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Auto-Regressive with Exogenous Input Model Predictive Controller for Water Activity in Esterification

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In this work, the Auto-Regressive with Exogenous Input Model Predictive Controller (ARX-MPC) was designed and implemented to control the water activity of the lipase-catalysed esterification process. The empirical model, which was embedded in the MPC was developed using the Autoregressive with Exogenous input (ARX) model. The parameter estimation and model validation for the ARX model were carried out using the recursive least squares estimation (RLSE) system identification toolbox in MATLAB®. The capability of the models to capture the dynamics of the input and output variables was also verified. ARX models were solved using the quadratic programming (QP) method in the MPC toolbox in MATLAB®/Simulink. The ARX-MPC parameters were tuned to determine the best controller performance. Then, the performances of the best-tuned ARX-MPC were evaluated in terms of set point tracking and disturbance rejection. According to results, the ARX-MPC was considered suitable and reliable for tracking the set-point changes of the controlled process variable and able to eliminate the presence of disturbance in the process.

1. Introduction

The rising demand for the natural products which are environmentally friendly leads the application of lipases as catalyst in many chemical processes. The rate and equilibrium yield as well as the stability of lipases can be influenced by many factors such as temperature, enzyme concentration, water activity, biocatalyst loading, initial molar substrate ratio and different solvents. Among these factors, the most critical is water activity (Wehtje et al., 1997). Most lipase catalysed need a certain amount of water activity in order to work. Continuous control of water activity for esterification process is a must. Control of water activity in the lipase-catalysed esterification process is very important to achieve high yields and rates, as well as to reduce side products. A small number of studies has been done in controlling the esterification process, and most of them implemented conventional controllers, such as Proportional-Integral (PI) controller (Won and Lee, 2002). This type of controller is expected to perform efficiently only when the process operates in a genuinely linear behaviour. The control system has to cope with the process uncertainties, as well as the changes in operations conditions, in the presence of disturbances. Due to these difficulties, studies of advanced control strategies during batch processes have received considerable interest in the past decades (Hosen et al., 2011). Previous studies have proven that the Model Predictive Control (MPC) is a good control for batch reactor processes because its algorithms can cope with multivariable systems and can be formulated to handle process constraints explicitly (Santos et al., 2013).

The MPC can be defined as a control system in which the control algorithm optimises the manipulated variable profile over a finite future time horizon in order to maximise an objective function subjected to plant models and constraints (Eaton and Rawlings, 1992). The MPC has been successfully implemented in a number of chemical processes. The implementation of the MPC controller in an esterification system is still scarce. Among the major issues in the MPC development are the developments of a suitable internal model that can represent the real process (Mohd and Aziz, 2015). A proper internal model with an efficient optimisation algorithm must be embedded in the MPC in order to achieve better performance in controlling the esterification process. ARX modelling was regularly used as time series models. Just like any other empirical modelling approaches pertaining to the given time series data, the key problem is to determine the most

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suitable model complexity that can also depict the dynamic structure of the objective system. The complexity of the ARX modelling is determined by the number of model orders which is the number of the past consecutive measurable input and output response under a constant time interval.
In this work ARX model has been developed and used as internal model that can capture the dynamics relating the inputs to the output of the esterification process. For control purposes, the developed ARX model is embedded in the MPC and known as ARX-MPC. Finally, ARX-MPC performance is evaluated for set-point tracking, set-point change and disturbance rejection.

2. Water activity control system in batch esterification reactor

In this work, Citronellyl laurate ester was synthesised from Citronellol and lauric acid using immobilised Candida Rugosa lipase as a biocatalyst. The esterification process was carried out in a jacketed batch reactor with the presence of iso-octane as a solvent. In the water activity control loop system, water activity was measured in the gaseous phase with a humidity sensor and connected to a computer for monitoring. The MATLAB® software was used to design the program for the controller to control the inflow of dry air, which was needed to ensure the water activity was retained at the set point value (MATLAB, 2016). The measured value in the reactor was compared with the set point and the air flow was controlled via a proportional valve, and directed into a desiccating column to dry the air, respectively. The air was bubbled into the reactor through small holes in a narrow steel tube. Details on the process can be found in Zulkeflee et al. (2013).

