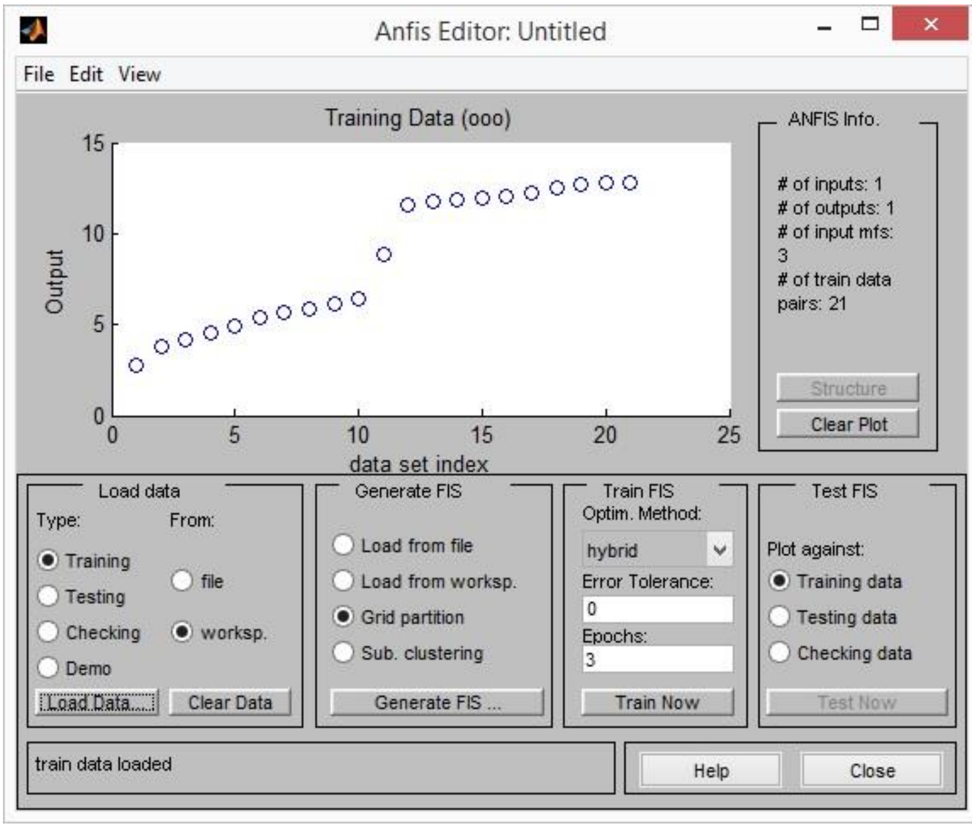

Fig. 1. ANFIS editor.

The set of experimental data used is from [7]. In Table 1, there are presented the used data set for training the hybrid structure (the pH variation with NaOH volume).

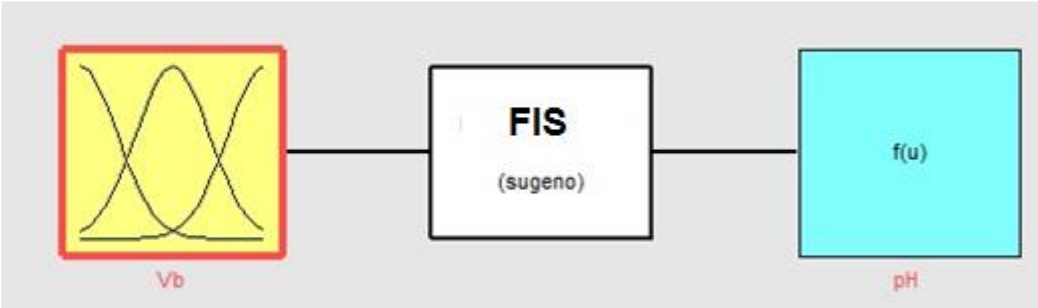

Fig. 2. Input-output representation.

Table 1. pH variation in case of titrating 50 mL acetic acid (0.2 M concentration) with sodium hydroxide (0.2 M concentration).

