

Model predictive control of pH neutralization processes: A review

A.W. Hermansson^{a,b,*}, S. Syafie^b

^a Faculty of Engineering and the Built Environment, SEGi University No. 9 Jalan Teknologi, Kota Damansara, 47810 Petaling Jaya, Selangor, Malaysia

^b Department of Chemical and Environmental Engineering, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia



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ABSTRACT

The paper provides a review of the different approaches of Model Predictive Control (MPC) to deal with the nonlinearities and transient behavior associated with pH and its control.

Firstly a description of the pH system and what makes it difficult to control is presented, followed by the general description of the structure of MPC. The different applications of MPC vary mostly in the way the model is described and how the optimization is carried out to obtain the desired control action. The different modeling techniques applied to the MPC, which is used to describe the behavior of the pH are ranging from simple linear models, multiple linear models like piecewise linear descriptions and fuzzy models, to nonlinear descriptions like Wiener models and the use of artificial neural networks. The models and their respective ways of application are reviewed. Finally, the areas where more research is needed are addressed.

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1. Introduction

The control of pH is an integral part of many areas in chemical and biotechnological engineering, with wastewater neutralization probably being the most studied case, where the objective is to make sure that the discharged water is neutral. Examples, where a particular pH range is required for optimum conditions, include fermentation (Todaro & Vogel, 2014), absorption of metals from water (Mandal, Mahapatra, & Patel, 2015), coagulation as part of water treatment (Bello, Hamam, & Djouani, 2014d) and algae growth in biomass production (Pawlowski et al., 2014). The common denominator for the different cases is a liquid system in which the pH exhibits a nonlinear behavior. This has led to claims that among the most commonly used process variables, pH is the most difficult to control (Love, 2007). The nonlinearity and difficulty controlling pH in a process can also be highlighted by studying the common range for the controller gain in tuning tables for PID controllers (Couper, Penney, & Fair, 2009; McMillan, 2000) where the variational range of the gain setting recommendation for a pH controller is 100 times greater than the process with the second highest range of gain.

The paper is organized as follows. Section 2 describes the general properties of pH and what factors lead to the nonlinear

behavior. In Section 3 the problems faced when control of pH are desired, followed by Section 4, giving a short introduction to model predictive control (MPC). The review of the different pH control approaches utilizing MPC, arranged by the type of model used, appears in Section 5 and finally the paper is concluded in Section 6.

2. General properties of pH

2.1. Definition of pH

The pH is the logarithmic value of hydrogen ion activity (a_{H^+} in mol/l) in an aqueous solution defined as

$$pH = -\log_{10} a_{H^+} \quad (1)$$

where the hydrogen-ion activity is defined as

$$a_{H^+} = \gamma_{H^+} [H^+] \quad (2)$$

where γ is the activity coefficient and $[H^+]$ is the hydrogen ion concentration. The activity and the concentration of hydrogen ion have to be distinguished as in solutions with high ionic concentration the hydrogen ion activity is less than the actual hydrogen ion concentration, while in ionically dilute solutions they can be considered to be equal, hence $\gamma \approx 1$.

The use of pH with its logarithmic scale and hydrogen-ion activity is largely due to the standard measurement device, an ion-selective electrode, which will create a potential difference that is proportional to the negative logarithmic value of the hydrogen ion

* Corresponding author. Present address: School of Engineering and Physical Sciences, Heriot-Watt University Malaysia, No. 1 Jalan Venna P5/2, Precinct 5, 62200 Putrajaya, Wilayah Persekutuan Putrajaya, Malaysia.

E-mail addresses: a.hermansson@hw.ac.uk (A.W. Hermansson), syafie@eng.upm.edu.my (S. Syafie).

activity, which is adding additional nonlinearity to the problem of neutralization.

2.2. Equilibrium behavior of water

Nonlinearity is also part of the equilibrium behavior associated with the dissociation of the acids and bases when put into an aqueous solution. Water will weakly dissociate into hydrogen ions and hydroxyl ions in equal parts according to



which at 25 °C have the following equilibrium relation:

$$K_w = [\text{H}^+][\text{OH}^-] = 10^{-14}. \quad (4)$$

Any hydrogen in water will react with the water to form hydronium ion according to



For simplicity this is not explicitly stated in most cases using $[\text{H}^+]$ in the place of $[\text{H}_3\text{O}^+]$ for brevity, which is also generally applied to the case of Eq. (1) using hydrogen-ion concentration in the place of the hydrogen-ion activity.

For water, equal parts dissociate, hence the concentration of the two ions has to be equal and both have the value 10^{-7} according to Eqs. (3) and (4) giving a pH, for pure water, of 7, which is the definition for neutrality at the given temperature, with pH below 7 being acidic and above 7 alkaline.

2.3. Acids and bases in aqueous solution

Acids are also referred to as proton donors as they can release at least one hydrogen ion under certain conditions. The acids that can donate only one ion is called monoprotic, which is described as HA. If more than one hydrogen ion can be released the acid is polyprotic (diprotic (H_2A), triprotic (H_3A) etc.). Bases can accept a proton instead and are hence referred to as proton acceptors and can be monoprotic and polyprotic as well. They are commonly written in the standard form as BOH or $\text{B}(\text{OH})_i$ for polyprotic bases. Some of the dissociation reactions are summarized in Table 1.

The equilibrium constant for each reaction specifies to what extent the acid or base gives or accepts protons which is referred to as thermodynamic dissociation coefficient. The definitions of dissociation coefficients are also summarized in Table 1. The tabulated value for any acid/base dissociation is using the logarithmic value to simplify the tabulation, using

$$\text{p}K_i = -\log_{10} K_i. \quad (6)$$

Table 1
Examples of dissociations reactions and coefficients for different agents.

Agent	Dissociation reaction(s)	Dissociation coefficients
Monoprotic acid	$\text{HA} \rightleftharpoons \text{H}^+ + \text{A}^-$	$K_a = \frac{[\text{H}^+][\text{A}^-]}{[\text{HA}]}$
Monoprotic base	$\text{BOH} \rightleftharpoons \text{B}^+ + \text{OH}^-$	$K_b = \frac{[\text{B}^+][\text{OH}^-]}{[\text{BOH}]}$
Triprotic acid	$\text{H}_3\text{A} \rightleftharpoons \text{H}^+ + \text{H}_2\text{A}^-$	$K_{a1} = \frac{[\text{H}^+][\text{H}_2\text{A}^-]}{[\text{H}_3\text{A}]}$
	$\text{H}_2\text{A}^- \rightleftharpoons \text{H}^+ + \text{HA}^{2-}$	$K_{a2} = \frac{[\text{H}^+][\text{HA}^{2-}]}{[\text{H}_2\text{A}^-]}$
	$\text{HA}^{2-} \rightleftharpoons \text{H}^+ + \text{A}^{3-}$	$K_{a3} = \frac{[\text{H}^+][\text{A}^{3-}]}{[\text{HA}^{2-}]}$

2.3.1. Strong and weak agents

A strong agent is an acid or base that completely dissociates upon contact with water. Common examples of a strong acid and a strong base respectively are hydrogen chloride (HCl) and sodium hydroxide (NaOH). When HCl is dissolved in water, all hydrogen from the acid will be present in the form of hydrogen ions (H^+) and all of the hydroxyl in the NaOH will be in the form of hydroxyl ions (OH^-). This means if a single strong agent is present in an aqueous solution, the pH could be directly obtained from the concentration of the acid or the base using Eq. (1), as long as the ionic concentration is not too great (i.e. $\gamma_i \approx 1$). Weak agents would only partially donate or accept protons, leaving part of the acid or base unreacted in the solution, which would make it possible to shift the equilibrium by adding or removing any of the components relating to the dissociation of that particular agent.

2.3.2. Buffering

The effect that the incomplete dissociation of weak acids or bases has on the pH system is to dampen the effect of the additional base or acid added to the system. This effect of resisting changes of pH, when agents are added, is referred to as buffering and occurs due to the shifting of the equilibrium by the neutralization of the hydronium ion or the hydroxyl ion in the solution. This will make the acid donate more protons or the base accept more protons, hence the hydrogen ion activity will not change by the amount expected based on the amount of base or acid added. Buffering will take place as long as the agent is not completely dissociated, which in the case of single weak agent is as long as the agent has not been completely neutralized. For even more efficient buffering a salt of the agent would be added to the system resisting pH changes even further, by introducing precipitation and dissolution to the system.

2.3.3. Titration curves

The nonlinear behavior of the pH system is illustrated by plotting how the pH, for a set of initial concentration of acid(s) and/or base(s), varies with the addition of an agent to the system. The shape of the titration curve is determined by the participating acid (s) and base(s), particularly by their dissociation coefficients as well as their initial concentrations, however for a monoprotic case the curve will always be s-shaped, as seen in Fig. 1. For a polyprotic case there would be multiple s-shaped segments though only the beginning of the second s-shape is indicated in Fig. 1 as a triprotic acid would require thrice as much base for neutralization.

For a strong acid, the behavior would be concave as the hydrogen ions are continuously neutralized by the added base until the vertical equilibrium point where all acids have been neutralized. The weak acid would only be partially dissociated so when the base is added it will neutralize the hydrogen ions shifting the equilibrium making the acid donate more of the protons to achieve a new equilibrium leading to a behavior with an inflection point occurring at the value of the dissociation constant (the $\text{p}K_a$) and then following a concave behavior like for the strong acid until the equilibrium point. For polyprotic acids, the behavior is similar with every inflection point specified by the different dissociation constants as well as an equilibrium point for each proton donor in the acid. The behavior of the base would be analogous to the acid, but dealing with proton accepting instead of proton donation with the inflection point appearing at a point specified by $(14-\text{p}K_b)$. As seen in Fig. 1 the behavior after neutralization is identical as the same base are used in all three cases. Changing the base would change the behavior after neutralization, which in the case of ammonia would create a mirror image of the acetic acid, just as the sodium hydroxide is mirroring the hydrochloric acid, which is due to diffusion coefficients of the acid and the base having the same numerical value.