3. Auto-regressive with exogenous input model predictive control (ARX-MPC)

The control objective for the lipase-catalysed esterification process is to control the water activity (a_w) by manipulating the air flowrate (F_{air}). The idea of the MPC is to attain the current control action by providing an optimal solution in every sampling time through a finite horizon open-loop optimal control problem based on the plant's current state as the primary state. Based on the difference between the required and actual output response, there is a reduction of the required objective function within the optimisation method that is linked to an error function. The earliest optimal input is attached to the plant at time t, while other optimal inputs that come later will be rejected. In the meantime, another size of the optimal control problem is solved at time t + 1, while the regressing horizon mechanism offers the preferred feedback mechanism for the controller (Nagy et al., 2007). A formulation of the MPC online optimisation used in this work is as follows:

$$\min_{u[t|t],\dots u[m+p|t]_{i=0}} J(y(t), u(t)) \tag{1}$$

$$\min_{u[t|t],\dots u[m+p|t]_{k=0}} \sum_{k=1}^{P} w_k(y[t+k|t] - y_{sp})^2 + \sum_{k=1}^{M} r_k \Delta u[t+k|t]^2 \tag{2}$$

where $u(t)$ and $y(t)$ are the input and output variables. P and M are the length of the process output prediction and the manipulated process input horizons. $u[t+k|t]_{k=0,\dots P}$ is the set of future process input values. The vector w_k and r_k represent the weight vector for output and input control response. The notation shows the value of the variable at instant $t+k$ calculated at instant t.
At each time step t, the current state $y(t)$ of the process and the reference input over the finite horizon were provided to the controller which then computed the optimal input for the process response.

$$y_{sp}(t) = [y_{sp}(t+1) y_{sp}(t+2) \dots . y_{sp}(t+P)]^T \tag{3}$$

In this work, the ARX model was developed used as the internal model embedded in the MPC. This structure is known as ARX-MPC. Figure 1 depicts the structure of the proposed ARX-MPC.
ARX-MPC controller was formulated by considering the objective function, the constraints imposed by the empirical model, and input and output variables. The ARX model error, $e(t)$ is:

$$e[t|t] = y(t) - \sum_{i=0}^{n_u} a(i). u(t-i) - \sum_{j=1}^{n_y} b(j). y(t-j) \tag{4}$$

The prediction of future outputs is:

$$y(t+k) = \sum_{i=0}^{n_u} a(i). u(t-i+k) + \sum_{j=1}^{n_y} b(j). y(t-j+k) + e(t) \tag{5}$$

Substitution of Eq(4) and Eq(5) into Eq(2) yields Eq(6):

$$\min_{u[t|t],\ldots u[m+p|t]_{k=0}} \sum_{k=1}^{P} w_k \left(\sum_{i=0}^{n_u} a(i).u(t-i+k + \sum_{j=1}^{n_y} b(j).y(t-j+k+y(t) - \sum_{i=0}^{n_u} a(i).u(t-i) - \sum_{j=1}^{n_y} b(j).y(t-j) - y_{sp} \right)^2 + \sum_{k=1}^{M} r_k \Delta u[t+k|t]^2 \quad (6)$$

