

## Advanced Control of a Fluidized Bed Using a Model-predictive Controller

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**Abstract:** The control of fluidized-bed processes remains an area of intensive research due to their complexity and the inherent nonlinearity and varying operational dynamics involved. There are a variety of problems in chemical engineering that can be formulated as Nonlinear Programming (NLP) problems. The quality of the solution developed significantly affects the performance of such a system. Controller design involves tuning of the process controllers and their implementation to achieve a specified performance of the controlled variables. Here we used a Sequential Quadratic Programming (SQP) method to tackle the constrained high-NLP problem, in this case a modified mathematical model of gas-phase olefin polymerisation in a fluidized-bed catalytic reactor. The objective of this work was to present a comparative study; PID control was compared to an advanced neural network-based MPC decentralised controller, and the effect of SQP on the performance of the controlled variables was studied. The two control approaches were evaluated for set-point tracking and load rejection properties, both giving acceptable results.

**Key words:** Model predictive control, proportion integral derivative control, neural networks, optimisation

### Nomenclature

$u(t)$	Manipulated variable
$J$	Cost function
$P$	Prediction horizon
$C$	Control horizon
$\hat{y}_k$	$(t + i)$ Predicted process output
$\hat{B}_k$	Hessian, approximation matrix
$d_k$	Search direction
$L_q$	Lagrangian function
$u_o$	Initial velocity, m/sec
$Q_c$	Catalyst flowrate mg/sec
$C_{\text{ethylene}}$	Mole fraction of ethylene
$C_{\text{butene}}$	Mole fraction of butene
$C_{\text{hydrogen}}$	Mole fraction of hydrogen
$T_{\text{in}}$	Inlet temperature °k

### Greek letters

$\xi$	Suitably large number
$I_k$	Continuously differentiable function
$\lambda$	Weighting coefficient
$\alpha$	Scalar-valued step length parameter

### Letters

MPC	Model-predictive controller
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NLMPC	Nonlinear model predictive model
SQP	Sequential Quadratic Programming
LMPC	Linear model predictive model
PID	Proportional-integral-derivative controller
ANN	Artificial neural network

## INTRODUCTION

The incentive for process control may vary depending on the processes application under consideration. The objectives include maintaining high product quality, avoiding or minimising losses, maximising throughput, minimising operational costs, and ensuring safe and environmentally friendly operation. Furthermore, studying the control of fluidized-bed polymerisation operations has continually been an active research area due to their complexity and non-linearity, which obscure the design of optimum control strategies capable of handling the entire range of operation. This is further complicated by the availability of a variety of contacting geometries, and the use of diverse processing techniques. The processes entailed in fluidisation are highly complex and often require extensive coordination and management in order to ensure that they are handled efficiently and with high safety standards. The ability of a process to achieve and maintain the desired equilibrium value is termed the controllability of the process. This is measured by considering a range of properties of the non-linear process (Ahmed S Ibrehem *et al.*, 2008). However, in engineering practice, a plant is called controllable if it is possible to achieve the specified control objectives (Rao *et al.*, 1999). Control strategy involves the design of control systems and their study concerning stability and robustness. Controller design involves tuning of the process controllers and their implementation to achieve a specified performance of the controlled variables. Nevertheless, most industrial polymerisation processes are still controlled using linear controllers based on a linear process model. However, starting in the last decade, some researchers (Mc Auley *et al.*, Aswin N *et al.* and Ang W.L. *et al.*) began proposing non-linear controller designs to control certain severely non-linear processes where tight control is required. Furthermore, most of the non-linear control problems related to polyethylene reactors are highly complex. This process represents one of the major challenges facing process engineers in the chemical process industries, and this process requires optimisation and control of product quality while keeping process variable costs as low as possible.

Modern control algorithms attempt to address these difficulties and to solve the polymerisation control problem under variable operating conditions in order to achieve optimal performance. Many such algorithms have been proposed during the last two decades.

Recently, model predictive control (MPC) has motivated researchers as well as process engineers to implement it as one of the most recommended advanced process algorithms, both in academia and industry. The combination of new control design concepts in MPC, such as model prediction, receding horizon optimisation, and real time correction, makes it possible to yield high performance characteristics, and the neural network-based control system design is gaining a great deal of attention due to these networks' universal approximation ability, on and off learning features and their parallelism.

Control studies for the polyethylene production process span a variety of schemes and algorithms. A list of relevant studies is given in Table (1) for the period 1990-2008.