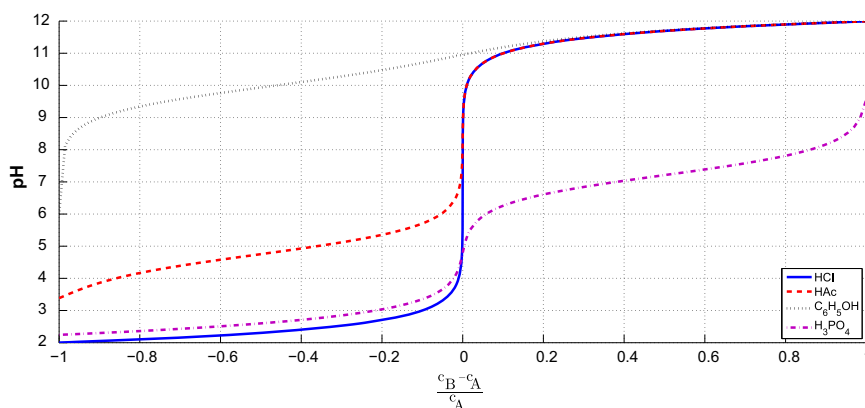


Fig. 1. Titration curves for 0.01 mol/dm³ of hydrochloric acid, acetic acid, phenol and phosphoric acid, in water, titrated with 0.01 mol/dm³ sodium hydroxide.

2.3.4. Buffer capacity

Additional characteristics found in the titration curves in Fig. 1 are the almost vertical behavior around the equivalence point, which is more prominent for strong agents. Those characteristics are related to the sensitivity of pH to changes in concentration of any of the mediums in the system and are closely related to the buffering of the system. The sensitivity and hence the buffering effect of a liquid system are commonly evaluated using the buffer capacity, β , that is defined as

$$\beta = \frac{dc_B}{dpH} = - \frac{dc_A}{dpH} \quad (7)$$

Hence, the buffering capacity is describing the differential change of base or acid with regard to changes in the pH, which is essentially describing the inverse of the gradient of the titration curve. In Fig. 2 the buffer capacity of the acids and base used in Fig. 1 are plotted as a function of pH. The figure shows that the highest buffer capacity is occurring at the pK values as they are the equilibrium points for the agents and hence the additional addition of agents will shift the equilibrium slowing down the change of pH. The opposite will occur around the neutralization points where a small change will give a quick effect of the pH as all agents are by then neutralized.

3. Control of pH

3.1. The neutralization system

The most common setup used to study the nonlinear control behavior in a neutralization process is a continuously stirred tank reactor (CSTR) with at least two inlets, the first being the influent

with an undesired pH that is to be adjusted. Additional streams are the means to adjust the pH, in the simplest case an acid solution if the original solution is alkaline or vice versa. When the feed can vary between acidic and alkaline two reagents are needed, both an acidic and an alkaline. A buffer may also be included to simplify the control problem either as a separate stream or mixed together with the reagents. Additional equipment includes a pH meter positioned in the reactor effluent and control valves for the reagent. Other approaches include using a static mixer, a so-called in-line mixer, which can handle minor changes well, but may develop a problem when the pH of the influent fluctuates too much. However, the in-line mixer has found its niche as a pre-mixer before the CSTR.

Different design considerations to achieve good control has to be followed to minimize the problems associated with pH control, like the selection of control valves, the design of the CSTR and the positioning of the pH measurement instrument. This will not be covered here but are well described to various degrees in books like Shinsky (1973), McMillan (1984), Love (2007), and Lipták (2005). The lab-scale systems commonly used for trying different control schemes are commonly simpler setups as the important part is to demonstrate the handling of the nonlinearities.

3.2. Issues in pH control

The general behavior of the pH has been described in Section 2 and the major problems faced when dealing with pH control are threefold, the nonlinearity of the process, the high sensitivity (low buffering/buffer capacity) around the equilibrium point and the time variant behavior that develops as a function of varying concentrations of the inlets hence changing the process behavior and hence the description of the process (the titration curve).

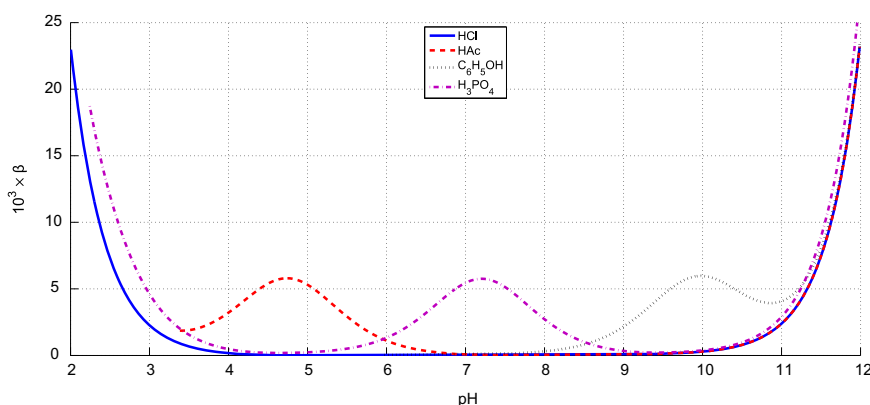


Fig. 2. Buffer capacity curves for 0.01 mol/dm³ of hydrochloric acid, acetic acid, and phenol in water, neutralized with 0.01 mol/dm³ sodium hydroxide.

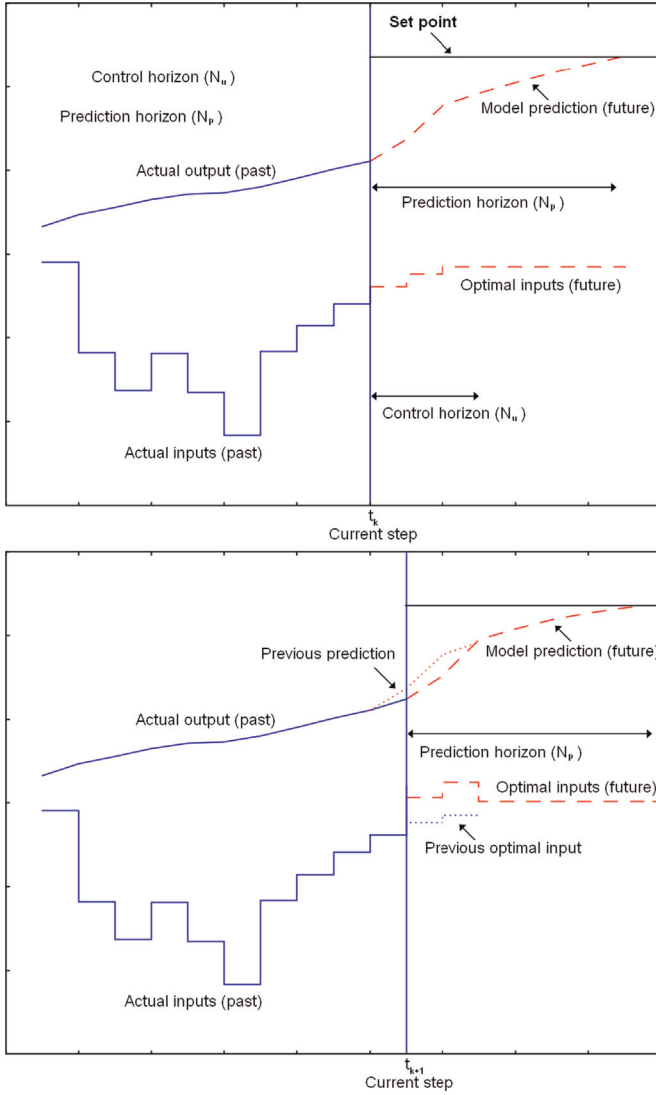


Fig. 3. The receding horizon approach illustrated.

These are the circumstances for which the controller has to be designed to deal with. There are some additional remedies like adding a buffer to the system making the system less sensitive around the equilibrium point, if the required pH is in that region, though this is not a general solution to the control problem as the buffering may cause problems in itself. This is particularly true for biological systems and wastewater treatment (Gustafsson, Skrifvars, Sandström, & Waller, 1995). It should also be noted that not all pH control systems are problematic, as the required pH may be in an area with high buffer capacity, which would make a simple linear controller work well. The control sections are presented with the assumption that buffering is not applied or a more or less linear behavior is not possible to accommodate or achieve.

The traditional way of achieving good control of the pH when dealing with neutralization is to use three tanks in series in combination with a simple linear PI or PID controller at each stage with different set points approaching the desired value. This approach is generally not favored as it constitutes a considerable capital investment, hence creating a need for more advanced controllers that could handle the nonlinearities.

4. Model Predictive Control

The Model Predictive Controller (MPC) is based around the three following characteristics:

1. A model is used to predict the future behavior of the process over a predetermined time interval, commonly referred to as the prediction horizon.
2. A sequence of controller inputs is obtained by minimizing a cost function over another time interval, the control horizon.
3. A receding horizon approach, so that at each time interval, when a predicted behavior and a control sequence are obtained the two horizons are shifted another step into the future, while the first entry in the control sequence is applied to the process.