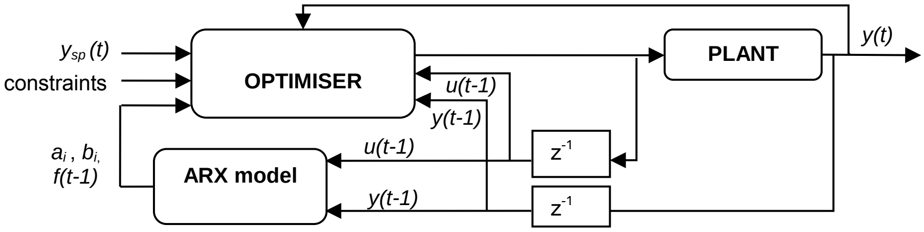

Figure 1: Structure of the ARX-MPC

The issue of online optimisation as shown above can also incorporate a few limitations. In this work, the normal operating condition for the air valve was at 50 %. The valve opening for the jacket and air was set to be in the range between 15 % and 85 %. The minimum and maximum constraints of input changes [Δu_{min}, Δu_{max}] can be set as [-35 %, 35 %]. The process constraints for this work can be seen in the following equations:

$$16.67\ L/s \le F_{air}[t+k|t] \le 83.30\ L/s \quad (7)$$

$$0 \le a_w[t+k|t] \le 0.8 \quad (8)$$

The tuning of the MPC parameter is based on the rule of thumb suggested by Bemporad et al. (2010) for application in the MPC toolbox in the MATLAB software. The sampling period, T_s, is approximated to one fifth of the process time constant, the small control horizon is selected with the default; M ≥ $1/3\,(T_{sett}/T_s)$ where T_{sett} is the settling time and the default prediction horizon is initially based on, P ≥ M. The weighting factor (w_k and r_k) is set to default value, 0.1. The value of the controller parameters is increased until further increases have a minor impact on the controller performance. The controller performance of the process response in following and tracking the set-point is evaluated based on the error value, rise-time, overshoot, and settling time. In this work, ISE is used to evaluate the performance of the developed controller. The ISE criterion formula is written as follows:

$$ISE = \int_0^{\infty} \left|y_{sp}(t) - y(t)\right|^2 dt \quad (9)$$

4. Identification of ARX model

As a linear recurrence equation, the ARX model is used to join the current value of an objective variable together with its past finite time series, as well as other exogenous input variable's finite time series. This can be written as follows:

$$y(t)_{ARX} = \sum_{i=0}^{n_u} a(i).u(t-i) + \sum_{j=1}^{n_y} b(j).y(t-j) + e(t) \quad (10)$$

where $a(i)$ is the coefficient of the originating exogenous terms; $b(i)$ is the coefficient of the autoregressive terms and $e(t)$ is the process noise. Here, n_u and n_y are the input and output orders of the dynamical model in which $n_u \ge 0$, $n_y \ge 1$. The matrix form of the ARX model in Eq(10) can be written as follows:

$$\begin{bmatrix} y(t) \\ y(t+1) \\ \vdots \\ y(t+n_y) \end{bmatrix}_{ARX} = a.u^T + b.y^T + e(t) \quad (11)$$

where:

$$a = [a(0)\ a(1) \ldots a(n_u)]^T \quad (12)$$

$$b = [b(1)\ b(2) \ldots b(n_y)]^T \quad (13)$$

$$u = [u(t)\ u(t-1) \ldots u(n_u)] \quad (14)$$

$$y = [y(t-1)\ u(t-2) \ldots u(n_y)] \tag{15}$$

Eq(12) can be alternatively expressed as:

$$y(t)_{ARX} = [u^T y^T]\begin{bmatrix} a \\ b \end{bmatrix} \tag{16}$$

The constants a and b are the coefficients of the term cluster which contains the form $u^{n_u}(t-i)y^{n_y}(t-j)$ for $n_u + n_y \leq n_l$, where i and j are any time lag. Such coefficients are called cluster coefficients and are represented as $\theta_{n_u n_y}$. Eq(18) can be represented in a simpler form:

$$\bar{Y} = \bar{U}.\theta_{n_u n_y} \tag{17}$$

where:

$$\bar{Y} = y(t) \tag{18}$$

$$\bar{U} = [u^T y^T] \tag{19}$$

$$\theta_{n_u n_y} = [a\ b]^T \tag{20}$$

The estimation of the model constant in Eq(19) can be solved by:

$$\theta_{n_u n_y} = \bar{U}/\bar{Y} \tag{21}$$

With full state measurements, choosing the number of input and output lags is crucial and the process conditions can be initially described by the current states and inputs. The state and input transition matrices are estimated by regressing a matrix of concatenated states and inputs on a matrix of forward shifted states. In this work, the input of pseudo random binary signal (PRBS) has been implemented in the process simulation system and the output signal has been verified to be used in the ARX model identification. The minimum and maximum of air flowrate is equal to 16.67 L/s and 83.30 L/s.