In this work, we have utilised the advantages of both methods within a neural network model-based model-predictive controller to control the fluidized bed polyethylene reactor. The model used for the control is a modification of the model developed recently by Ahmed Saadi Ibrehem *et. al.*, (2008). Control studies were done for set-point tracking and disturbance rejection and comparison made with the PID controller.

### ***Descriptive Behaviour of the New Mathematical Model:***

Heterogeneous models are widely used, especially in polymerisation system. Current research in this important area can be divided into two classes, namely, mathematical models for fixed-bed catalyst reactor systems and mathematical models for fluidized-bed catalytic reaction, e.g., for the production of polyethylene. Chatzidoukas, *et al.*, (1974) improved the heterogeneous model; however, they did not consider solid phase effects. Varma (1981) included mixing in the axial direction. R. Sala, F. Valz-Gris and L. Zanderighi Paterson developed a two-dimensional mathematical model where concentration and temperature patterns in the reactor can be predicted. R. J. Zeman and N. R. Amundson, Xuejing Zheng, Makarand S. Pimplapure, Günter Weickert, and Joachim Loos, Victor M. Zavala, Antonio Flores-Tlacuahuac and Eduardo Vivaldo-Lima improved the dynamic optimisation of a semi-batch reactor for polyurethane production, H.Hatzantonis, H. Yiannoulakis, A. Yiagopoulos, C.Kiparissides further improved the two-phase model of the polymerisation

system. In previous works, mass transfer with chemical reaction in fluidized-bed systems either considered all phases (D. Kunii and O. Levenspiel 1969) or the emulsion phase alone (Choi & Ray, 1985; McAuley *et al.*, 1994; Hatzantonis, 2000).

Modified modelling is done by including the catalyst phase and considering all three phases as compared to the other models, i.e., the constant bubble size model, the well-mixed model and the bubble growth model. Simulations were also performed to study the effects of superficial velocity and catalyst flow rate in the bubble and emulsion phases. Comparisons with actual plant data at steady state were also performed.

In this model, the reactant gas enters the bottom of the bed and flows upward in the reactor in the form of bubbles. As the bubbles rise, mass transfer of the reactant gases takes place between the bubbles and the clouds without chemical reaction, between the clouds and the emulsion without chemical reaction, and between emulsion and solid with a chemical reaction occurring on the surface of catalyst particles. The type of catalyst particles, porous or rigid, can also be specified, as catalyst porosity has pronounced effects on the reaction rate. All the relevant details of this type of model are elucidated in Ahmmed S Ibrehem *et al.*, (2008).

#### **Nonlinear Model Predictive Control:**

Motivated by the advances in computer technology and control analysis techniques, more sophisticated control system design procedures have appeared during the past two decades, including the non-linear model-predictive controller mentioned in the previous section. Model Predictive Control (MPC) refers to a class of algorithms that compute a sequence of manipulated variable adjustments in order to optimise the future behaviour of a plant. Originally developed to meet the specialised control needs of power plants and petroleum refineries, MPC technology can now be found in a wide variety of application areas including chemicals, food processing, automotive, aerospace, metallurgy and pulp and paper.

There have been great accomplishments in the application of MPC for many industrial processes over the past two decades and it is gaining popularity as an efficient and reliable control algorithm due to the following features [Arkun, 1994; Ogunnaiké *et al.*, 1994]:

- Deals with uncertainty in the process characteristics due to parameter variations.
- Handles uncertainty in the environment from external disturbances.
- Manages the nonlinearities of the process introduced by multiple operating regimes.
- Can be used for situations of changing control objectives.
- Used for the characterisation of a performance index amenable to controller design.
- Handles processes with time delays, inverse response and other difficult process dynamics encountered by most industrial processes.
- Manages situations where there is interaction between variables involved in the control strategy.
- Eliminates problems of stability created by constraints. These constraints restrict the use of the tuning guidelines for the unconstrained case (Zafiriou, 1990).

Due to the versatile nature of the neural network model for non-linear systems, it is an excellent candidate to use for modelling the polymerisation system and incorporation within the model-predictive framework.

Figure (1) shows a neural network MPC scheme. The non-linear optimiser in an MPC is used to select the manipulated variable that minimises a cost function, which is quadratic in the set-point/process output error. To do so, the non-linear optimiser uses the ANN process model to predict the possible future responses of the process to future manipulated variable sequences and the current measured disturbances.

By using the ANN model to predict multiple steps ahead, the control scheme can anticipate the process trajectory and compensate for measured disturbances before their impact on the process output is detected.

