

APPLIED ADAPTIVE DYNAMICAL IDENTIFICATION TO THE PREDICTION OF CHEMICAL PROCESS EVOLUTION A Case Study

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Abstract

A Self Tuning/Adaptive Control Algorithm has been developed and tested. This control has proved to be efficient to maintain the pH effluent of the bench set-up at neutrality.

It has been compared with other conventional controllers showing its greater capacity to stand the high changing dynamic of the controlled plant.

The minimal control equipment has been chosen in order to approach experimental conditions to industrial real cases. This selection increases the difficulty of the control. Adaptation has proved to be a reliable strategy even under additional constraints.

The control goal has been achieved: The developed Self Tuning/Adaptive Regulator guarantees, in a satisfactory way, pH neutralization without having to use holding stages and even standing in front of hard perturbations.

Keywords: prediction of chemical process evolution, adaptive dynamical identification.

1. Introduction

What happens when a process is non-linear, when it is too complex to be properly modeled, when it shows an 'unpredictable' time-dependent character or when it is submitted to 'uncontrollable' disturbances? How can we design a control strategy that copes with such a system?

Human beings success in universal evolution is based on our ability to learn and to modify, in consequence, our behaviour; if fact, to 'adapt' our behaviour to conform unpredictable and uncontrollable external conditions, taking in account our own time-changing capabilities. Control Theory uses the same strategies, the same 'conceptual blocks', to design *Adaptive Controllers* (Fig. 1).

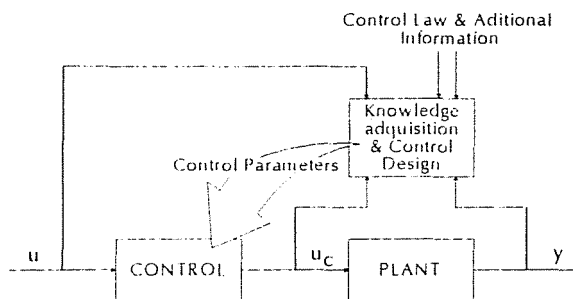


Fig. 1. Block diagram of an Adaptive Control Scheme

The work presented here describes the application of an adaptive scheme to the control of a system characterized by the above described undesirable properties: non-linear, time-dependent, high disturbed. In fact, we will discuss the application of Adaptive Control to pH-neutralization for wastewater treatment.

pH is a well-known measurement, but sometimes it seems to be a confusing concept in relation with control in chemical processes. Its logarithmic character and the presence of dynamic non-linearities, due to the measurement system, difficult the action of controllers. Although this peculiarities, our everyday experience shows the real need for accurate pH-controllers in chemical industry; in includes stationary and dynamic chemical processes.

One of the most common applications is wastewater treatment. Industrial wastewater may contain strong and week acids, bases and their salts in solution. Control goal is to keep pH of the effluent into the range of neutrality. The main difficulties, listed below (WILLIAMS *et al.*, 1990), are derived not only from the pH behaviour. The changing nature of the pH influent is in this case very important, too.

- 1) Depending on base addition, 10 orders of magnitude variations may be expected.
- 2) Feed composition and buffer capacity is unknown.
- 3) Flow rate is variable.
- 4) Small disturbances cause fast displacements of the system from neutrality to acid or base zone.

Traditional control systems are not efficient in most cases. Although under certain conditions they achieve good performances, they cannot cope with the wide range of the work conditions that pH-Controllers must stand. For instance, P.I.D. controllers become unreliable due to the variability of the titration curve.

There are some works which contemplate the use of adaptive controllers: GUSTAFFSON and WALLER (1983, 1984) propose a linear adaptive control based on the reaction invariant model (WALLER et al, 1980); WILLIAMS et al, (1990) incorporate information of the process non-linearities to design a nonlinear adaptive control with more flexibility.

Our aim is to develop a simple, but robust, *Adaptive Control strategy for on-line wastewater neutralization*, without having to consider great holding stages for off-line pH-neutralization, that increase the overall costs.