In ARX model identification, the model matrices function is estimated using the recursive least squares estimation (RLSE) function block in the MATLAB®/Simulink. The Kalman filter is chosen as the ARX model estimation method since it allows a prediction of the output response and then updates the output based on the available measurement. The parameters obtained from the model is exported in the MATLAB® workspace and used in the model validation procedure. For validation, the multiple step input signal is introduced into the process system to generate the validation data set. In developing the ARX models, the important phase that should be taken into account is the choice of the model order. (Eq)22 represents the calculation of the Mean Square Error (MSE) between the model output response and the real process output response.

$$MSE \Longrightarrow \forall u \in \mathbb{U}: \xi\left\{\left|y(t,u,y) - y_m\left(t,u,y,n_u,n_y,\theta_{n_u n_y}\right)\right|^2\right\} \tag{22}$$

The model $y_m(t,u,y,n_u,n_y)$ converges in mean square sense to a system $y(t,u,y)$, if all the column vectors of the model residuals, $\varepsilon > 0$, $\exists M_\varepsilon$, is independent of $\theta_{n_u n_y}$.

5. Results and discussion

Different orders of the ARX models, which involved mapping the past input (n_u) and output (n_y) terms to future outputs, were tested and the best were selected according to the MSE criterion. The results for the variations in the model order and the corresponding MSE values for the ARX model are tabulated in Table 1.

Table 1: MSE values for different numbers of n_u and n_y

(n_u, n_y)	MSE (x 10^{-2})	
	Training	Validation
0,1	3.0849	7.9382
1,1	2.6833	5.5213
2,1	2.2910	5.0042
2,2	2.0628	4.9017
2,3	2.1735	4.9834

For the first identification, all the model orders were set to n_u = 0 and n_y = 1 to keep the models as simple as possible. As can be seen from the results, the ARX model orders, n_u = 2 and n_y = 2 was selected as the best models with MSE = 4.9017 for validation. It can be observed that the MSE value decreased by increasing the model order. The MSE values started to increase after the model reached a certain model order, which showed a larger value of error. Based on this result, it is important to consider the input terms in the model since the variations of the input determine the direction of the output.

Then, the best developed ARX model was used as the predictive models in the MPC. Table 2 shows the compilation results for the tuning parameters and the ISE criteria for the developed controllers in the set point tracking. Based on the results, the value of M = 4 gave the smallest error output response with ISE values =

195.43. The results indicated that smaller numbers of the M would lead to a better control performance if compared to a long control horizon. This was because the small value of the M had the tendency to increase the robustness of the system and reduce computational burden, whereas a long control horizon would result in unnecessary control action and a long settling time. The results also show that increasing the P would decrease the value of ISE. Further increase of the P led to higher ISE values. The best performances for the ARX-MPC was when P = 10. The longer P was required to determine the number of the output predictions that were used in the optimisation calculation and caused the control system to be less sensitive to model error. As can be seen, the controller performed the best at r_k = 0.1. For the w_k, controllers gave the lowest values of error at w_k= 1. The weighting factor penalised the tracking errors and guided the servo performance of the control system. Next, ARX-MPC with the best tuning was evaluated based on their performances on set point tracking, set point change and disturbance rejection.