The general philosophy of the ANN MPC is identical to that of the LMPC. The controller determines a set of future manipulated variable moves that minimise a cost function over a prediction horizon, subject to input and output constraints. The cost function usually includes the sum of squares of the errors between the predicted outputs and the set point values evaluated over the prediction horizon, and also commonly includes a term which penalises the rate of change of the manipulated variable. For such a cost function, the MPC problem can be posed as follows:

$$\min u(t) \quad J = \sum_{i=P1}^{i=P2} (\hat{y}(t+i) - r(t+i))^2 + \lambda \sum_{i=1}^{i=C} (u(t+i-1) - u(t+i-2))^2 \quad (1)$$

where  $u(t+i) = u(t+C-1), \quad i \geq C \quad (2)$

$$u_{\min} \leq u(t) \leq u_{\max} \tag{3}$$

$J$  is the cost function to be minimised,  $P1$  to  $P2$  define the prediction horizon,  $C$  is the control horizon,  $(t + i)$  is the predicted process output for time  $t + i$ ,  $u(t)$  is the vector of manipulated variable values of length  $C$  and  $\lambda$  is a weighting coefficient. In common with linear MPC, corrections should be made to the model output to account for process/model mismatch and unmeasured disturbances (Fine, T. L., 1999, Smith, M, 1996), and this can be done with an additive disturbance,  $e(t)$ , such that:

$$\bar{y}(t+i) = \hat{y}(t) + e'(t) \tag{4}$$

where  $\hat{y}(t+i)$  is the  $i$ th-step ahead ANN model prediction. A simple approach, which was adopted here, is to use the process/model mismatch to estimate this disturbance.

$$e'(t) = y(t) - \hat{y}(t) \tag{5}$$

Next we introduce the modified set point,  $r'(t)$  :

$$r'(t+i) = r(t+i) - e'(t) \tag{6}$$

Combining equations (4), (5), and (6) in equation (2) gives:

$$\min u(t) \quad J = Q \sum_{i=P1}^{i=P2} (\hat{y}(t+i) - r'(t+i))^2 + \lambda \sum_{i=1}^{i=C} (u(t+i-1) - u(t+i-2))^2 \tag{7}$$

In this study,  $y(t)$  represents the emulsion temperature and molecular weight, which are the controlled variable, while the variable  $u(t)$  represents the superficial velocity and catalyst flow rate. The optimisation problem outlined by equation (7) is solved using the sequential quadratic programming algorithm described in the next section.

**Sequential Quadratic Programming:**

The SQP method allows us to mimic Newton’s method for constrained optimisation. For each iteration, a method similar to Newton’s method is used to generate a quadratic programming sub-problem whose answer is used to determine a search direction for solution.

$$X = t_1 p_1^T + t_2 p_2^T + \dots + t_A p_A^T = T_p^T + E \tag{8}$$

$$Y = u_1 q_1^T + u_2 q_2^T + \dots + u_A q_A^T = uQ^T + F \tag{9}$$

Since the iterative optimisation algorithm employs an analytical gradient method, each term in the control model should be everywhere differentiable. Therefore, the discontinuous binary variable  $I_k$  in the objective function needs to be converted into a continuously differentiable function. In this work,  $I_k$  is approximated by the following smooth function:

$$I_k X_k = 1 - \sec h\{\xi(X_k^o - X_k)\} \tag{10}$$

$$I_k X_k = 1 - (1/(1/ e^{-\xi}(X_k^o - X_k))) \tag{11}$$

where  $\xi$  is a suitably large number. It tends to rapidly converge from zero to one, as  $x_k^o - x_k$  goes from zero to a large value. Therefore, a suitably large  $\xi$  ensures that it is not only binary but also differentiable. With this approach,  $I_k$  can be converted to a continuously differentiable function at the price of some inaccuracy due to approximation. A number of other smooth approximation functions are also available from Biegler, (1998).

The computational efficiency associated with solving an optimisation problem is often the key concern in the online implementation of MPC methods. However, the conventional MPC methods experience an extremely large computational burden for large-scale manufacturing processes. The computational burden rapidly increases as the problem size expands. Therefore, to improve the computational efficiency of on-line optimisation, it is necessary to reduce the dimensionality of the optimisation problem. For this purpose, we transformed the controllable and fixed variables into reduced-score variables in the pulsed prediction model and then optimised for the score variables.