2. Description of the System

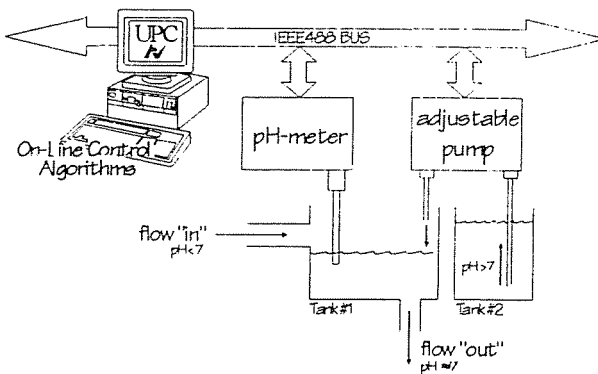


Fig. 2. Block diagram of the experimental set-up

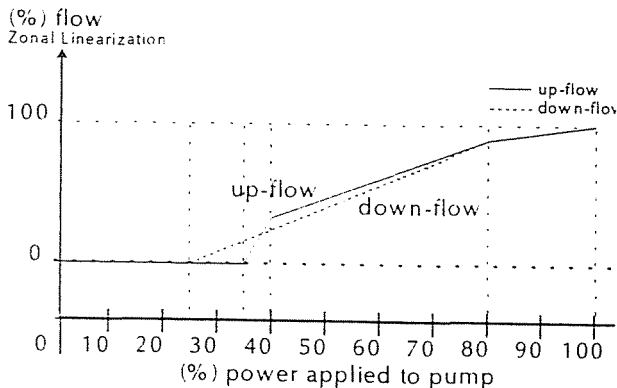


Fig. 3. Zonal linearized description of pump's flow/power ratio

The control algorithm has been tested in an experimental bench scale set-up. The plant was designed in order to minimize complexity, reducing the

variables involved for control purpose and the needed instrumentation to acquire information (*Fig. 2*).

pH is on-line neutralized in tank#1. The neutralization is achieved by adjusting the flow of base, coming from tank#2 through the pump (see in *Fig. 3*). The pH of the influent, effluent and neutralization base and also the flow rates are neglected.

3. The Adaptive Control

3.1. Structure

We consider a control algorithm based on the Self Tuning Regulator (S.T.R). This adaptive regulator can be thought of as composed of two loops; an inner loop for linear ordinary feedback; an outer loop for acquiring knowledge about the process and for the application of the knowledge to the recalculation of the controller in the inner loop.

- 1) When the process is worth-known the outer loop adjusts the parameters of the controller, that is, the outer loop 'tunes' autonomously the controller process (Self Tuning Reg.).
- 2) When the process changes (dynamic process) the outer loop has to recalculate, also autonomously, the parameters of the controller to 'adapt' its performance to the new process behaviour (Self Adaptive Reg.).

The most important topic for pH-control purposes is the 'adaptation' to the changing conditions of the controlled plant.

3.2. Dynamic Identification

Self Adaptive Regulation uses dynamic identification to build an on-line model of the controlled process. Many strategies may be used for this purpose. In this work Least Squares has been used to adjust the parameters of an ARMAX model. The result is a local linearized model of the controlled process. Least Squares has been chosen for its simplicity. Additional features, such as recursivity and memory are of great importance and will be further discussed.

3.2.1. The Structure of the Model

The selected ARMAX model can be expressed as follows:

$$y(i) + \sum_{j=1}^{n_a} \alpha_j y(i-j) = \sum_{j=1}^{n_b} \beta_j u(i-j) + \sum_{j=1}^{n_c} \gamma_j \varepsilon(i-j).$$

Equation can be easily rewrite using the 'delay operand' q^{-1} :

$$A(q^{-1})y(i) = B(q^{-1})u(i) + C(q^{-1})\varepsilon(i).$$

n_a , n_b and n_c should be experimentally chosen, for instance, applying the final identification algorithm.

3.2.2. Least Squares Algorithm

The last expression can be rewritten as:

$$\hat{y}(i) = \varphi_1(i)\vartheta_1(i) + \varphi_2(i)\vartheta_2(i) + \dots + \varphi_n(i)\vartheta_n(i)$$

or vectorially expressed:

$$\hat{y}(i) = \phi^T(i)\theta(i),$$

$\hat{y}(i)$ model output/model estimation,

φ_i collected in vector ϕ , are known functions,

ϑ_i collected in vector θ , are the 'adjustable' parameters, computed by the algorithm.