Table 2: Tuning parameters and ISE criteria for set point tracking

Tuning M	ISE	Tuning P	ISE	Tuning w_k	ISE	Tuning r_k	ISE
M = 2	385.04	P = 7	185.02	w_k = 10	318.02	r_k = 10	581.01
M = 3	200.87	P = 8	181.58	w_k = 1	174.75	r_k = 1	174.75
M = 4	195.43	P = 9	176.92	w_k = 0.1	190.04	r_k = 0.1	138.17
M = 5	231.57	P = 10	174.75			r_k = 0.01	152.22
		P = 11	190.11				
with P = 5; w_k = 1; r_k = 1		with M = 4; w_k = 1; r_k = 1		with P = 10; M = 4; r_k = 1		with P = 10; M = 4; w_k = 1	

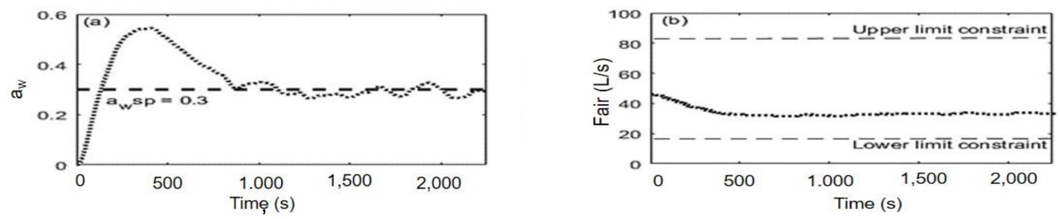

Figure 2: (a) Water activity control responses of the ARX-MPC controllers for set-point tracking and (b) their respective manipulated variable actions

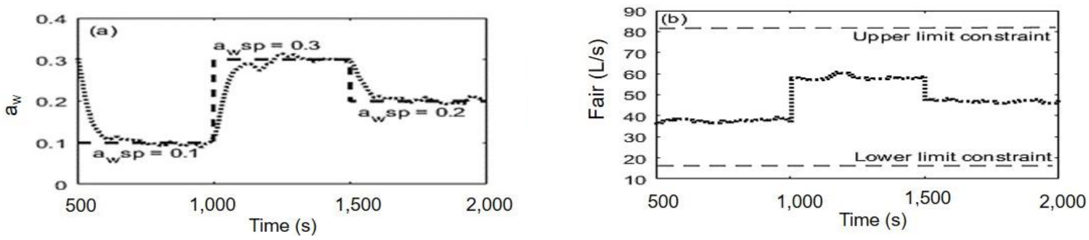

Figure 3: (a) Water activity control responses of the ARX-MPC controllers for set-point changes and (b) their respective manipulated variable actions

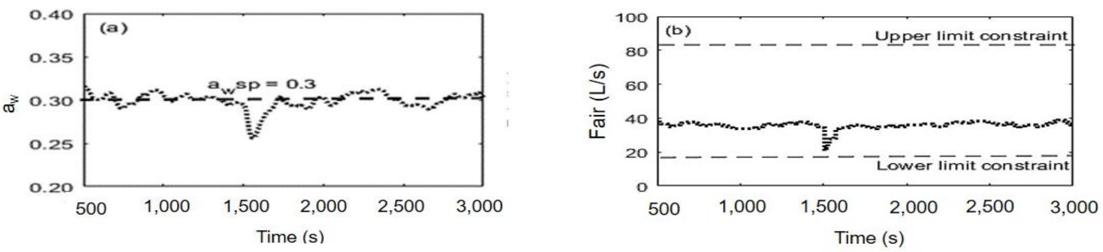

Figure 4: (a) Water activity control responses of the ARX-MPC controllers for disturbance rejection and (b) their respective manipulated variable actions.