The objective of optimisation was to minimise (or maximise) a function of one or more parameters, as in Figure (2). A set of equality and/or inequality constraints that are also functions of the parameter set, and which confine the parameter values to specified regions of the search space, may also be imposed as part of the optimisation problem. A minimisation problem may be stated more formally in the following mathematical format:

$$\begin{aligned} &\text{minimise } F(x) \\ &\text{subject to: } g(x) \\ &h(x) \geq 0 \end{aligned} \tag{12}$$

where  $x$  is a real-valued vector of variable parameters,  $F(x)$  is a scalar-valued cost function, and  $g(x)$  and  $h(x)$  are vectors of constraint functions. The solution to the general optimisation problem is obtained by Lagrange Multiplier analysis. The Lagrangian for the standard optimisation problem may be written as:

$$L(x, \lambda, \mu) = F(x) - \lambda^T g(x) - \mu^T h(x)$$

Where  $\lambda$  and  $\mu$  are Lagrange multiplier vectors. The following Kuhn-Tucker necessary conditions for a local minimum (Baker, 2002 and Fine, T. L., 1999) may be applied to gain potential solutions to this problem:

$$\begin{aligned} \frac{\partial L}{\partial x_i} &= \frac{\partial F(x)}{\partial x_i} - \lambda^T \frac{\partial g(x)}{\partial x_i} - \mu^T \frac{\partial h(x)}{\partial x_i} \\ \mu^T h(x) &= 0 \\ \mu_j &\geq 0 \end{aligned} \tag{13}$$

In cases where it is unclear if a point satisfying the necessary conditions is a minimum, maximum or otherwise, a set of second-order sufficient conditions may be applied for clarification of (10). If the analytical representation of  $F(x)$  or the constraint set is not available, or not tractable, then numerical methods may be applied to find an approximation to the solution of (12). At present, the most efficient numerical approach to solving nonlinear optimisation problems is the Sequential Quadratic Programming (SQP) method (Smith, 1996). The SQP method produces iterative estimates of the optimal parameter values and the Lagrange multipliers. As the numerical algorithm converges, these iterative estimates approach the optimal parameter values and Lagrange multipliers that would result from the analytical method (13), if it were applied. The primary computational components of a sequential quadratic program are responsible for the formation of an iterative locally quadratic approximation to the Lagrangian function and a sufficient decrease line search of an augmented Lagrangian merit function. An iterative quadratic approximation to the Lagrangian is given by,

$$L_q(x_k, \lambda_k, \mu_k) = L_q(x_{k-1}, \lambda_{k-1}, \mu_{k-1}) + d_k^T \nabla \lambda^T g(x) - \mu^T h(x) L_q(x_{k-1}, \lambda_{k-1}, \mu_{k-1}) + \frac{1}{2} d_k^T B_k d_k \tag{14}$$

where  $\nabla$  is the gradient operator (with respect to  $x$ ),

$$d_x = x_k - x_{k-1} \tag{15}$$

and  $x_k$  and  $x_{k-1}$  are the values of the parameter vector  $x$  at the current iteration and the previous iteration, respectively. The second-order partial derivative, or Hessian, approximation matrix,  $B_k$  in (14), is generated by variable metric update equations. The update that is typically applied is the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update (Shahaf *et al.*, 1985, Biegler, L., 2001, M.J.D. Powell, 1978, E.L. Baker, 1992), which was modified by Powel M.S. Bazaraa *et al.*, 1993:

$$B_k = B_{k-1} - \frac{B_{k-1}SS^T}{S^TB_{k-1}S^T} + \frac{\eta\eta^T}{\eta^T S} \tag{16}$$

Where

$$S = x_{k-1} - x_{k-2} \tag{17}$$

$$\eta = \theta\omega - (1 - \theta)B_{k-1}S$$

$$\omega = \nabla L_q(x_{k-1}, \lambda_{k-1}, \mu_{k-1}) - \nabla L_q(x_{k-1}, \lambda_{k-1}, \mu_{k-1})$$

and

$$\theta = \left[ \begin{array}{l} 1 \text{ if } S^T\omega > 0.25S^TB_{k-1}S \\ 0.8 \\ \frac{0.8}{S^TB_{k-1}S} \end{array} \right] \tag{18}$$