The Least Squares method applies to the minimization of the error between *system real output* and *linear model estimation*:

$$\varepsilon(i) = y(i) - \hat{y}(i) = y(i) - \phi^T(i)\theta,$$

$$V(\theta, i) = \frac{1}{2} \sum_{k=1}^i \varepsilon^2(k) = \frac{1}{2} \sum_{k=1}^i [y(k) - \phi^T(k)\theta]^2.$$

Recursivity: The amount of information used by the standard algorithm increases continuously. Recursivity fixes the order of the equations by using in each sampleperiod the processed information of the past one.

Memory: To develop the adequate learning capability involved in the identification's algorithm, forgetting must be implemented. By introducing

factor λ in the recursive least squares equations we achieve a desired exponential decreasing ponderation of the past.

Recursive Least Squares algorithm, with exponential forgetting factor, is described by the following set of tree equations:

$$\theta(i) = \theta(i-1) + K(i) \left[y(i) - \varphi^T(i)\theta(i-1) \right],$$

$$K(i) = \frac{P(i-1)\varphi(i)}{[\lambda I + \varphi^T(i)P(i-1)\varphi(i)]},$$

$$P(i) = \frac{[I - K(i)\varphi^T(i)]P(i-1)}{\lambda}.$$

3.3. Controller Design

The design of the Linear Controller

$$R(q)u(i) = T(q)u_c(i) - S(q)y(i)$$

(see the Controller Block – Fig. 4 –) is based on the method of Pole Placement.

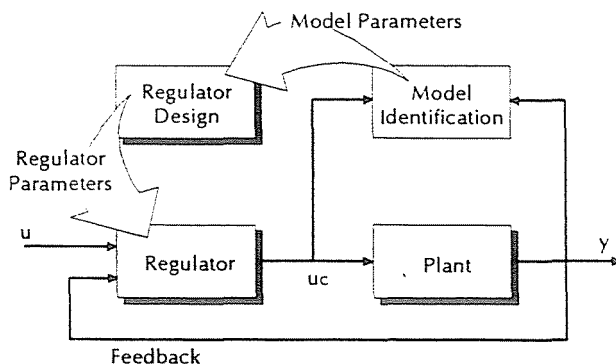


Fig. 4. Block diagram of the Self-tuning/adaptive Regulator

Two concepts have to be remarked:

The Identification block provides the Controller Designer block with a full process model $H(q)$. User/Programmer fixes the observer A_0 and the desirable model for the whole process $H_m(q)$.

An extended stability region D may be defined, too.

$$H(q) = \frac{B(q)}{A(q)} \quad \& \quad H_m(q) = \frac{B_m(q)}{A_m(q)}.$$

$B(q)$ must be factored taking into account the defined D region:

$$B(q) = B^-(q)B^+(q),$$

$$B_m(q) = B^-(q)\widehat{B}_m(q).$$

$B^+(q)$ is a monic polynomial with all its roots in the stability region D .

The following expression shows the objective of the control design algorithm:

$$\frac{B(q)T(q)}{A(q)R(q) + B(q)S(q)} = H(q) = H_m(q) = \frac{B_m(q)}{A_m(q)}.$$

Additional considerations drive us to the following Diophantic equation:

$$(q-1)^l A(q)\widehat{R}(q) + B^-(q)S(q) = A_0(q)A_m(q).$$

In order to solve this polynomial equation some physical constraints may be considered:

$$\text{gra}(S) < l + \text{gra}(A),$$

$$\text{gra}(\widehat{R}) = \text{gra}(A_0) + \text{gra}(A_m) - \text{gra}(A) - l.$$

The control law is finally defined with the help of the following equations:

$$S(q),$$

$$R(q) = B^+(q)(q-1)^l \widehat{R}(q),$$

$$T(q) = T(q) = \widehat{B}_m(q)A_0(q).$$

3.4. The Extended Controller

To cope with some unstabilities found during Self Adaptive Regulator experimentation, a non-linear self adaptive controller (*Fig. 6*) has been added to the original structure. The resulting Extended Dual Self Adaptive Regulator is described in *Fig. 5*.