V_b	[acetic acid]	[acetate]	$[OH^-]$	$[H_3O^+]$	pH
0	0.2	0	0.0019	5.345E-12	2.7280
5	0.163636364	0.018181818	-	-	3.8058
10	0.133333333	0.033333333	-	-	4.1579
20	0.085714286	0.057142857	-	-	4.5839
30	0.05	0.075	-	-	4.9361
40	0.022222222	0.088888889	-	-	5.3621
45	0.010526316	0.094736842	-	-	5.7142
46	0.008333333	0.095833333	-	-	5.8207
48	0.004081633	0.097959184	-	-	6.1402
49	0.002020202	0.098989899	-	-	6.4502
50	0	0.1	0.0000	-	8.8760
52	-0.003921569	0.101960784	0.0039	2.55E-12	11.5935
53	-0.005825243	0.102912621	0.0058	1.717E-12	11.7653
54	-0.007692308	0.103846154	0.0077	1.3E-12	11.8861
55	-0.00952381	0.104761905	0.0095	1.05E-12	11.9788
56	-0.011320755	0.105660377	0.0113	8.833E-13	12.0539
60	-0.018181818	0.109090909	0.0182	5.5E-13	12.2596
70	-0.033333333	0.116666667	0.0333	3E-13	12.5229
80	-0.046153846	0.123076923	0.0462	2.167E-13	12.6642
90	-0.057142857	0.128571429	0.0571	1.75E-13	12.7570
100	-0.066666667	0.133333333	0.0667	1.5E-13	12.8239

The resulted titration curve (figure 3) is highly nonlinear. There are three sections that describe the titration curve: above equivalence point, near equivalence point and under the equivalence point. The steady state behavior is highly nonlinear due to the strong variation of pH process gain (1:50000). The ANFIS approach can provide an alternative to conventional modeling methods.

A neuro-fuzzy system is capable to learn new rules or membership functions, to optimize the existing ones. The starting point is the training data in creating the rule base and membership functions. There are three possible situations:

- the rule base is empty and the ANFIS creates rules until the problem is solved;
- the rule base is complete and the proper training lead to some rule elimination;

- the initial rule base has a fixed number of rules. After learning process old rules are replaced in order to maintain system size.

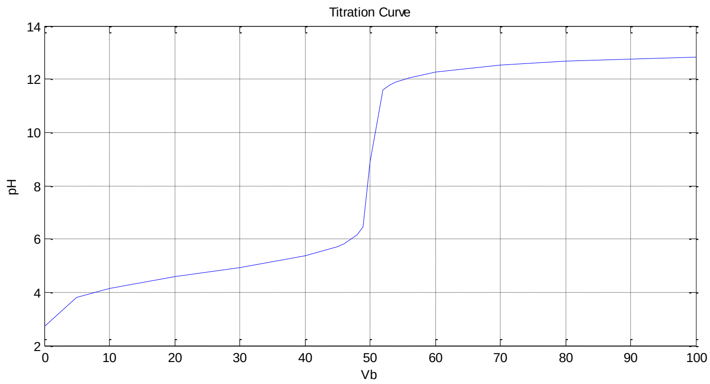

Fig. 3. The titration curve from experimental data from table 1.

The rule base must be checked for completeness, consistency and continuity. The presented case study starts with an empty rule base. The modelling methods applied to generate the FIS structure are grid partition (figure 1) and subtractive clustering. The ANFIS structure is Sugeno type. Using the grid partition method with hybrid optimization algorithm the training error is 0.93247 (after 5000 epochs, figure 4a.), while the backpropagation yields an error of 0.23371 (figure 4b).

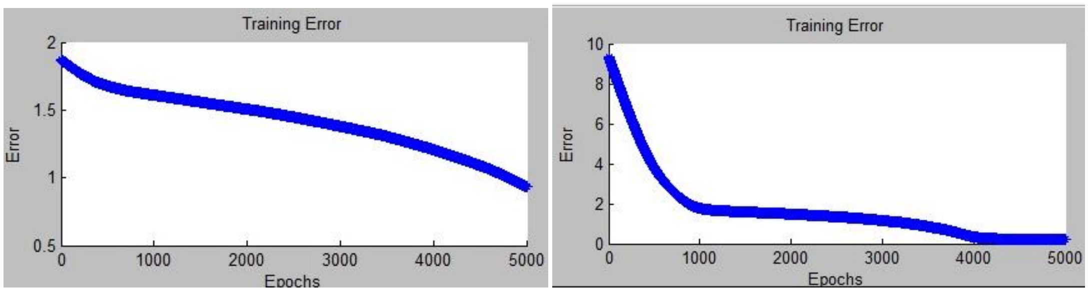

Fig. 4. The resulted training error – grid partition method.

a. hybrid algorithm b. back propagation algorithm

The model validation was done testing the trained FIS structure and verifying the model response ("*") versus experimental data ("o"). The results were better in the case of back propagation algorithm (figure 5b).