The quadratic approximation to the Lagrangian function is solved for the direction,  $d_k$ , in parameter space that points in a minimising direction of the quadratic. The variable metric matrix,  $B_k$ , must remain positive definite to ensure a bounded solution for the search direction,  $d_k$ . In practice, a positive definite  $B_k$  is maintained by the Levenberg-Marquardt method or by storing the variable metric updates in Cholesky decomposed form (Y. Ye, 1988, P.E. Gill, 1981). The positive definite state of  $B_k$  enables (14) to be solved as a minimisation problem. In a numerical setting, the quadratic approximation to the Lagrangian may be recast, through primal-dual relationships, as the following quadratic sub-problem with linearised constraints:

$$\begin{aligned} \min_{d_k} & F(x_{k-1}) + d_k^T \nabla F(x_{k-1}) + d_k^T B_k d_k \\ \text{subject to:} & g(x_{k-1}) + d_k^T \nabla g(x_{k-1}) = 0 \end{aligned} \tag{19}$$

The maintenance of a positive definite  $B_k$  ensures that the local approximation given in (16) can be readily solved for the search direction,  $d_k$ , through standard convex quadratic programming methods. In practice, other numerical techniques may be applied to prevent the linearised constraint approximations from completely closing off the feasible region (Fine, T. L.1999, Smith, M, 1996). An active sets strategy (Y. Ye, 1981 and Evangelhos Zafiriou, 1992) is also employed so that only the inequality constraints that are satisfied to within some small tolerance of an equality are included in the quadratic model, thereby reducing the overall computational effort.

Following solution of the quadratic sub-problem, a one-dimensional line search along the minimising direction,  $d_k$ , is conducted. Another class of approximations to the Lagrangian (augmented Lagrangian merit functions) is typically used for this phase of the analysis. The following merit function was used for this analysis:

$$W(x_k, \lambda_k, \mu_k) = F(x_k) + \lambda_k^T g(x) + \mu_k^T h(x) \tag{20}$$

The iteration point,  $x_k$ , is determined by evaluating (14) at successive candidate points,  $x_k$ , until a sufficient decrease in the value of (20) is found. The candidate points are generated from the line search update equation

$$x_k^- = x_{k-1} + \alpha d_k \tag{21}$$

The variable  $\alpha$  is a scalar-valued step length parameter that is iteratively adjusted by a step-length algorithm. In program NLQPEB18,  $\alpha$  is initialised to one at the beginning of each line search, and the candidate point,  $x_k^-$ , from (21) is tested for a sufficient decrease in (20) by applying Armijo's step-length criteria (P.E. Gill, 1996, Evangelhos Zafiriou and Hung-Wen Chiou, 1992).



#### ***Non-linear Model-Predictive Control:***

This network can be used in a successive recursive way in a general NMPC structure to obtain the model prediction. This model can be used for prediction in several ways. Below are presented two types of d-step-ahead predictors to compensate for the influence of the time-delay.

This leads to a non-convex non-linear optimisation problem, for which the global solution is difficult to find; thus, special optimisation algorithms should be used. The schematic representation of the dynamic MPC is presented in Figure (1).

#### ***Neural Network Modelling:***

This mathematical technique was first used to help cognitive scientists to understand the complexity of the nervous system. They have evolved steadily and have been adopted in many areas of science. Basically, the ANNs are numerical structures inspired by the learning process of the human brain. They are constructed and used as alternative mathematical tools to solve a diversity of problems in the fields of system identification, forecasting, pattern recognition, classification, financial systems and many others (Huang and Mujumdar, 1993; Joaquim and Dente, 1997, Shaw *et al.*, 1997; Baker and Richards, 2002, Al-Asheh *et al.* 2006). The interest in ANN as a mathematical modelling tool resulted in the consolidation of its theoretical background and the development of its underlying learning and optimisation algorithms.

Modelling and simulation of chemical processes is one of these research areas of interest that made use of ANN modelling techniques. The implementation of mechanistic models that rely on fundamental material and energy balances as well as empirical correlation, such as for this polymerisation process, involves a great deal of mathematical difficulty and in many instances lacks accuracy. Neural network-based modelling can be used confidently as a substitute for such situations due to the favourable features entailed in their use. Among these features are simplicity, fault and noise tolerance, a plasticity property (Shahaf and Marom, 2001) (the ANN can retain its prediction efficiency while tolerating some neuron damage or loss), black box modelling methodology and the capability to adapt to process changes (Baker *et al.*, 2002). The ANNs can be categorised in terms of topology, such as single- and multi-layer feed-forward networks (FFNN), feedback networks (FBNN), recurrent networks (RNN) and self-organised networks. In addition, they can be further categorised in terms of application, connection type and learning methods. FFNNs are the most commonly used type for function approximation. In this topology, the network is composed of one input layer, one output layer and a minimum of one hidden layer. The term feed-forward describes the way in which the output of the FFNN is calculated from its input layer-by-layer throughout the network. In this case, the connections between network neurons do not form cycles. It performs a weighted sum of its inputs and calculates an output using certain predefined activation functions. Activation functions for the hidden units are needed to introduce the non-linearity into the network. The sigmoid functions, such as *logistic* and *tanh*, and the *Gaussian* function, are the most common choices for the activation functions. The neural system architecture is defined by the number of neurons and the way in which the neurons are interconnected. The network is fed with a set of input-output pairs and trained to reproduce the outputs. The training is done by adjusting the neuron weighting using an optimisation algorithm to minimise the quadratic error between observed data and computed outputs. A good reference on the FFNN and their applications is given by Fine (1999).

