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NORTCLIFFE, Anne <http://orcid.org/0000-0001-6972-6051> and LOVE, J



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# A VARIABLE TRANSFORMATION APPROACH TO IN-LINE pH CONTROL

A. L. Nortcliffe and J. Love

University of Sheffield, UK

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**Abstract:** Current practice and research into pH control principally entails the use of Continuous Stirred Tank Reactors (CSTRs). Whilst the over-design of this process does indeed damp out disturbances, it is expensive and leads to problems with control. Industry requires systems that are:

- economical, both in terms of capital and operating costs
- robust from a control point of view
- operable and flexible from a process point of view

pH control of neutralisation is a difficult non-linear control problem. This is largely due to the gross non-linear behaviour of pH measurement, but also due to the variable time delays inherent in the process. Non-linear processes have traditionally been controlled by a combination of linear control methods and gain scheduling. However in the last few years much progress has been made in the development of non-linear control systems. This paper outlines a variable transformation approach, that is an anti-logging technique which removes the non-linearity at source and yields an hydrogen ion concentration which is easier to handle.

## Introduction

Many industrial processes entail the use of pH control. Applications are very diverse; Latrille et al[1] applied neural-networks to the production of lactic acid during the fermentation of milk and recently Deshpande et al[2] applied pH control to the wastewater from the sago industry. The most common process that calls for pH control is waste-water effluent treatment.

Historically the neutralisation process has largely been used as a test-bed for determining the effectiveness of innovative non-linear control methods. For example; Aoyama et al[3] used the neutralisation process to examine a control affine model approach identified by fuzzy neural networks. Many advances have been made in non-linear control methods and can be considered suitable for pH control, as reviewed by Gokhale et al[4]. Another review by Bequette[5] on the development of non-linear control systems utilised in the process industry also covered advanced methods applied to pH control.

Researchers in the pH control domain have mainly adhered to and concentrated on McMillian[6] plant design advice. The processes are over designed and consist of CSTRs. Research in this area is considered complete, as briefly demonstrated in a review by Nortcliffe et al[7], although studies on existing plant continue. For example; Palancar et al[8] recently reported on applying model reference adaptive control to neutralising a variety of streams of weak and strong acids with buffering in a CSTR. Also Lakshmi Narayanan et al[9] combined non-linear IMC, strong acid equivalent and an adaptive mechanism to control the pH in a CSTR.

However industry's need is for a cheap but effective solution to the problem to enable the legal requirements to be met the latest being the Environmental Act (1995) and to satisfy media pressure. Seider et al[10] illustrated that advances in non-linear predictive control enable these criteria to be satisfied simultaneously. End of pipe solutions are much cheaper and more attractive to industry. Research in this area is incomplete and minimal. Examples of studies in this field; Rhinehart's[11] research concluded that dual in-line base injection is preferable to single in-line base injection for acidic effluent streams. Following this study Williams et al[12] applied Process Model-Based Control (PMBC) to a dual base injection system and yielded results that were more than comparable with CSTR solutions. More recently Shukla et al[13] applied heuristic model control.

Gustafsson[14] and Pröll et al[15] studied control methods applied to plant design that combined the effective mixing of a CSTR with the in-line base injection approach. Karim et al[16] used a process model based on the same system to test an adaptive radial basis function network.

## Anti-logging Approach

The anti-logging approach is based upon research by Love[17,18] and is a variable transformation approach. The pH measurement is anti-logged yielding a linear signal: the concentration of hydrogen ions, as depicted in Figure 1.

The conversion from pH to $[H^+]$ is calculated from:

If $pH \le 7$ then $[H^+] = 10^{(6-pH)}$ (mg/m$^3$)

If $pH \ge 7$ then $[H^+] = -10^{(pH-8)}$ (mg/m$^3$)

Alkaline solutions are considered to be negative acids. The hole in the scale at pH 7 is in significant: consequently, the concentration of hydrogen ions at this point is considered to be equal to zero. Note also that a factor of $10^6$ has been introduced to enable the $[H^+]$ concentration scale to be handled numerically within standard control algorithms and displays.