The description of the parts used in MPC is one of the most common forms used though many variations occur in the literature. The process is commonly described by state-space models in discrete time as

$$\hat{x}(k+1|k) = f(\hat{x}(k|k), u(k)) \quad (8)$$

$$\hat{y}(k|k) = g(\hat{x}(k|k)) \quad (9)$$

or in linear form as

$$\hat{x}(k+1|k) = A\hat{x}(k|k) + Bu(k) \quad (10)$$

$$\hat{y}(k|k) = C\hat{x}(k|k) \quad (11)$$

where \hat{x} is the model description of the state vector, u is the vector of manipulated inputs, \hat{y} is the model description of the vector of outputs, f and g are nonlinear functions and A , B and C are matrices. The discrete time k is at the current time and $(k+i|k)$ signifies a prediction of the variables at time $(k+i)$ when the current time is k for any value i , which is a step length toward the future. The optimal control sequence is obtained by minimizing a cost function, which is given as

$$J(k) = \sum_{j=0}^{N_p} \|\hat{x}(k+j|k) - x_{sp}(k)\|_Q^2 + \sum_{j=0}^{N_u} \|u(k+j) - u_{sp}(k)\|_R^2 \quad (12)$$

where R and Q are symmetric positive semidefinite weight matrices to specify the cost of deviation from the desired values of the states (x_{sp}) and inputs (u_{sp}), and N_p and N_u are the prediction- and control-horizons respectively. Eq. (12) is one of the most common cost function representations, where the most common alternative addition is a term including the change in input (Δu) as well as adding a terminal cost function forcing the system to be close to the desired value at the end of the prediction horizon.

The controller output, u , is obtained by minimizing the cost function using u as the variable over the control horizon thus obtaining the optimum control sequence $\{u(k), u(k+1), \dots, u(k+N_u)\}$ of which only the first entry $u(k)$ is applied as the manipulated variable to the process. The procedure is then repeated at the next time instant, $k+1$, hence the horizons keep receding further into the future. The procedure is illustrated in Fig. 3 for a single input single output case, but the procedure would work just as well for multiple input multiple output cases. Another common addition is to include constraints in the minimization problem, particularly to ensure that the magnitude and rate of change of the manipulated variable are physically realizable. In fact, the straightforward translation into a multiple cases and the inclusion of constraints are the major reasons for the popularity of MPC.

Just as for standard controllers like PID, there is a requirement for robustness and stability of the MPC. The first approach to incorporating stability into the MPC setup was to use infinite prediction horizons, followed by dealing with a terminal condition, keeping the control horizon finite. The terminal condition was either in the form of a terminal cost (Rawlings & Muske, 1993), which would be an additional term in the cost function (12),

severely penalizing deviation from the set point at the last step of the prediction horizon, or a terminal constraint set (Michalska & Mayne, 1993), as an additional constraint for Eq. (12), whereby the state is forced into a specified set by the end of the horizon. Combinations of the two terminal conditions have also been applied. These strategies work well when the system is well known, but for uncertain systems additional measures have to be taken and hence robust control techniques have to be incorporated. The robustness steps taken include using a tube based approach (Chisci, Rossiter, & Zappa, 2001; Mayne & Langson, 2001; Mayne, Kerrigan, Van Wyk, & Falugi, 2011), whereby the system is kept within a stable set, the tube, which guarantees stability for bounded disturbances specified in the setup or using min–max methodology (Kothare, Balakrishnan, & Morari, 1996; Løvaas, Seron, & Goodwin, 2008) relying on finding the worst case scenario for Eq. (12) encompassing all specified uncertainties as a pre-step before the minimization of the cost function. For more details on the setup of the MPC, including choices of cost function, optimization techniques and stability and robustness amongst others the following books are good starting points (Camacho & Bordons, 2004; Kwon & Han, 2006; Maciejowski, 2002; Rawlings & Mayne, 2009; Rossiter, 2013).

5. MPC for pH control

Applying MPC to nonlinear cases such as pH control requires careful consideration with regard to how the different parts in the MPC setup are specified. This is essential in creating good handling of the nonlinearities while at the same time not making the computational cost too high, hence making the controller too sluggish to handle fast changes. Selections that have to be made include but are not limited to the type of model to use for the predictions, what cost function to use, the optimization algorithm to apply to the cost function and finally how to compensate for deviation between the model and the actual process. The research literature is mainly focusing on the model selection and the optimization algorithm used for the cost function minimization. The different considerations are interconnected thus requiring some consideration of each part to some extent. For example a simpler choice of model, which would make the optimization easier, would commonly require more focus on the compensation for the model–process mismatch.

The cost function is predominantly a quadratic function like in Eq. (12) though the variables included in it may vary. A linear cost function is also possible, which is mostly used when dealing with huge systems though it creates a more erratic behavior as the optimum point would commonly jump between different constraints.

The selection of optimization algorithm would generally be a matter of choosing the fastest algorithm that could handle the requirements specified. For simpler cases, an analytical solution is possible while a variety of nonlinear solution techniques have been used for the more complex requirements.

When it comes to obtaining the model to be used the general questions center around whether to use a linear or a nonlinear model and what techniques should be used to obtain the model. The effect of these modeling decisions are more profound for a nonlinear system like pH, as more care is needed to obtain a good description of a nonlinear process while at the same time not making it too complicated causing the optimization problem to become too time-consuming. The three classes of models, as specified by Sjöberg et al. (1995), are as follows:

- Fundamental modeling (White box modeling) based on physiochemical understanding of the process.

- Empirical modeling (Black box modeling) based on identifying the process without applying any prior knowledge of the process, but using model parameters that are easily adaptable to different processes but do not have a particular physical meaning.
- Hybrid modeling (Grey box modeling) uses a combination of physiochemical understanding and empirical modeling. The combination is either applied when the fundamental model cannot be or is not desired to be completely derived from knowledge or when the physiochemical understanding is used as a basis for empirical modeling.

The following review of the different applications of MPC to the pH control problem is organized based on what type of model is applied inside the MPC loop, which in its general form is nonlinear, even though for most cases the model used for optimization is linear. The setup of the system with regard to, for example, cost function or optimization techniques is only mentioned when they deviate from the standard setup, with quadratic cost function and using standard quadratic programming software for the optimization.

5.1. Linear models

Linear models have a use in nonlinear control problems, such as pH, as it simplifies controller design and reduces computational time. This is the case for MPC as well, which in the case of having a quadratic cost function and not enforcing any constraints analytical solutions are possible. When constraints are present the optimization problem is convex, hence have a global minimum that can be obtained quickly using standard optimization tools. However, describing the pH system with linear models creates discrepancies between the model and the process that has to be compensated for in some way, if good control is required. Different approaches have been proposed to deal with the modeling error; using a single linear model in conjunction with some adaptive scheme, using a model bank of linear models that when combined creates a nonlinear description of the process or using a hybrid model that includes some nonlinearity, while keeping the nonlinearity outside the optimization leaving the problem convex.

There have been some approaches using a single linear model without any model error compensation though those are usually highlighting other findings. Villanueva Perales, Ollero, Gutierrez Ortiz, and Gómez-Barea (2009) applies the simple linear model case to a wet limestone flue gas desulfurization plant and Altınten (2007) used a single ARIMAX model to lab scale set. The former paper demonstrated the MPC application to a particular process while the main target of the latter paper was to show the applicability of the genetic algorithm for modeling of pH control systems. Annal and Jerome (2014) also used a simple MPC approach with the aim to compare linear MPC to a PID controller, which showed that MPC made more of a difference for disturbance rejection compared to set-point tracking. These papers show good control performance, which lends credence to the general idea that if the desired control range does not include both the inflection point and the equilibrium point a linear control strategy will work nicely.

5.1.1. Linear models in adaptive schemes

The adaptive schemes applied to the MPC take the form of adding a compensator that updates some of the parameters in the MPC scheme.

Maiti, Kapoor, and Saraf (1994) applied an adaptive approach whereby the model was updated by running an updating algorithm, however, this was not an automated implementation, but was initiated and run separately when deemed necessary. The

adaptive update was recommended to be done at least daily or more frequently if changes occur frequently, which worked fine in the paper but seem impractical. However, the idea could be a put to good use if the update of the model was automatically implemented by a controller when the controller exceeds some control or modeling error criteria.

Automatic adaptive updating scheme was implemented by Zhang and Zhang (2006) whereby a pseudo-derivative description was used to model the nonlinear behavior using a linear description. The linear model was continuously updated through an adaptive learning algorithm to ensure that the process was described as accurately as possible by a linear model. Another approach was demonstrated by Obut and Özgen (2008) by adding an adaptive updating scheme to the move suppression factor (equivalent of R in Eq. (12)), which was based on an estimation of the gradient of the changes. For the lab scale experiment, they also made the assumption that the gradient of the disturbance is constant as an approximation of the behavior of the disturbance.

Pawlowski, Fernández, Guzmán, Berenguel, Ación, and Normey-Rico (2014) and Pawlowski, Mendoza, Guzmán, Berenguel, Ación, and Dormido (2014) applied an event-based MPC approach whereby the application of controller depends on different events affecting the process and using different specifications for the MPC depending on what event most closely matches the current situation. This was applied to bioreactors where the pH is a measurement of the CO_2 that has to be supplied to maximize the microalgae photosynthesis and minimize that wastage of CO_2 . The event-based approach proved superior to an on-off controller or single linear MPC for the respective trials.

The performance of any of the adaptive MPC shows an improvement over using a linear PI controller, but in the case of Obut and Özgen (2008) a fuzzy logical controller actually outperformed their adaptive MPC setup. This is not totally surprising as the fuzzy controller incorporates the nonlinearity directly into the design, while their MPC approach does it indirectly, through adaptation. The adaptive approaches can obviously handle the nonlinearities better than the simple linear MPC, but still seem limited to areas where pH behaves fairly linearly.