The water activity was controlled at its set point value of 0.3. Based on Figure 2(a), the ARX-MPC presented a large output overshoot with the ISE value of 46.27. Based on Figure 2(a), the ARX-MPC presented a large output overshoot (ISE = 46.27) as the water activity increased rapidly at the beginning of the reaction caused from the water production from the esterification process. With some overshoot and fluctuation, the results showed that the ARX-MPC controller can drive the water activity to the desired set points. As shown in Figure 3, the ARX-MPC controllers were able to bring the water activity to the new set point. The ARX-MPC showed small fluctuating responses around the set point trajectory. In this test, the ISE value of the the ARX-MPC was 41.49. A step input with 2 % increase of the jacket temperature variable is introduced after the measured process response becomes steady which at allocated time the cooling line was closed and the heating system was allowed to run for a few minutes until the jacket temperature has reached a 2 % increase from the initial value. In Figure 4(a), it is clear that when the process was disturbed, water activity responses by the ARX-MPC deviated from the original set-point. A similar behaviour response can be observed from the manipulated profiles in Figure 4(b). For all tests, it can be observed that the manipulated variable profiles for ARX-MPC controllers fluctuated within the input constraints. In this test, the ISE value for the ARX-MPC was 31.79. As observed, the ARX-MPC showed a good performance in rejecting the process disturbance

6. Conclusions

The ARX-MPC controller had been proposed in this work. The identification of the ARX models for lipase-catalysed esterification process was presented. The ARX model with model order n_u = 2 and n_y = 2 was selected as the best predictive models for the water activity control loop system. The identified model served as the basis for the design and evaluation of the MPC controllers. The important MPC were tuned to obtain the best controller performance. The ARX-MPC with controller parameters: P = 10, M = 4, w_k = 1, and r_k = 0.1 was selected since these controllers showed the best performances in controlling water activity. Finally, all the controllers were evaluated based on their performances on set point tracking, set point change, and disturbance rejection. The performance results of the ARX-MPC controllers revealed that the closed-loop responses were satisfactory and effective in tracking the optimal set point. Aim of the future work is to embed the nonlinear empirical model in the MPC which can provide better prediction on the reaction process and thus will be able to bring the process variable to the set point quickly with smaller amount of overshoot.

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References

Bemporad A., Morari M., Ricker N.L., 2010, Model predictive control toolbox, user's guide, The Mathworks Inc., Massachusetts, USA.

Eaton J.W., Rawlings J.B., 1992, Model-predictive control of chemical processes, Chemical Engineering Science 47 (4), 705-720.

Hosen M.A., Hussain M.A., Mjalli F.S., 2011, Control of polystyrene batch reactors using neural network based model predictive control (NNMPC): An experimental investigation, Control Engineering Practice 19, 454-467.

Matlab, 2016, The Mathworks Inc., Massachusetts, USA.

Mohd N., Aziz N., 2015, Control of Bioethanol Fermentation Process: NARX-based MPC (NARX-MPC) versus Linear-based MPC (LMPC), Chemical Engineering Transactions 45, 1297-1302.

Nagy Z.K., Mahn B., Franke R., Allgower F., 2007, Evaluation study of an efficient output feedback nonlinear model predictive control for temperature tracking in an industrial batch reactor, Control Engineering Practice 15, 839-850.

Santos R.R.C., Santos B.F., Fileti A.M.F, Da Silva F.V., Zemp R.J., 2013, Application of Artificial Neural Networks in an Experimental Batch Reactor of Styrene Polymerization for Predictive Model Development. Chemical Engineering Transactions 32, 1399-1404.

Wehtje E., Kaur J., Adlercreutz P., Chand S., Mattiasson B., 1997, Water activity control in enzymatic esterification processes, Enzyme and Microbial Technology 21 (7), 502-510.

Won K., Lee S.B., 2002, On-line conversion estimation for solvent-free enzymatic esterification systems with water activity control, Biotechnology and Bioprocess Engineering 7 (2), 76-84.

Zulkeflee S.A., Abd Sata S., Aziz N., 2013, Kinetic Model with Effect of Water Content for Enzyme-Catalyzed Citronellyl Laurate Esterification Process, Applied Mechanics and Materials 284 -287, 423-428.