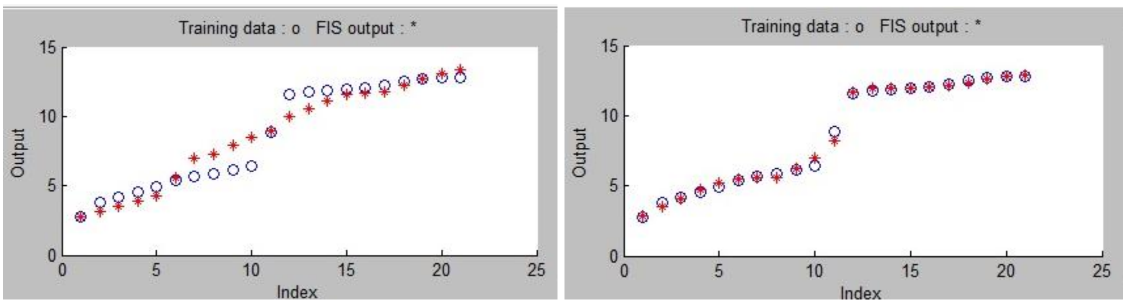

Fig. **5**. Resulted training data – grid partition method:

a. hybrid algorithm b. backpropagation algorithm

The second method for generating the rule base is subtractive clustering. The same data set is used but the training error is better in the case of hybrid algorithm (0.15284 instead of 0.94496 in the case of back propagation, figure 6).

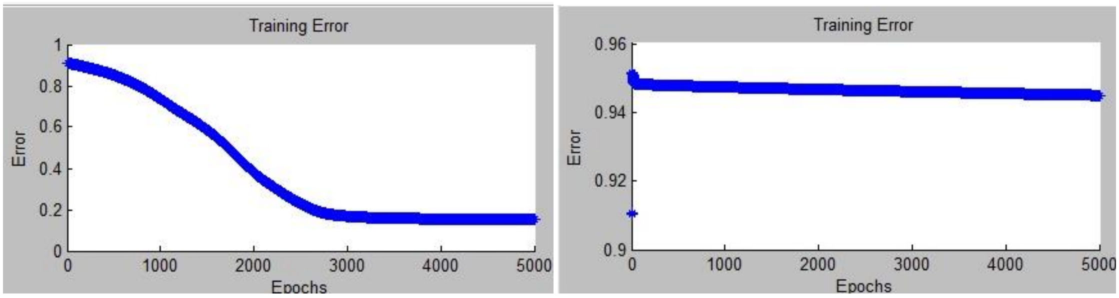

Fig. 6. The resulted training error – subtractive clustering method.
a. hybrid algorithm b. back propagation algorithm

The low values of error give a measure of model accuracy as seen in figure 7. The hybrid algorithm provides better results than back propagation algorithm; the resulted model better fits the experimental data (figure 7).

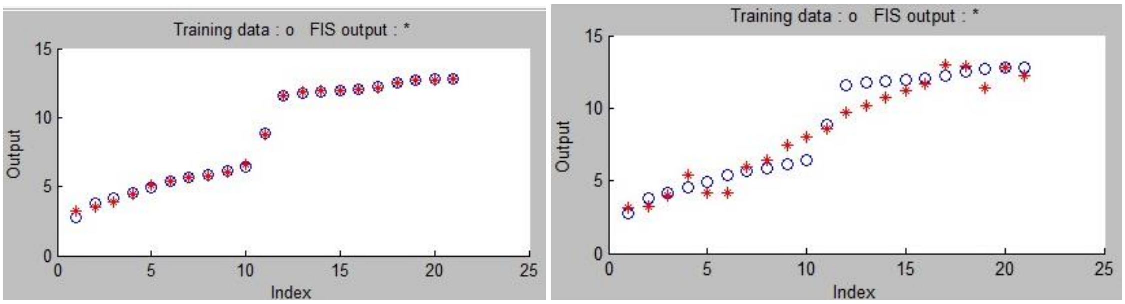

Fig. 7. Resulted training data – subtractive clustering method.
a. hybrid algorithm b. backpropagation algorithm

The methods for generating the rule base have different results. The best results are obtained with subtractive clustering method combined with hybrid optimization algorithm (figure 6 and 7). The resulted rule base is simple and formed by three rules according to the three zones in titration curve (figure 8)