5.1.2. Multiple linear models

The shortcoming of linear MPC is that even with adaptive action it cannot handle the nonlinearities very well. Adding adaptive action improves the behavior, but it may still be outperformed by other controllers that have been regionally tuned, hence handling the nonlinear behavior of pH better. The combination of using linear MPC and regional handling of the nonlinearities have resulted in the use of multiple linear models in the MPC scheme. The nonlinear behavior is captured by separating the range into different regions and obtaining a linear model for each region, rendering a piecewise linear (PWL) representation of the nonlinear behavior. The common way of obtaining the set of linear models is to start with obtaining a fundamental nonlinear model and then linearize that model at different operating points. After obtaining the PWL description the way of utilizing them has to be decided, particularly how to deal with the transition from one model to another, as well as the standard considerations with regard to cost function and optimization.

Johansen and Foss (1992) were among the first to demonstrate the use of multiple linear models to describe the nonlinear behavior of the pH system, where the different linear models were obtained by Taylor expansions of the nonlinear model in the regions of interest. Different models were weighted together to generate a single linear model to be used at the current time instant. The weight for each model was obtained by computing the model error, as the difference between the actual output and the output predicted by the model. This was done for each model

followed by normalization of the error by dividing by the sum of the model errors.

Weighting the models together gives the possibility of capturing the nonlinear behavior when the system is far away from any of the operating points. However, if the system is undergoing rapid changes the update of the averaged model may lag behind as the average is based on the previous best model, using a model that is not ideal. Dougherty and Cooper (2003) used a linear weighting between the two models with the closest proximity to the current pH giving a simpler and more direct weighting technique with less lag. Other forms of weighting have been used by Hermansson, Syafie, and Mohd Noor (2010) applying a Bayesian weighting scheme that enables a gradual move between two or more models, at the price of introducing additional lag to the system. To make any type of weighting work some additional function, possibly an adaptive scheme, would have to be incorporated into the system.

The most common technique to speed up the update and avoid lag is to do direct switching between different models. A model is selected as describing the process best based on a comparison to the actual current state or the desired state. This would of course come at the price of not handling the nonlinearities as well when being far from any points of linearization. Halldorsson, Ali, Unbehauen, and Schmid (2002) used a rectangular division operating areas, hence the model description was using more than the current pH as an input variable for the linear models. The switching was done based on the desired pH and applied to lab equipment, utilizing steepest descent optimization. Zhou and Zhou (2006), Sivakumaran and Radhakrishnan (2007), Costa, Fileti, Oliveira-Lopes, and Silva (2014) and Bello, Hamam, and Djouani (2014a) used a similar setup but with one-dimensional linearization using pH as the only variable. The three former ones applied the setup to a lab scale process while the latter applied it to a coagulation process in a water treatment plant. The drawback of the switching, however, is the erratic behavior that occurs when the controller starts cycling between two models. Bello, Hamam, and Djouani (2014b) suggested a way around this by applying fuzzy weighting, linearly combining two models at the intersection instead of a direct switching, which was applied to the pH control in a waste water treatment plant. Xie, Zhou, Ma, and Zhou (2008) combined fuzzy weighting with a fuzzy clustering, where the models are combined using fuzzy clustering to minimize the number of models and assign operating regions for the different models. When the system operates outside any operating region, fuzzy weighting is used to combine the neighboring models to a single model, while a single model is used if the system operates inside an operating region. Further development in the area of switching was the re-initialization technique proposed by Gu and Gupta (2008), whereby in conjunction with the switching they reset the system forcing the system to initialize at the current state if necessary. Shamsaddinlou, Fatehi, and Sedigh (2014) added a supervisor agent to switch between using an adaptive MPC and a standard linear MPC approach. The most applicable of these techniques seem to be the simple fuzzy weighting. This has also been shown by Shamsaddinlou, Fatehi, Sedigh, and Karimi (2013) whereby fuzzy weighting provides good control, but it also included the additional supervisor part which seems a bit redundant.

Bagheri, Mardanlou, and Fatehi (2011) compared three different techniques; firstly the weighting and switching used by researchers in previous paragraphs, while the third technique added an adaptive weighting to the switching technique, aimed on the weighting matrix Q in the cost function, varying how the control error is penalized. The values of Q are obtained using step tracking and an integrated absolute error tuning, giving a high penalty when buffering capacity is low and low penalties when the buffering capacity is high. Applying an analytical solution to the

optimization problem, they found that switching performed better than weighing and that the addition of adaptation of Q reduces any oscillations as it will act to reduce the control action. As the weighing for Q has much higher resolution than the weighing and switching of models it is not sure how much of the improvement is due to the increased resolution and how much is due to the approach itself.

The previous examples have achieved good control, which is partially due to applying the control to some of the simpler neutralization systems, which is why an analytical solution of the optimization problem is possible. To obtain the same level of control for a more complicated system would require a more robust control scheme, which gives rise to a more complicated optimization problem. Lu, Arkun, and Palazoglu (2004) attacked the problem of robustness by using a quasi-min-max approach which was basically an update on an approach by Kothare et al. (1996), by minimizing the quasi-worst case instead of the worst case, rendering a less restrictive optimization, leading to improvements in the performance of the controller. The min-max approach was also taken up by Hermansson and Syafie (2014) but tackled the sluggish behavior as well as applied it under conditions where the state was unknown and the disturbance unmeasured by adding a separately acting I-controller. Both the robust approaches generate control of situations with more uncertainty that are at par with the cases assuming little or no uncertainty.

Lastly, we look at two cases with new approaches to deal with the issues related to the MPC setup. Åkesson, Toivonen, Waller, and Nyström (2005) used the standard PWL description, but they modeled the optimization of the cost function as a neural network description using the state, the reference behavior of the states and the output setpoint as inputs and applied it instead of the solving of the optimization problem. This creates additional steps in the preparation, but it showed good results for lab scale neutralization as the optimal control sequence is obtained very fast though to avoid steady state error additional corrections had to be added. Azimzadeh, Palizban, and Romagnoli (1998) used the MPC as a way of obtaining the set point of the system, which was fed to a PID controller, that would bring the system to its desired value. This was applied to a fermentation process for which it was required to control the fermentation by adjusting the temperature as well as the pH under the assumption of no constraint and using an analytical solution of the cost function.

The use of multiple linear models in MPC shows an improvement of the control compared to the single linear MPC, as a set of models is able to capture the nonlinearities better. The approach does not add any additional cost when it comes to computing time as the multiple model case will use a single linear model in the optimization, though some additional steps in modeling are required as more models are needed. The choice how to combine the different models, using switching or weighing, has to be taken into consideration as well. Switching has generally proved to perform better, though weighing has an advantage in giving a better overall description of the process, probably mostly applicable for slow processes as it adds some lag to the process.

5.1.3. Fuzzy model

Fuzzy modeling is a type of black box modeling based on fuzzy rules on how to apply different models that are either obtained as part of a parameter identification process or by using some pre-specified regions, in which case the model would be considered gray box model. As part of the identification process the designation of the weighting procedure, the fuzzy rules, are obtained as well. Commonly the rules and models are checked for validity as well as possibly being subjected to clustering to reduce the number of models and rules. There are many different approaches to obtain the models and do the clustering, though the one attracting the

most attention is the Takagi–Sugeno (T–S) fuzzy model, which is suitable for modeling of the dynamic behavior of complex nonlinear systems, like pH. The fuzzy models are placed under the linear model category, even though they are not necessarily linear, but when used inside an MPC scheme the fuzzy models are generally linear, creating a very similar setup compared to the multiple model MPC approaches in the previous section.

Kelkar and Postlethwaite (1994) used fuzzy modeling based on the integral square error to obtain the model in conjunction with a simple MPC setup, where the optimization was carried out using a Fibonacci search. As only one model was identified the result are very similar to the linear model case described in Section 5.1.1.

The first application of the Takagi–Sugeno approach was done by Kavsek-Biasizzo, Skrjanc, and Matko (1997). They obtained a nonlinear model from the fuzzy modeling, while applying triangular weights, hence just linearly combining two models at the time, to obtain the linear model applied at each time step. The result was good, however, it was applied to a simple process, as the main task was to show the applicability of the fuzzy modeling to pH control using an MPC approach. Marusak (2009) followed along the same lines as Kavsek-Biasizzo but developed a simple algorithm synthesis demonstrated for MIMO cases for pH control as well as a van de Vusse reactor. Li, Liu, and Yuan (2014) and Bello, Hamam, and Djouani (2014c) used similar setups for the MPC, where in the latter case it was applied to a wastewater treatment plant. The pH level was maintained to optimize the amount coagulation in the process, showing that the fuzzy linearized controller performs just as well as a nonlinear MPC, but with a lower computational load.

The use of fuzzy models in MPC was extended by Mollov, Babuska, Abonyi, and Verbruggen (2004), by using a linear time-variant model approach, which meant that different models may be used along the prediction horizon. This was done to increase the accuracy of the description of the nonlinear behavior as the most accurate model was used at every time step along the predicted trajectory. The approach relies on an iterative approach, starting with applying the best initial model and if the trajectory was reaching into the region of another model, the prediction is redone using the other model in the regions for which it is deemed most accurate. This change of model was repeated until the optimal model is used at every time step of the prediction horizon. This approach was combined with a more advanced optimization technique incorporating constraints.

Novák, Chalupa, and Bobál (2011) and Novák and Chalupa (2013) also used the approach letting the models possibly vary along the prediction horizon and they did further development in the latter paper where an extended Kalman filter was added for state and disturbance estimation. These estimations are done for each model and weighted together in the same manner as for the controller.

The fuzzy approach has much in common with the linear model cases when it comes to the MPC approach itself using a linear model for optimization. The difference is in the way of obtaining the model as well as applying the tools associated with the fuzzy modeling to decide on the number of models to be used.

5.2. Nonlinear models

A well tuned nonlinear model has the ability to describe the nonlinear process more accurately than a single linear model as well as a set of linear models. However, the increased accuracy comes at the price of making the MPC algorithm more complicated and time consuming, particularly with regard to the optimization of the cost function that does not have guaranteed convergence anymore. The most successful approaches rely on using a linear model for the optimization problem, while keeping the nonlinear model to enable a good description of the process or as a corrector

of the control sequence.