During 'fine-tuning' operation, non-linear self-adaptive control (see Fig. 6), adjusts hysteresis cycle and out-power levels of the on-off controller.

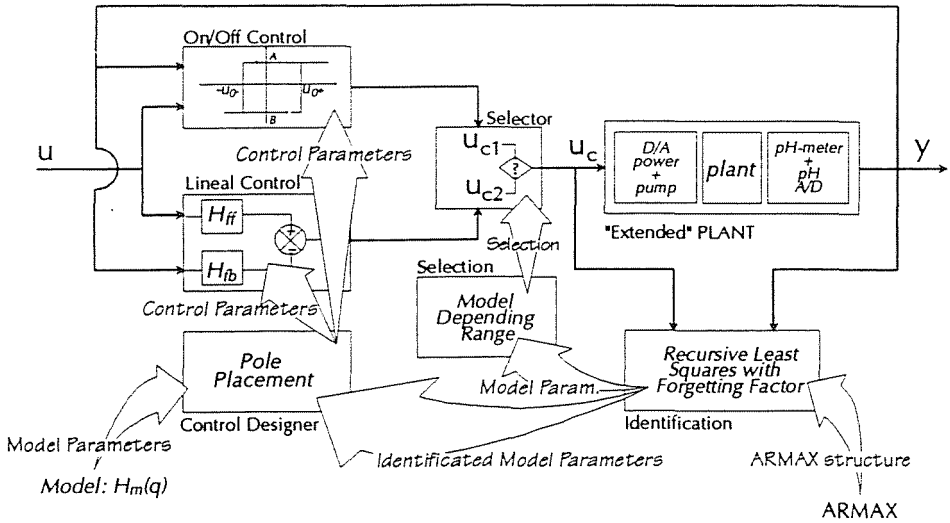


Fig. 5. Detailed block diagram of the Extended Dual Regulator

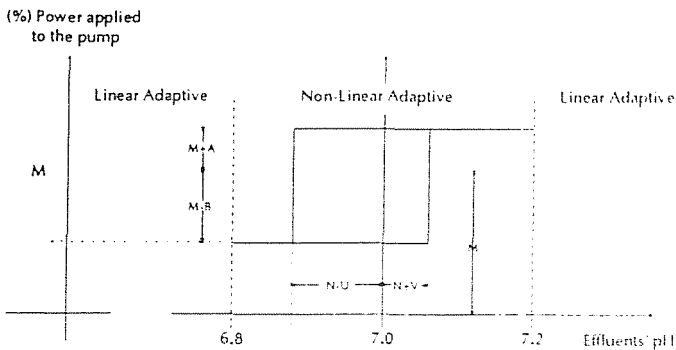


Fig. 6. Self-Adaptive non-linear controller description

3.5. Additional Control Data

Sample Time: 1.5 seconds

Look forward prediction: 5 sample time periods

ARMAX structure:

$$y(i) = -a_1y(i - 1) - a_2y(i - 2) + b_0u(i - 5) + b_1u(i - 5 - 1) + c_0\varepsilon(i).$$

Control Model:

$$H_m(q) = \frac{0.01}{q^2 - 1.49q + 0.5}$$

4. Experimental

The experimental design is shown in *Fig. 7*. Its simplicity makes it attractive from the industrial point of view. The influents, an acid mixture of variable composition and buffer capacity, flow through a stirred tank reactor of capacity 6l, where pH is measured and then base feed adjusted. Flowrates and composition of the streams are indicated in *Table 1*. Control goal is to maintain pH of effluent at neutrality.