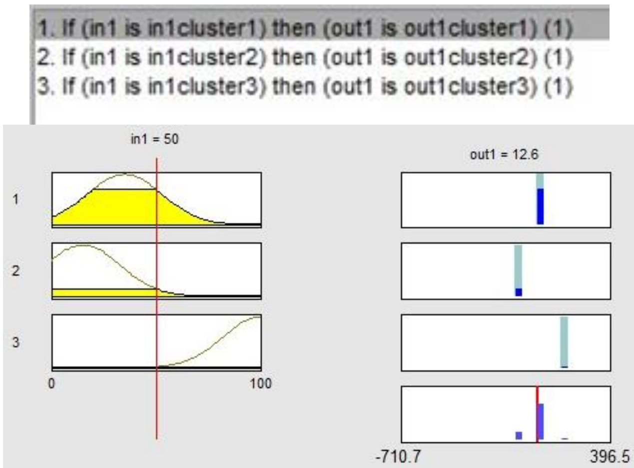

Fig. 8. The resulted rule base.

The membership functions used in subtractive clustering methods are from Gaussian type, while the membership functions used in grid partition method are in triangular shape.

Conclusions

ANFIS method is a proper solution in the case of highly nonlinear pH neutralization process. MATLAB ANFIS editor provides useful tools for comparing different solutions for ANFIS problems. The studied titration curve is typical for strong base weak acid titration. The acid volume is kept constant while the sodium hydroxide varies within safety range. The ANFIS method can be extended for other titration curves dependent on the pH of the solution to be neutralized. The rising of epoch's number leads to smaller error for the resulted models (in the same time the computing effort increases).

Modelling the titration curve is the first step in obtaining by inverse modelling the proper control algorithm for pH control.

References

1. Nie, J., Loh, A.P., Hang, C.C. – Modeling pH neutralization processes using fuzzy-neural approaches, *Fuzzy Sets and Systems*, **78**, Issue 1, 1996, p. 5.
2. Oprea M., Dragomir E.G., Mihalache S.F., Popescu M. – *Capitolul 11. Metode şi tehnici de predicţie a concentraţiei particulelor PM2.5 în mediul urban*. In: Iordache Ş., Dunea D. (editori) - *Metode de evaluare a efectelor poluării aerului cu particule în suspensie asupra sănătăţii copiilor*, Editura MatrixRom, Bucureşti, 2014, pp. 387-428.
3. Pishvaie, M.R., Shahrokhi, M. – Control of pH processes using fuzzy modelling of titration curve, *Fuzzy Sets and Systems*, **157**, Issue 22, 2006, p. 2983.
4. Salehi, S., Shahrokhi, M., Nejati, A. – Adaptive nonlinear control of pH neutralization processes using fuzzy approximators, *Control Engineering Practice*, **17**, Issue 11, 2009, p. 1329.
5. Saoud, L., Rahmoune, F., Tourtchine, V., Baddari, K. – Modelling pH Neutralization Process using Dynamic Neural units Approaches. *International Journal of Computer Applications*, **28**, 4, 2011, p. 22.
6. Zanil, M.F., Norhuda, A.M., Hussain, M.A., Omar, R. – Hybrid model of pH neutralization for a pilot plant, *Journal of Intelligent and Fuzzy Systems*, **26**, 2014, p. 551.
7. * * * – http://chemwiki.ucdavis.edu/
8. * * * – http://www.mathworks.com/help/fuzzy/anfis-and-the-anfis-editor-gui.html

Modelarea caracteristicii statice a procesului de neutralizare a pH-ului: abordarea neuro-fuzzy

Rezumat

În această lucrare este modelată caracteristica statică puternic neliniară a procesului de neutralizare a pH-ului utilizând o metodă bazată pe ANFIS. Metoda hibridă neuro-fuzzy este aplicată pentru cazul titrării unui acid slab cu o bază tare. In funcţie de pH-ul soluţiei de intrare de neutralizat se poate determina familia de caracteristici statice neliniare. In mod obişnuit curba de titrare are trei porţiuni distincte ce descriu comportamentul neliniar al procesului: deasupra punctului de echivalenţă, în vecinătatea punctului de echivalenţă sau sub punctual de echivalenţă. Pentru reglarea procesului este foarte importantă cunoaşterea factorului de proporţionalitate al procesului, care în cazul studiat are o variaţie foarte mare determinând puternice neliniarităţi. Metoda hibridă neuro-fuzzy este o soluţie potrivită în modelarea caracteristicii. Modelul obţinut poate fi utilizat pentru reglarea pH-ului.