5.2.1. NARX models

The earliest examples of using nonlinear models inside the MPC scheme relied on using NARX models that were used for all parts of the MPC, including the optimization.

Pröll and Nazmul Karim (1994) obtained an NARX model through online identification and used a modified Marquardt algorithm to solve the nonlinear optimization problem. They applied the control setup both to computer simulations, using a physiochemical model to simulate the neutralization as well as applying it to a small test rig. The major result showed that using nonlinear models has a profound positive effect on the control of the system compared to using linear models in the MPC. It can also be noted that the simulations were as a demanding task as the application to the real process. Hong, Morris, Karim, Zhang, and Luo (1996) extended the work done by Pröll and Nazmul Karim by creating what they referred to as adaptive NARX based predictive control. They added an adaptive updating scheme using a recursive parameter estimation algorithm to update the model, using the offset as the input to the algorithm. This by itself creates some other problems in the pH control which they solved by adding a set point perturbation, which gives a satisfactory result handling varying buffering capacity problems. Bello et al. (2014d) applied the NARX based NMPC to a water treatment, where the pH was used to optimize the coagulation rate by varying the chemical dosing rate. The NMPC approach was compared to a linearized version without showing a great difference, which might be attributed to the coagulation taking place at fairly high pH where the titration curves are quite linear.

The general consensus is that using a nonlinear model for all parts of the MPC has too many drawbacks. This is particularly true with regard to the optimization, especially when constraints are required.

5.2.2. Volterra models

A Volterra model is essentially a linear combination of polynomials of varying degree characterized by a power expansion analytic representation. The series in itself is truncated, just using the terms up to a certain degree, to simplify identification and application, but at the cost of model errors. To enable a good nonlinear description, it cannot be truncated too much. As at least a quadratic behavior is incorporated into the general optimization problem, the optimization would be non-convex requiring different optimization algorithms, commonly relying on some type of search technique.

Díaz-Mendoza and Budman (2010) incorporated the Volterra series model into a robust framework relying on structured singular value approach, which was a min–max approach creating robustness by applying the worst model into an MPC setup. A difference from many MPC approaches was that the constraints and terminal conditions are directly incorporated into the optimization problem as additional costs, making the optimization problem in itself bigger but with the benefit of not having any constraints. The optimization setup may not be able to obtain a global minimum as well as slow due to the size, but the robustness feature makes the approach interesting for further investigation. Kumar and Budman (2014) extended the work of Díaz-Mendoza and Budman by incorporating a polynomial chaos expansion (PCE) as way of describing the uncertain Volterra model coefficients, which made it possible to estimate the output prediction error, which can be used to compensate for model errors. The PCE approach will maintain robustness while at the same time speeding up the computation of the optimal input as well as showing better control characteristics in their comparison.

The Volterra models have a similar effect to the MPC as the NARX models, with increased computational load and not being

able to guarantee finding the global optimum, while giving a more accurate description of the process. The possibility of incorporating robustness into the problem is also interesting though the approach may be getting too complicated of the general practitioner.

5.2.3. Wiener and Hammerstein models

Wiener and Hammerstein models are examples of cascade type models, also referred to as serial models, as they are a combination of a dynamic linear model in series with a steady-state nonlinear model. In the case of Wiener models, the static nonlinear model block is followed by a dynamic linear model while in Hammerstein models the blocks are placed in the opposite order. The different models are commonly obtained empirically. When applied to MPC the common approach is to just use the linear part for prediction/optimization while leaving the nonlinear part on the outside as a compensator to incorporate the nonlinear behavior.

Fruzzetti, Palazoglu, and McDonald (1997) simulated a pH system for which they then obtained a Hammerstein model. This was then used for in MPC, where the optimization was carried out using an ellipsoidal cutting plane algorithm.

The improvement of using cascade models compared to a single linear model has been demonstrated (Gerškšič, Juricic, Strmcnik, & Matko, 2000; Norquay, Palazoglu, & Romagnoli, 1999; Patwardhan, Lakshminarayanan, & Shah, 1997, 1998), using fairly simple cases with only strong agents. Patwardhan et al. (1997, 1998) did a comparison between linear MPC, NMPC using Wiener model and NMPC using Hammerstein model. The models were obtained using a partial-least-square approach on a simulated pH system. Norquay et al. (1999) used the same basic setup with regard to acid and base but used a laboratory neutralization reactor instead, applying a Wiener model for the MPC. The use of laboratory equipment would add additional buffering effects. For the Wiener model approach, they used step response modeling. The result showed that the cascade models were generally an improvement over using a single linear model, though there were cases when the linear model MPC or a PID controller could perform just as well. Gerškšič et al. (2000) did a more wide comparison, applying many different approaches of Wiener models in NMPC, including different types of observers and optimization techniques as well as varying the input to the optimization between just using the linear part as well as including a linearization of the nonlinear model. The improvement over linear models at the cost of slower optimization was showed again, but also that using cascade models has a wider range of applicability and better stability properties.

Gómez, Jutan, and Baeyens (2004) incorporated an observer, to approximate the buffer flow and to correct for model discrepancies. They modeled a system with a buffer stream using a subspace-based Wiener model. The control would at a first glance look worse than the other cases but the added complication of not knowing the state or disturbances was a much harder system to control and went to show that the setup is far superior to a single model MPC, particularly when it comes to stability. Though it was noted that when dealing with unconstrained cases a PID controller was on a comparable level with the MPC.

A Hungarian research group led by Abonyi has put forward two different approaches, the first approach (Abonyi, Chován, Nagy, & Szeifert, 1999) was basically using a Wiener model approach, applying a fuzzy model as the steady state nonlinear part and predictor–corrector approach instead of the receding horizon applied in the standard MPC approach, which in all makes it less flexible. The second approach (Abonyi, Nagy, & Szeifert, 2001) showed more promise in that sense, being based around fuzzy Wiener models, which were linearized at each sampling interval to be able to feed linear models to the optimization in the MPC. The approach is promising, but the test setup is not a very demanding one with an

unconstrained optimization and control in a linear region of a case with little buffering activity. The use of Fuzzy–Wiener model has also been tried by [Shaghghi, MonirVaghefi, and Fatehi \(2013\)](#) applying the inverse of the nonlinear model for the correction.

[Mahmoodi, Poshtan, Jahed-Motlagh, and Montazeri \(2009\)](#) and later [Wang and Zhang \(2011\)](#) used Laguerre filters to model the linear part in the Wiener model, also referred to as Wiener–Laguerre model. The two approaches differ in the way the Laguerre part was obtained where the former use standard least square and the latter use a least squares support vector machine and thereby being able to show better results than the former. Both approaches incorporated a correction term to minimize the effect of unmeasured disturbances and being able to show improvement over linear MPC as well as previous approaches of Wiener–Laguerre attempts. [Dubravić, Šehić, and Burgić \(2014\)](#) continued with the same approach, but used Legendre polynomials as well as Laguerre functions to describe the process and demonstrated that the model of choice varies with the application problem. These three approaches were contrary to the standard cascade model approaches as they feed the whole model set into the MPC optimization requiring nonlinear programming in the form of sequential quadratic programming, which makes the optimization more computationally demanding that raise the question about the applicability of the approach.

Another recent approach involves using a piecewise linear model bank to describe the nonlinear part in the Wiener model, in the same way as discussed in [Section 5.1.2](#). This approach has been used by [Shafiee, Arefi, Jahed-Motlagh, and Jalali \(2006\)](#), [Oblak and Škrjanc \(2010\)](#) as well as [Ipanaqué and Manrique \(2011\)](#). In all three papers, the standard setup was applied and the differences between the approaches were in the way of obtaining the model and that Oblak and Škrjanc used continuous models instead of discrete models. They all show that the approaches apply well to the pH control though it can be questioned whether using a Wiener or Hammerstein model is better than just applying a multiple model description by itself as that would not require a correction step. [Zou et al. \(2013\)](#) used model algorithmic control with a Hammerstein model, which as an additional part had a trajectory generator and that past events were included in the model. Their simulation showed improvement over linear MPC and nonlinear PID controller, but no comparison is made to other nonlinear MPC.

A robust approach has recently been tested by [Khani and Haeri \(2015\)](#), which is an extension of the approach discussed in [Section 5.1.2](#). For the Hammerstein model, it basically leaves the nonlinear model outside the min–max approach as the standard correction, while for the Wiener the nonlinear model has to be included into the min–max setting. This was done by considering the nonlinearity to be a Lipschitz nonlinearity and hence bounded, which enables its inclusion without affecting the convexity of the optimization problem. The approach showed an improvement over the multiple linear models considerably reducing settling time.

The implications of using cascade models are more or less the same as for using multiple models or fuzzy models as long as only the linear part is used in the prediction and optimization or if the nonlinearity can be reduced to simpler forms. Overall they work well compared to the single model linear MPC, with better control particularly when the nonlinearity is profound as well as improving the stability properties. As seen in the paper by [Khani and Haeri \(2015\)](#) it is shown that cascade models can improve the control, compared to the multiple model linear case, however that try is for setpoint change only and without studying the increase in computational cost.

5.2.4. Artificial neural network

The basic principle of artificial neural networks (ANN) is to simulate the neural behavior in the brain by creating a system of

nodes, commonly referred to as neurons, that are linked together and ultimately links the inputs to the outputs. The modeling is achieved by having an adaptive updating scheme or a learning scheme, which changes the weights of the interaction between the different neurons to get an appropriate nonlinear model of the system. Considerations are based on what algorithm to use for the training of the ANN, how different functions in the neurons should look like and how the neurons should be interconnected. The application of ANNs has grown rapidly since the 1980s ([Ławryńczuk, 2013a](#)) as computing power has increased and the advent of new structures of ANN, particularly the multi-layer cases. This has made ANN a widespread tool for modeling nonlinear systems though it has one major drawback in all its applicability, which is its black-box nature. The empirical formulation limits, if not totally removes, the understanding of the process itself, which has led to ANN being described as a model-free approach as a model in the traditional sense is not obtained.