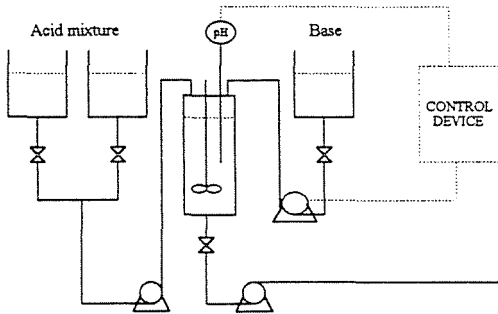


Fig. 7. Detailed experimental setup

Table 1
Experimental conditions

	Conditions 1	Conditions 2
Acid composition	0.04 – 0.06 M CH ₃ COOH 0.025 M (NH ₄) ₂ SO ₄ 0.025 M CH ₃ COONa	0.04 – 0.06 M CH ₃ COOH 0.006 M (NH ₄) ₂ SO ₄ 0.006 M CH ₃ COONa
Basic composition	0.15 M. NaOH	0.15 M. NaOH
Total flow	1.0 – 1.5 l/min	1.0 – 1.5 l/min
Case studies	case 1, case 4	case 2, case 3

Four cases have been analyzed (see *Table 1*). First, the behaviour of the self-adaptive controller under two different buffer capacities is considered. Then the system is perturbed with an acid pulse. Finally the performance of an adjusted P.I.D. controller and the self adaptive controller developed are compared, by applying them to the stabilization of the same experiment.

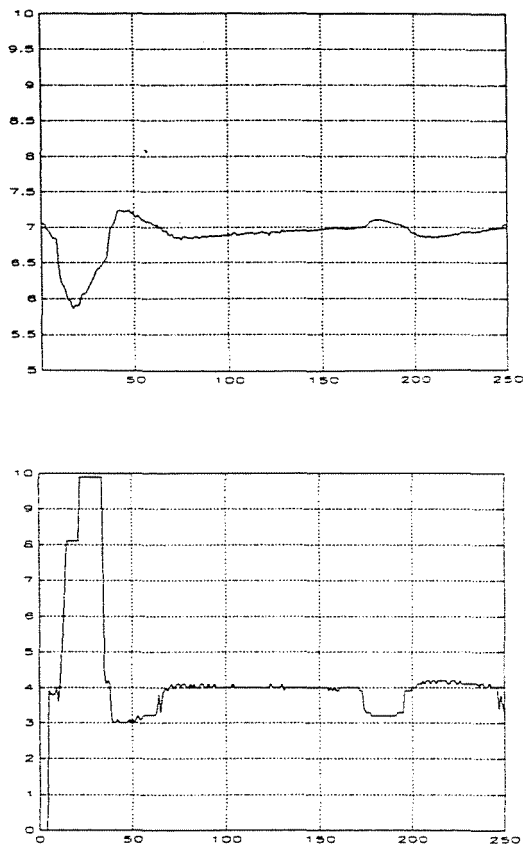


Fig. 8. a) pH evolution, case 1, b) Power to pump, case 1

Case 1

Although the behaviour of the self adaptive controller needs some time to identify the process then it drives the system near the neutrality with a high stability. In order to avoid pH oscillations of the starting time, it can be considered, as it was suggested by SHIMSKEY (1979), to feed back the effluent to the reactor.

Case 2

In this case buffer capacity of the solution is reduced. Consequently pH sensitivity is increased, and the system becomes more difficult to control. The controller gives also good results and maintains the neutrality, but it has more problems to stabilize the system than in case 1.