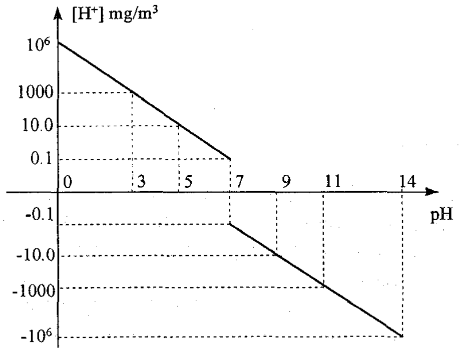


Figure 1: pH versus the hydrogen ion concentration

The hydrogen ion concentration in the stream leaving the mixing junction is the result of injecting the basic stream into the wild acidic stream, as illustrated in Figure 2.

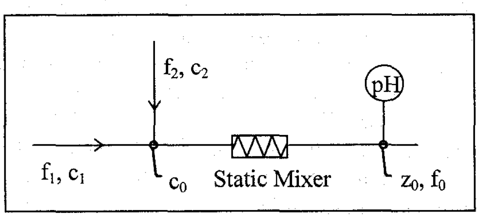


Figure 2: Mixing Junction

The unsteady state mass balance for concentration across the mixing junction;

$$f_0.c_0 = f_1.c_1 + f_2.c_2$$

If the desired pH of the mixed stream is neutrality then $c_0$=0, therefore

$$f_2 = -c_1.f_1/c_2$$

The concentration of hydrogen ions at the point of the pH measurement downstream of the in-line mixer is the same as the concentration $c_0$, except that it is delayed by time L due to distance velocity effects.

$$z_0 = c_0(t - L)$$

This is a variable transformation approach as infers pH control from hydrogen ion concentrations of the inlet streams.

## Neutralisation Plant Design

The pH control pilot rig design is similar to the Gustafsson[13] process, but replaces the CSTR with a back mixing tank, see Figure 3. Walsh[19] concluded that the time delays associated with mixing effects in a CSTR and distance velocity effects in the external circulation loop of a back mixed tank are comparable, but it should be noted that both are small relative to the dominant first order lag of the vessel itself. In terms of cost advantage, the back mixing tank design is better value than a CSTR as;

- a centrifugal pump is cheaper than a motor/agitator assembly for a given mixing duty.
- the pipe work associated with the pumped external circulation loop is cheaper than the supports, bearings and seals required for an agitator, especially if the vessel is under pressure or vacuum.
- there is invariably a need for a pump for product discharge anyway. This can be specified to meet the dual function of discharge and mixing.

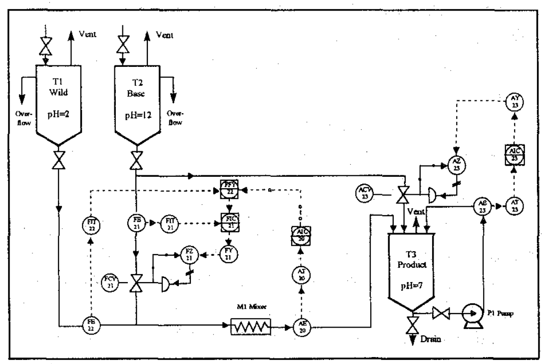


Figure 3: Pilot Neutralisation Plant P&I

## Control Strategy

The wild acid stream (HCl) is neutralised by mixing it with two alkali streams (NaOH), the products of reaction being salt (NaCl) and water ($H_2O$).

$$HCl + NaOH \rightleftharpoons NaCl + H_2O$$

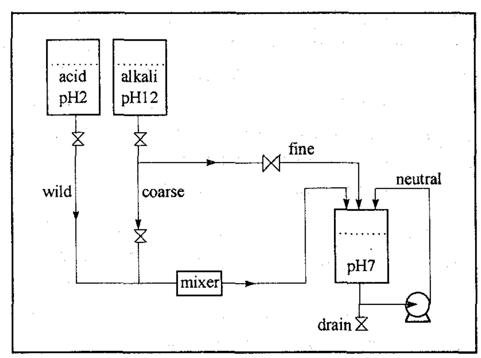


Figure 4: Two Control Stages of the Neutralisation Process

The neutralisation is carried out in two stages, as depicted in Figure 4. Firstly, a coarse adjustment is made using an 'in-line' mixer in which most of the neutralisation occurs. This in-line approach is typical of many effluent treatment plants. The second stage is a fine adjustment made using a mixing vessel and pump which completes the neutralisation. The use of the vessel is typical of many chemical process plants.