The first application known to the authors of ANN to MPC was done by [Draeger, Engell, and Ranke \(1995\)](#). The ANN was obtained by a back-propagation algorithm and applied to an MPC setup using an extended approach, similar to the idea of Wiener and Hammerstein models, which means that the linear part of the ANN is used as the internal model inside the cost function optimization, while the full use of the nonlinear ANN description was used externally to correct for errors associated with the linear approximation. The approach showed improvement compared to a PI controller when applied to a lab scale plant. [Gomm, Doherty, and Williams \(1996\)](#) studied in-line control, obtaining the ANN model of the neutralization using a radial basis function. They also included a dead time estimator through the MPC setup, using an 'iterative' optimization algorithm, where the estimated number of dead time sampling intervals is blocked out in the MPC optimization. [Kuo and Melsheimer \(1998\)](#) also used a time-lag recurrent radial basis function applied to a lab scale CSTR using an extended genetic algorithm for the optimization problem in the MPC.

Further applications of ANN in MPC were the major difference in the way the model was obtained or incorporated into the MPC. [Wior, Boonto, Abbas, and Werner \(2010\)](#) applied a linearized ANN to form ARX models incorporated into the MPC algorithm. [Tang and Nazmul Karim \(2011\)](#) used recurrent neural network modeling, for three different regions of pH that was selected using fuzzy switching and a genetic algorithm for the selection of nodes. [Tharakan, Benny, Jaffar, and Jaleel \(2013\)](#) developed the use of the ANN further by using a neural network description both as a model of the process and a substitution for the on-line optimization. The results are promising, but the drawback is the extensive training required to make the ANN carry a satisfactory substitute for the optimization. [Yang, Xiao, Qian, and Li \(2012\)](#) was demonstrating an approach for control of an MIMO system, using a back-propagating for the neural network to describe the nonlinear steady-state behavior in conjunction with a dynamic linear model. This setup was then incorporated into a parameter varying NMPC approach, which adds an adaptive element to the MPC. The adaptive component carries out a model update when the process-model mismatch exceeds a certain level. The full steady-state dynamic model was used, hence requiring a sequential quadratic programming to solve the optimization problem. [Wysocki and Ławryńczuk \(2015\)](#) used Elman neural networks to model the process which was used in conjunction with linearization of the ANN around the trajectory. The neural networks were linearized around the trajectory of the previous prediction horizon so that a set of linear models are available along the prediction horizon. The combination of linear description and a model development along the horizon enables efficient computation of the new control sequence.

There have also been some approaches that were referred to as neuro-fuzzy modeling, whereby the process was described using a

global model, describing the overall linear behavior, and a set of linear models describing the nonlinear behavior. The nonlinear description in the MPC is obtained by fuzzy logic. Waller and Toivonen (2002), Fatehi, Sadeghpour, and Labibi (2013) and Saadat, Alvanagh, and Rezaei (2013) all used neuro-fuzzy modeling for their MPC. The different approaches mainly differ in the way the neuro-fuzzy model was obtained. Waller and Toivonen were using a quasi-ARMAX approach applying fuzzy clustering utilizing a Gaussian function applied to a lab-scale system. Fatehi et al. used a multilayer perceptron ANN combined with a clustering of the operating data points before the identification process using a Gath–Geva fuzzy clustering resulting in five operating regions. Finally, Saadat et al. used the LOLIMOT algorithm to model the process and applied to lab scale process showing generally better result than a PID controller, but there were regions where the PID performed better.

To incorporate more physical understanding of the ANN model the idea of making the ANN a part of a Wiener or a Hammerstein model has been proposed. This relies on using the ANN to describe the nonlinear static model inside the cascade model, while the dynamic linear model is obtained by other means leaving at least part of the model explicitly known, making it a gray model case. As per the standard procedure for cascade model the linear part is incorporated into the MPC framework.

Zhao, Guiver, Neelakantan, and Biegler (2001), Saha, Krishnan, Rao, and Patwardhan (2004), and Arefi, Montazeri, Poshtan, and Jahed-Motlagh (2006) based the description of the system around a Wiener model approach that in the former case used partial least squares for the linear model plus the addition of an extended Kalman filter for state estimation, while the second described the linear part by Laguerre filters and comparing the ANN and a polynomial description for the nonlinear part and the latter compared it to a linear case. Both comparisons showed that the ANN approach was better than polynomial model fit for the nonlinearities and that the whole setup gave good result in a lab scale trial. Chi, Fei, Liu, and Liang (2015) presented a way to make the solving of the nonlinear optimization problem more efficient. This is done by casting the model in a partial least square framework and incorporating a latent-variable space to make the input variables serve as input to the optimization. This generates a latent-variable dynamic optimization that makes the computation swifter. The results showed an improvement over the standard ANN-NMPC approach.

Ławryńczuk (2010) applied ANN as part of a Hammerstein model, but changed some of the techniques commonly used for cascade models, most significantly was the change in approach for the optimization using a suboptimal approach instead. The sub-optimal approach was not simply using the linear dynamic model in the MPC optimization, the ANN was used to obtain a free response trajectory to describe how the nonlinearity of the system would progress if the input(s) obtained was applied for the whole control horizon. This in conjunction with a linearization of the nonlinear model, for use as part of the predictive model, leads to an optimization that has more of the nonlinearities of the process incorporated into it, which was shown to give a better control compared to using the standard polynomial based Hammerstein model. The idea was extended, Ławryńczuk (2011), by applying a multilayer control to the approach from the former paper with the inclusion of a disturbance estimation, to deal with control levels, basic control and supervisory control, and then using Hammerstein model for economic optimization on different layers as well. The addition of disturbance estimation shows promise, but the economical optimization seems to need more work. In 2013 Ławryńczuk (2013b) used a Wiener model instead of a Hammerstein model, but applying the same modeling approach as in Ławryńczuk (2010). The laboratory tests showed that the sub-optimal approaches were an improvement over a simple

linearization of the model, but not as good as using nonlinear optimization using the nonlinear model directly, however the saving in computational time compared to the nonlinear case makes the linearization worthwhile.

Additional work using ANN has been done by Villanueva Perales, Gutiérrez Ortiz, Vidal Barrero, and Ollero (2010) using ANN in MPC to control model case to a wet limestone flue gas desulfurization, where the pH was the controlled variable for the achieved desulfurization, using nonlinear optimization.

Recently the use of ANN has become the most popular model type to use for NMPC. This is particularly an effect of the development of algorithms for modeling and rapid development of computing power making the modeling practical and easily accessible. Applying the ANN to MPC means that the same considerations as for any other model type has to be considered. The biggest issue is the black box structure not giving any knowledge of the particular process though that issue has been considered by making the system a gray box model by incorporating some physical models into process description.

6. Conclusions

The application of MPC to controlling the pH in neutralization processes and other processes has been extensively studied during the last decades, where the major issue is incorporating the nonlinear behavior of the pH system without making the prediction and optimization too computationally demanding and hence slow. The favored approach is still to use a linear model as the computational model for dealing with the optimization at a low cost, where piecewise linear descriptions are preferred and obtained either through linearization of a nonlinear fundamental model or using a fuzzy model description employing empirical modeling. When it comes to more direct approaches of incorporating the nonlinearities, cascade models, which contain the both a linear dynamic model and a nonlinear static model, and artificial neural networks are used. The former uses the linear part internally and applies the nonlinear description to correct the discrepancies while the latter pretty much does the same with the linear model being obtained by repeated linearization of the nonlinear ANN.

The different approaches will generally show an improvement compared to using simple linear MPC cases as well as PI and PID controllers. However, in many cases fairly simple problems are posed, with small or nonexistent changes of the buffer capacity as well as controlling the system in fairly linear parts of the operating region. The variety of applications of the different approaches makes a direct comparison likely to be a bit inaccurate. This withstanding the general point would be that if it is a fairly linear case, a well tuned PI controller or a single linear MPC would work just fine. However when it comes to problems with more severe nonlinearities, possibly including precipitation of salts in the system, greater demand would be made on describing the nonlinear behavior as correct as possible, hence requiring incorporating the nonlinearities into the MPC in some form. As seen in this review there have been several approaches doing this well.

Looking to the future further development would be required to more complex processes to incorporate robustness into the process as well as incorporate time delays into the setup, particularly when using nonlinear models in the MPC optimization and prediction.

Appendix A. Supplementary data

Supplementary data associated with this paper can be found in the online version at <http://dx.doi.org/10.1016/j.conengprac.2015.09.005>.