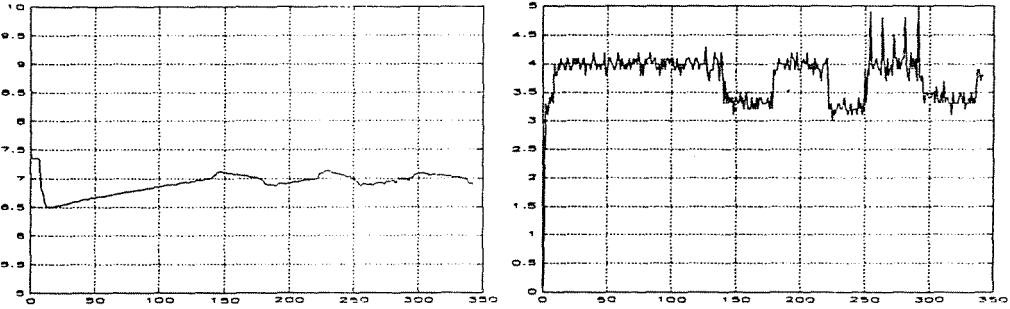


Fig. 9. a) and b) pH and power to pump, case 2

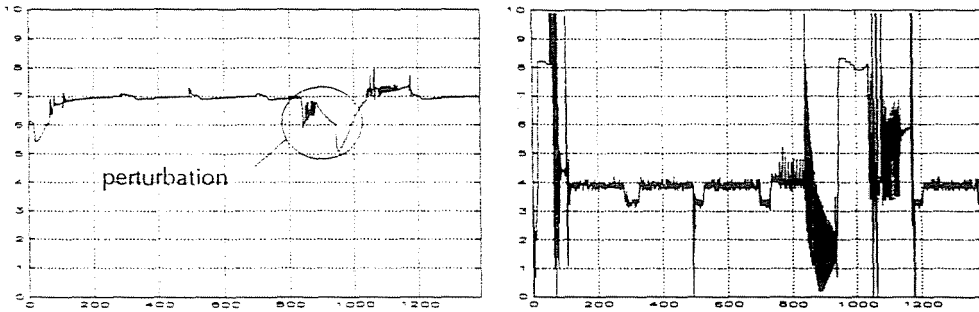


Fig. 10. a) and b) pH and power to pump, case 3

Case 3

An acid pulse has been introduced into the reactor. The controller reacts increasing the flow base addition and when pH is near 7 the flowrate is reduced. At this time pH decreases dramatically, probably because the solution is not homogeneous until some time after the pulse introduction. Then the controller returns the system to neutrality.

Case 4

A P.I.D. controller has been tested which was designed for different operating conditions. The controller is not capable to maintain the system at neutrality without oscillations because of the variations of the system from

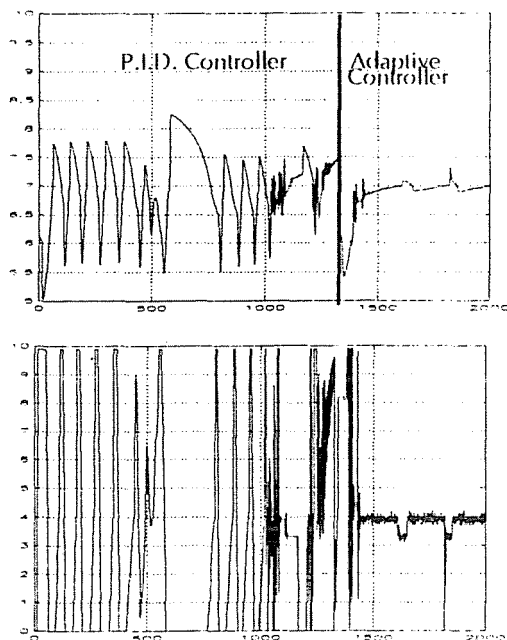


Fig. 11. a) and b) pH evolution and power to pump, case 4

the initial tuning conditions. When the self adaptive controller is activated, the system reaches quickly the neutrality.

References

- MAHULI, S. K. - RHINEHART, R. R. - RIGGS, J. B.: pH Control Using a Statistical Technique for Continuous On-line Model Adaptation. *Computers Chem. Engng.*, Vol. 17, No. 4, pp. 309-317, 1992.
- GUSTAFSSON, F. G.: An Experimental Study of Algorithms for Adaptive pH Control. *Chemical Engng. Sci.*, Vol. 40, No. 5, pp. 827-837, 1984.
- GUSTAFSSON, T. K. - WALLER, K. V.: Myths about pH and pH control. *AICHE Journal*, Vol. 32, No. 2, pp. 335-337, 1986.
- SHIMSKEY, F. G.: *Process-Control Systems*. Mc Graw Hill, pp. 263-272, 1979.
- WALLER, K. V. - MÄKLLÄ, P. M.: Chemical Reaction Invariants and their Use in Reactor Modelling, Simulation and Control. *Ind. Eng. Chem. Process Des. Dev.*, Vol. 20, No. 1, pp. 1-11, 1980.
- WILLIAMS, G. L. - RHINEHART, R. R. - RIGGS, J. B.: In-line Process-model-based Control of Wastewater Using Dual Base Injection. *Ind. Eng. Chem. Res.*, Vol. 29, pp. 1254-1259, 1990.