Whereas feedback control is retrospective, i.e. it corrects for errors that already exist, feedforward control predicts the control action required to prevent errors from occurring. Knowing the flow rate of acid $f_1$ and the strengths of the acid and alkali, the flow rate of alkali required for complete neutralisation may be calculated. The set point $f_R$ of the coarse alkali flow control loop is set at about 95% of this value, as depicted in Figure 5.

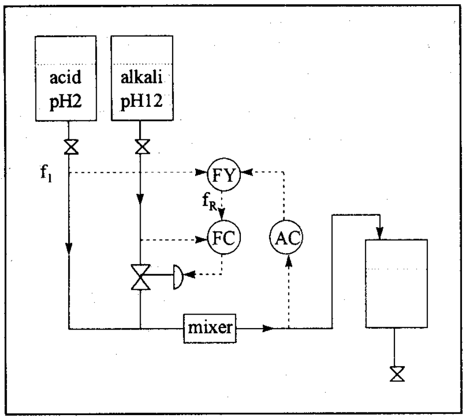


Figure 5: Coarse Control Loop

It is a well-known fact that feedforward controllers are susceptible to measurement errors, resulting in an off-set which may be substantial. So, a feedback controller using the downstream value $z_0$ is used to counter-act any offset. The feedback controller yields a scaling factor which trims the feedforward output $f_R$, to generate the remote set point for the cascade flow control loop on the coarse stream. The cascade flow control loop insulates the concentration control loop from disturbances due to pressure changes.

Good mixing is achieved in the receiver vessel by pumping the process liquor through an external circulation loop. The strength of the liquor is measured downstream of the pump and a conventional feedback controller is used to manipulate the fine alkali flow rate, as depicted in Figure 6. This flow corresponds to the remaining 5% or so of alkali required for neutralisation.

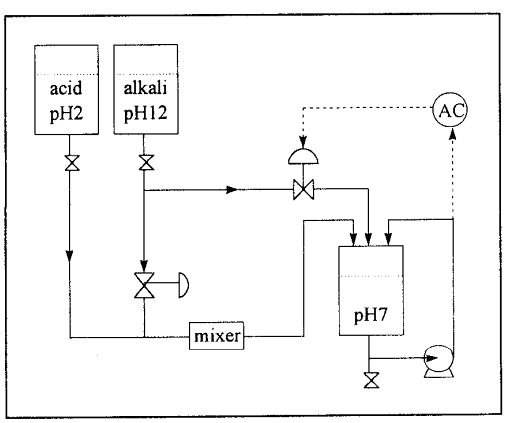


Figure 6: Fine Control Loop

**Current Position**

The effectiveness of the anti-logging approach combined with the control strategy has been demonstrated by means of simulation by Love[17].

A pilot scale rig comprising the neutralisation process and industrial instrumentation for realising the control strategy has been developed. It is interfaced to both a Eurotherm SCADA and Honeywell DCS system and is currently being commissioned.

Empirical results of tests on the rig will be presented at the conference. Whereas the approach is known to be robust for strong acid/base neutralisations, it is not known how effective it is in the presence of buffering. It is hoped that the results on weak acid/base neutralisation will also be presented.

**Future Work**

There are two main components to the future work. Firstly, modifications may need to be made to accommodate buffering effects. One approach is to employ a model that describes the titration of a weak acid with a strong base as developed by Cardinali et al[20]. An alternative to this is to use Atkins[21] description of the titration curve. Another approach is to apply a modelling technique that characterises the flow of a plug of fluid along the mixing pipe and the rate of change of the chemical composition in the mixed stream, Bailey[22]

Secondly is the anti-logging technique is to be used in conjunction with various alternative classical and modern control techniques. For example; Smith Predictor, Fuzzy Logic and Model Based Predictive Control (MBPC). Empirical and simulation results of applying such advanced control methods to the pH process will be presented at the conference.