References

- Abonyi, J., Chován, T., Nagy, L., & Szeifert, F. (1999). Hybrid convolution model and its application in predictive pH control. *Computers & Chemical Engineering*, 23, S227–S230.
- Abonyi, J., Nagy, L., & Szeifert, F. (2001). Fuzzy model-based predictive control by instantaneous linearization. *Fuzzy Sets and Systems*, 120(1), 109–122.
- Åkesson, B. M., Toivonen, H. T., Waller, J. B., & Nyström, R. H. (2005). Neural network approximation of a nonlinear model predictive controller applied to a pH neutralization process. *Computers & Chemical Engineering*, 29(2), 323–335.
- Altunten, A. (2007). Generalized predictive control applied to a pH neutralization process. *Computers & Chemical Engineering*, 31(10), 1199–1204.
- Annal, W. P., & Jerome, J. (2014). Performance assessment of PID and MPC control algorithm subject to servo tracking and disturbance rejection. *Australian Journal of Basic and Applied Sciences*, 8(17), 265–273.
- Arefi, M. M., Montazeri, A., Poshtan, J., & Jahed-Motlagh, M. R. (2006). Nonlinear model predictive control of chemical processes with a Wiener identification approach. In *IEEE international conference on industrial technology, 2006, ICIT 2006* (pp. 1735–1740). IEEE, Mumbai.
- Azimzadeh, F., Palizban, H. A., & Romagnoli, J. A. (1998). Online optimal control of a batch fermentation process using multiple model approach. In *Proceedings of the 37th IEEE conference on decision and control, 1998* (Vol. 1, pp. 455–460). IEEE, Tampa, FL.
- Bagheri, P., Mardanlou, V., & Fatehi, A. (2011). Multiple model predictive control of multivariable pH process using adaptive weighting matrices. In *The 18th IFAC world congress* (pp. 12366–12371).
- Bello, O., Hamam, Y., & Djouani, K. (2014a). Coagulation process control in water treatment plants using multiple model predictive control. *Alexandria Engineering Journal*, 53(4), 939–948.
- Bello, O., Hamam, Y., & Djouani, K. (2014b). Control of a coagulation chemical dosing unit for water treatment plants using MMPC based on fuzzy weighting. *Journal of Water Process Engineering*, 4, 34–46.
- Bello, O., Hamam, Y., & Djouani, K. (2014c). Fuzzy dynamic modelling and predictive control of a coagulation chemical dosing unit for water treatment plants. *Journal of Electrical Systems and Information Technology*, 1(2), 129–143.
- Bello, O., Hamam, Y., & Djouani, K. (2014d). Nonlinear model predictive control of a coagulation chemical dosing unit for water treatment plants. In *Proceedings of the IFAC world congress, Cape Town* (Vol. 19, pp. 370–376).
- Camacho, E., & Bordons, C. (2004). *Model predictive control* (2nd ed.). Berlin: Springer.
- Chi, Q. H., Fei, Z. S., Liu, K. L., & Liang, J. (2015). Latent-variable nonlinear model predictive control strategy for a pH neutralization process. *Asian Journal of Control*.
- Chisci, L., Rossiter, J. A., & Zappa, G. (2001). Systems with persistent disturbances: predictive control with restricted constraints. *Automatica*, 37(7), 1019–1028.
- Costa, T. V., Fileti, A. M. F., Oliveira-Lopes, L. C., & Silva, F. V. (2014). Experimental assessment and design of multiple model predictive control based on local model networks for industrial processes. *Evolving Systems* (pp. 1–11), 1–11.
- Couper, J. R., Penney, W. R., & Fair, J. R. (2009). *Chemical process equipment revised 2E: Selection and design* (2nd ed.). Houston: Gulf Professional Publishing.
- Díaz-Mendoza, R., & Budman, H. (2010). Structured singular valued based robust nonlinear model predictive controller using Volterra series models. *Journal of Process Control*, 20(5), 653–663.
- Dougherty, D., & Cooper, D. (2003). A practical multiple model adaptive strategy for single-loop MPC. *Control Engineering Practice*, 11(2), 141–159.
- Draeger, A., Engell, S., & Ranke, H. (1995). Model predictive control using neural networks. *Control Systems, IEEE*, 15(5), 61–66.
- Dubravić, A., Šehić, Z., & Burgić, M. (2014). Orthonormal functions based model predictive control of pH neutralization process. *Tehnički vjesnik*, 21(6), 1249–1253.
- Fatehi, A., Sadeghpour, B., & Labibi, B. (2013). Nonlinear system identification in frequent and infrequent operating points for nonlinear model predictive control. *Information Technology and Control*, 42(1), 67–76.
- Fruzzetti, K. P., Palazoglu, A., & McDonald, K. A. (1997). Nonlinear model predictive control using Hammerstein models. *Journal of Process Control*, 7(1), 31–41.
- Gerkišić, S., Juricic, D., Strmcnik, S., & Matko, D. (2000). Wiener model based nonlinear predictive control. *International Journal of Systems Science*, 31(2), 189–202.
- Gómez, J. C., Jutan, A., & Baeyens, E. (2004). Wiener model identification and predictive control of a pH neutralisation process. In *IEE proceedings—control theory and applications* (Vol. 151, pp. 329–338). IET.
- Gomm, J. B., Doherty, S. K., & Williams, D. (1996). Control of pH in-line using a neural predictive strategy. In *UKACC international conference on CONTROL '96* (pp. 1058–1063). IET, Exeter.
- Gu, B. F., & Gupta, Y. P. (2008). Control of nonlinear process by using linear model predictive control algorithms. *ISA Transactions*, 47, 211–216.
- Gustafsson, T. K., Skrifvars, B. O., Sandström, K. V., & Waller, K. V. (1995). Modeling of pH for control. *Industrial Engineering Chemistry Research*, 34, 820–827.
- Halldorsson, U., Ali, A., Unbehauen, H., & Schmid, C. (2002). Adaptive predictive control of a neutralization plant using local model networks. In *Proceedings of the IFAC world congress, Barcelona*.
- Hermansson, A. W., & Syafie, S. (2014). Control of pH neutralization system using nonlinear model predictive control with I-controller. In *2014 IEEE international conference on industrial engineering and engineering management (IEEM)* (pp. 853–857). IEEE, Malaysia.
- Hermansson, A. W., Syafie, S., & Mohd Noor, S. B. (2010). Multiple model predictive control of nonlinear pH neutralization system. In *2010 IEEE international conference on industrial engineering and engineering management (IEEM)* (pp. 301–304). IEEE, Macau.
- Hong, T., Morris, A. J., Karim, M. N., Zhang, J., & Luo, W. (1996). Nonlinear control of a wastewater pH neutralisation process using adaptive NARX models. In *IEEE international conference on systems, man, and cybernetics, 1996* (Vol. 2, pp. 911–916). IEEE, Beijing.
- Ipanaque, W., & Manrique, J. (2011). Identification and control of pH using optimal piecewise linear Wiener model. In *World congress* (Vol. 18, pp. 12301–12306).
- Johansen, T. A., & Foss, B. A. (1992). Nonlinear local model representation for adaptive systems. In *Proceedings of Singapore international conference on intelligent control and instrumentation, 1992, SICIC'92* (Vol. 2, pp. 677–682). IEEE, Singapore.
- Kavsek-Biasizzo, K., Skrjanc, I., & Matko, D. (1997). Fuzzy predictive control of highly nonlinear pH process. *Computers & Chemical Engineering*, 21, S613–S618.
- Kelkar, B., & Postlethwaite, B. (1994). Fuzzy-model based pH control. In *Proceedings of the third IEEE conference on fuzzy systems, 1994. IEEE world congress on computational intelligence* (pp. 661–666). IEEE.
- Khani, F., & Haeri, M. (2015). Robust model predictive control of nonlinear processes represented by Wiener or Hammerstein models. *Chemical Engineering Science*, 129, 223–231.
- Kothare, M. V., Balakrishnan, V., & Morari, M. (1996). Robust constrained model predictive control using linear matrix inequalities. *Automatica*, 32(10), 1361–1379.
- Kumar, D., & Budman, H. (2014). Robust nonlinear MPC based on Volterra series and polynomial chaos expansions. *Journal of Process Control*, 24(1), 304–317.
- Kuo, L. E., & Melsheimer, S. S. (1998). Wastewater neutralisation control using a neural network based model predictive controller. In *Proceedings of the 1998. American Control Conference, 1998* (Vol. 6, pp. 3896–3899). IEEE, Philadelphia.
- Kwon, W. H., & Han, S. H. (2006). *Receding horizon control: model predictive control for state models*. London: Springer Science & Business Media.
- Ławryńczuk, M. (2010). Suboptimal nonlinear predictive control based on multi-variable neural Hammerstein models. *Applied Intelligence*, 32(2), 173–192.
- Ławryńczuk, M. (2011). On-line set-point optimisation and predictive control using neural Hammerstein models. *Chemical Engineering Journal*, 166(1), 269–287.
- Ławryńczuk, M. (2013a). *Computationally efficient model predictive control algorithms*. Cham: Springer.
- Ławryńczuk, M. (2013b). Practical nonlinear predictive control algorithms for neural Wiener models. *Journal of Process Control*, 23(5), 696–714.
- Li, S. Z., Liu, X. J., & Yuan, G. (2014). Application of supervisory predictive control based on TS model in pH neutralization process. In *Applied mechanics and materials* (Vol. 511, pp. 867–870). Trans Tech Publ, Dürnten.
- Lipták, B. G. (2005). *Instrument engineers' handbook, volume two: Process control and optimization* (Vol. 2). CRC press, Boca Raton.
- Løvaas, C., Seron, M. M., & Goodwin, G. C. (2008). Robust output-feedback model predictive control for systems with unstructured uncertainty. *Automatica*, 44(8), 1933–1943.
- Love, J. (2007). *Process automation handbook: A guide to theory and practice* (1st ed.). London: Springer Publishing Company, Incorporated.
- Lu, Y., Arkun, Y., & Palazoglu, A. (2004). Real-time application of scheduling quasi-min-max model predictive control to a bench-scale neutralization reactor. *Industrial and Engineering Chemistry Research*, 43(11), 2730–2735.
- Maciejowski, J. M. (2002). *Predictive control with constraints*. Englewood Cliffs, NJ: Prentice Hall.
- Mahmoodi, S., Poshtan, J., Jahed-Motlagh, M. R., & Montazeri, A. (2009). Nonlinear model predictive control of a pH neutralization process based on Wiener-Laguerre model. *Chemical Engineering Journal*, 146(3), 328–337.
- Maiti, S. N., Kapoor, N., & Saraf, D. N. (1994). Adaptive dynamic matrix control of pH. *Industrial & Engineering Chemistry Research*, 33(3), 641–646.
- Mandal, S., Mahapatra, S. S., & Patel, R. K. (2015). Neuro fuzzy approach for arsenic (iii) and chromium(vi) removal from water. *Journal of Water Process Engineering*, 5, 58–75.
- Marusak, P. M. (2009). Advantages of an easy to design fuzzy predictive algorithm in control systems of nonlinear chemical reactors. *Applied Soft Computing*, 9(3), 1111–1125.
- Mayne, D. Q., Kerrigan, E. C., Van Wyk, E. J., & Falugi, P. (2011). Tube-based robust nonlinear model predictive control. *International Journal of Robust and Nonlinear Control*, 21(11), 1341–1353.
- Mayne, D. Q., & Langson, W. (2001). Robustifying model predictive control of constrained linear systems. *Electronics Letters*, 37(23), 1422–1423.
- McMillan, G. K. (1984). *pH control*. Triangle Park: Instrument Society of America Research Triangle Park.
- McMillan, G. K. (2000). *Good tuning: A pocket guide*. Triangle Park: ISA.
- Michalska, H., & Mayne, D. Q. (1993). Robust receding horizon control of constrained nonlinear systems. *IEEE Transactions on Automatic Control*, 38(11), 1623–1633.
- Mollov, S., Babuska, R., Abonyi, J., & Verbruggen, H. B. (2004). Effective optimization for fuzzy model predictive control. *IEEE Transactions on Fuzzy Systems*, 12(5), 661–675.
- Norquay, S. J., Palazoglu, A., & Romagnoli, J. A. (1999). Application of Wiener model predictive control (WMPC) to a pH neutralization experiment. *IEEE Transactions on Control Systems Technology*, 7(4), 437–445.
- Novák, J., & Chalupa, P. (2013). Nonlinear state estimation and predictive control of pH neutralization process. In *Nostradamus 2013: Prediction, modeling and analysis of complex systems* (pp. 285–294). Springer, Ostrava.

- Novák, J., Chalupa, P., & Bobál, V. (2011). Multiple model modeling and predictive control of the pH neutralization process. *International Journal of Mathematical Models and Methods in Applied Sciences*, 5(7), 1170–1179.
- Oblak, S., & Škrjanc, I. (2010). Continuous-time Wiener-model predictive control of a pH process based on a PWL approximation. *Chemical Engineering Science*, 65(5), 1720–1728.
- Obut, S., & Özgen, C. (2008). Online identification and control of pH in a neutralization system. *Industrial & Engineering Chemistry Research*, 47(13), 4394–4404.
- Patwardhan, R. S., Lakshminarayanan, S., & Shah, S. L. (1997). Nonlinear model predictive control using PLS based Hammerstein and Wiener models. Presented at the AIChE Meeting, Los Angeles, CA.
- Patwardhan, R. S., Lakshminarayanan, S., & Shah, S. L. (1998). Constrained nonlinear MPC using Hammerstein and Wiener models: PLS framework. *AIChE Journal*, 44(7), 1611–1622.
- Pawlowski, A., Fernández, I., Guzmán, J. L., Berenguel, M., Ación, F. G., & Normey-Rico, J. E. (2014). Event-based predictive control of pH in tubular photo-bioreactors. *Computers & Chemical Engineering*, 65, 28–39.
- Pawlowski, A., Mendoza, J. L., Guzmán, J. L., Berenguel, M., Ación, F. G., & Dormido, S. (2014). Effective utilization of flue gases in raceway reactor with event-based pH control for microalgae culture. *Bioresource Technology*, 170, 1–9.
- Pröll, T., & Nazmul Karim, M. (1994). Model-predictive pH control using real-time NARX approach. *AIChE Journal*, 40(2), 269–282.
- Rawlings, J. B., & Mayne, D. Q. (2009). *Model predictive control: theory and design*. Madison, WI: Nob Hill Publishing, LCC.
- Rawlings, J. B., & Muske, K. R. (1993). The stability of constrained receding horizon control. *IEEE Transactions on Automatic Control*, 38(10), 1513–1516.
- Rossiter, J. A. (2013). *Model-based predictive control: a practical approach*. Boca Raton: CRC press.
- Saadat, A., Alvanagh, A. A., & Rezaei, H. (2013). pH control in biological process using mmpc based on neuro-fuzzy model by LOLIMOT algorithm. In *2013 9th Asian control conference (ASCC)* (pp. 1–6). IEEE, Istanbul.
- Saha, P., Krishnan, S. H., Rao, V. S. R., & Patwardhan, S. C. (2004). Modeling and predictive control of MIMO nonlinear systems using Wiener–Laguerre models. *Chemical Engineering Communications*, 191(8), 1083–1119.
- Shafiee, G., Arefi, M. M., Jahed-Motlagh, M. R., & Jalali, A. A. (2006). Model predictive control of a highly nonlinear process based on piecewise linear Wiener models. In *2006 1st IEEE international conference on e-learning in industrial electronics* (pp. 113–118). IEEE, Hammamet.
- Shaghghi, D., MonirVaghefi, H., & Fatehi, A. (2013). Generalized predictive control of pH neutralization process based on fuzzy inverse model. In *2013 13th Iranian conference on fuzzy systems (IFSC)* (pp. 1–6). IEEE, Teheran.
- Shamsaddinlou, A., Fatehi, A., & Sedigh, A. K. (2014). Switching-tuning adaptive multiple model predictive control. *Journal of Control Engineering and Technology*, 4(2).
- Shamsaddinlou, A., Fatehi, A., Sedigh, A. K., & Karimi, M. M. (2013). Study of multiple model predictive control on a pH neutralization plant. In *2013 9th Asian control conference (ASCC)* (pp. 1–6). IEEE, Istanbul.
- Shinsky, F. G. (1973). *pH and pION control in process and waste streams*. New York: John Wiley & Sons, Inc.
- Sivakumaran, N., & Radhakrishnan, T. K. (2007). Predictive controller design for non-linear chemical processes. *Indian Journal of Chemical Technology*, 14(4), 341–349.
- Sjöberg, J., Zhang, Q., Ljung, L., Benveniste, A., Delyon, B., Glorennec, P.-Y., Hjalmarsson, H., & Juditsky, A. (1995). Nonlinear black-box modeling in system identification: a unified overview. *Automatica*, 31(12), 1691–1724.
- Tang, W., & Nazmul Karim, M. (2011). Multi-model MPC for nonlinear systems: Case study of a complex pH neutralization process. In *21st European symposium on computer aided process engineering* (Vol. 29). Elsevier.
- Tharakan, L. G., Benny, A., Jaffar, N. E., & Jaleel, J. A. (2013). Neural network based pH control of a weak acid/strong base system. In *2013 international multi-conference on automation, computing, communication, control and compressed sensing (iMAC4s)* (pp. 674–679). IEEE, Chalkidiki.
- Todoaro, C. M., & Vogel, H. C. (2014). *Fermentation and biochemical engineering handbook*. Burlington: William Andrew.
- Villanueva Perales, A. L., Gutiérrez Ortiz, F. J., Vidal Barrero, F., & Ollero, P. (2010). Using neural networks to address nonlinear pH control in wet limestone flue gas desulfurization plants. *Industrial and Engineering Chemistry Research*, 49(5), 2263–2272.
- Villanueva Perales, A. L., Ollero, P., Gutierrez Ortiz, F. J., & Gómez-Barea, A. (2009). Model predictive control of a wet limestone flue gas desulfurization pilot plant. *Industrial & Engineering Chemistry Research*, 48(11), 5399–5405.
- Waller, J. B., & Toivonen, H. (2002). A neuro-fuzzy model predictive controller applied to a pH neutralization process. In *Proceedings of the 15th international federation of automatic control IFAC world congress*.
- Wang, Q., & Zhang, J. (2011). Wiener model identification and nonlinear model predictive control of a pH neutralization process based on Laguerre filters and least squares support vector machines. *Journal of Zhejiang University Science C*, 12(1), 25–35.
- Wior, I., Boonto, S., Abbas, H. S., & Werner, H. (2010). Modeling and control of an experimental pH neutralization plant using neural networks based approximate predictive control. In *Proceedings of 1st virtual control conference*, Denmark.
- Wysocki, A., & Ławryńczuk, M. (2015). Predictive control of a multivariable neutralisation process using Elman neural networks. In *Progress in automation, robotics and measuring techniques* (pp. 335–344). Springer, Cham.
- Xie, S. G., Zhou, L. F., Ma, A., & Zhou, L. W. (2008). A new switching scheme for multi-model predictive control using clustering modeling. In *Fifth international conference on fuzzy systems and knowledge discovery, 2008, FSKD'08* (Vol. 3, pp. 484–488). IEEE, Jinan.
- Yang, J.-F., Xiao, L.-F., Qian, H., & Li, J.-X. (2012). Nonlinear model predictive control using parameter varying BP-ARX combination model. *International Journal of Systems Science*, 43(3), 475–490.
- Zhang, B., & Zhang, W. (2006). Adaptive predictive functional control of a class of nonlinear systems. *ISA Transactions*, 45(2), 175–183.
- Zhao, H., Guiver, J., Neelakantan, R., & Biegler, L. T. (2001). A nonlinear industrial model predictive controller using integrated PLS and neural net state-space model. *Control Engineering Practice*, 9(2), 125–133.
- Zhou, L. W., & Zhou, L. F. (2006). Multi-model predictive control based on a new clustering modeling method. In *Intelligent control and automation, Lecture notes in control and information sciences* (Vol. 344, pp. 559–564). Springer, Berlin.
- Zou, Z., Yu, M., Wang, Z., Liu, X. H., Guo, Y. Q., Zhang, F. B., & Guo, N. (2013). Nonlinear model algorithmic control of a pH neutralization process. *Chinese Journal of Chemical Engineering*, 21(4), 395–400.