**Nomenclature**

- $c_1$ — $[H^+]$ for wild stream at the inlet to the mixing junction ($mg/m^3$)
- $c_2$ — $[H^+]$ for base stream at the inlet to the mixing junction ($mg/m^3$)
- $c_0$ — resultant $[H^+]$ at the outlet of the mixing junction ($mg/m^3$)
- $z_0$ — $[H^+]$ for the mixed stream at the point of pH measurement ($mg/m^3$)
- $f_1$ — the wild acid stream mass flow rate (Kg/s)
- $f_2$ — the base stream mass flow rate (Kg/s)
- $f_0$ — the resultant outlet stream mass flow rate (Kg/s)

## References


1. Latrille E., Corrieu G. and Thibault J., Neural Network Models for Final Process Time Determination in Fermented Milk Production, *Comput. Chem. Eng.*, vol. 40, pp 1171-1181, 1994

2. Desphande P.B., Nandy T. and Kaul S.N., Studies on Treatment of Wastewater from Tapioca Based Sago Industry, *Journal of Environmental Science and Health, Part A: Environmental Science and Engineering*, vol. 29, pp 2255-2268, 1994

3. Aoyama A., Doyle III F.J. and Venkatasubramanian V., Control-Affine Fuzzy Neural Network Approach for Nonlinear Process Control, *J. Proc. Cont. Control*, vol. 5, pp 375-386, 1995

4. Gokhale N.D., Shukla N.V. and Deshpande P.B., Advanced Control of Non-linear Processes, *Hydrocarbon Processing,* vol. 70, No. 40, pp 75-78, 1991

5. Bequette B.W., Non-linear Control of Chemical Processes: A review, *Ind. Eng. Chem. Res.*, vol. 30, pp 1391-1413, 1991

6. McMillian G.K., pH Measurement and Control, *Instrument Society of America,* 1991

7. Nortcliffe A. and Love J., In-line Approach to pH Control of Chemical Effluent, *Measurement and Control*, vol. 29, pp 198-200, 1996

8. Palancar M.C., Aragón J.M., Miguéns J.A. and Torrecilla J.S., Application of a Model Reference Adaptive Control System to pH Control. Effects of Lag and Delay Time, *Ind. Eng. Chem. Res.*, vol. 35, pp 4100-4110, 1996

9. Lakshmi Narayanan N.R.L., Krishnaswany P.R. and Rangaiam G.P., An Adaptive Internal Model Control Strategy for pH Neutralisation, *Chem. Eng. Sci.,* vol 52, pp 3067-3074, 1997

10. Seider W.D., Brengel D.D. and Widago S., Non-linear Analysis in Process Design-A Review, *AIChE J*, vol 37, pp 1-38, 1991

11. Rhinehart R.R., Wastewater pH Control, *InTech,* vol. 37, No. 7, pp 42-44, 1990

12. Williams G.L., Rhinehart R.R. and Riggs J.B., In-line Process Model Based Control of Waste-water pH using Dual Base Injection, *Ind. Eng. Chem. Res.*, vol. 29, pp 1254-1259, 1990

13. Shukla V. and Rhinehart R.R., Heuristic, In-line pH Control, *Advances in Instrumentation and Control,* vol. 51, pp.159-174, 1996

14. Gustafsson T.K., An experimental Study of a Class of Algorithms for Adaptive pH Control, *Chem. Eng. Sci.*, vol. 40, pp 827- 837, 1985

15. Pröll T. and Karim M.N., Model-Predictive pH Control using Real-time NARX Approach, *AIChE J,* vol. 40, pp 269-282, 1994

16. Karim W.L.M.N., Morris A.J. and Martin E.B., Control Relevant Identification of a pH Waste Water Neutralisation Process using Adaptive Radial Basis Function Networks, *Comput. Chem. Eng.*, vol. 20, pp S1017-S1022, 1996

17. Love J., Design of a pH Control System for Effluent Treatment", *Proceedings of SCSC Conference,* published by the Society for Computer Simulation, Baltimore, 1173-1180, 1991

18. Love J., An Alternative Approach to pH Controller Effluent Treatment, *Proceedings of DSP & Control Colloquium*, Belfast, 1995

19. Walsh S., Integrated Design of Chemical Waste Water Treatment Systems, *PhD Thesis,* (Imperial College of Science, Technology and Medicine, London, UK), 1993

20. Cardinali M. E., Giomini C., and Marrosu G., A Novel Approach to the Calculations Concerning the Titration Curves of Weak Monoprotic Acid or Bases, *L'Act. Chim.*, vol. 3, pp 217-220, 1991

21. Atkins P. W., Physical Chemistry, *Oxford Press University*, pp 300-303, 1994

22. Bailey S. G., pH Neutralisation, *Msc Thesis,* (University of Sheffield, UK), 1995