Input-target training data are usually pre-treated as explained above in order to improve the numerical conditions for the optimisation problem and to improve behaviour of the training process. Thus, the data are normally divided into three subsets: training, validation and testing subsets. The training subset data are used to accomplish the network learning and fit the network weights by minimising an appropriate error function, in the case of a feed-forward network by computing the gradient of the case-wise error function with respect to the weights. The performance of the network is then compared by evaluating the error function using the validation subset data, independently. The testing subset data are then used to measure the generalisation of the network (i.e., how accurately the network predicts targets for inputs that are not in the training set). Improperly trained neural networks may suffer from either *under-fitting* or *over-fitting*. The former describes the condition when a network that is not sufficiently complex fails to fully detect the signal in a complicated data set. On the other hand, the latter condition occurs when a network that is too complex may fit the noise, in addition to the signal; see Smith (1996).

Selecting network structure is a crucial step in the overall design of neural networks. The structure must be optimised to reduce computer processing, achieve good performance and avoid over-fitting. Experience in using an ANN for function approximation revealed that any non-linear function can be approximated by a three-layer ANN structure. The selection of the best number of hidden units depends on many factors. The size of the training set, amount of noise in the targets, complexity of the function to be modelled, type of activation functions used and the training algorithm all have interacting effects on the sizes of the hidden layers.

The final trained ANNs represent general relations linking ANN inputs to outputs for the modified mathematical model for the fluidized bed gas-phase olefin polymerisation reactor.

Thus, we can specify the inputs ( $u_o(k, k-1, \dots, k-n+1)$ ),  $Q_c(k, k-1, \dots, k-n+1)$ ,  $C_{\text{ethylene}}(k, k-1, \dots, k-n+1)$ ,  $C_{\text{butene}}(k, k-1, \dots, k-n+1)$ ,  $T_{\text{in}}(k, k-1, \dots, k-n+1)$  and  $C_{\text{hydrogen}}(k, k-1, \dots, k-n+1)$ ) and outputs ( $T_e(k, k-1, \dots, k-m+1)$  and MW( $k, k-1, \dots, k-m+1$ )). The feed-forward neural network shown in Figure (3) is in the process of being trained.

Based on previous experience with the new mathematical model (Ahmmed s ibrehem *et al.*, 2008) under consideration, the inputs, corresponding to ranges for the mole fractions of all gases (from 0.1 to 0.75) and for temperature input range from (300-395 K), were selected. The selected ranges cover the whole spectrum of the model system including flooding conditions and both outlet emulsion temperature and molecular weight. These data sets for the neural network-based predictive controller for controlling the temperature and molecular weight of the polyethylene reactor system are shown in Figures (4), (5) and (6). Data sets were divided into three subsets: training, validation and testing.

The neural network structure was selected based on testing different network configurations that vary in terms of structure and simulation parameters. The criterion for network structure selection was based on simplicity, performance and accuracy of model prediction. The finally selected network contained one hidden layer with eight neurons. The activation function used in the hidden layer is *tanh*, while output layer contains linear neurons.

The inputs and target are represented by an interval value [-1, 1] to make the neural network training more efficient. Network training was accomplished by manipulating weights and biases to achieve certain performance criteria. This was done by using an optimisation algorithm that searches for network parameters that minimise the prediction error described by equation (7).

The values of  $p$  were specified as per Eq. (8) and compared with values of  $\lambda$  and  $C$  (Eq. 1). Can notice that as  $p$  is decreased with respect to  $C$ , the control action becomes more aggressive and the transient response tends to become faster but closer to instability.

### **Simulation and Results:**

In a previous work, it was shown that the fluidized bed polyethylene process is highly non-linear, especially with excitations in the superficial gas velocity, and that the effects of non-linearity is more pronounced on emulsion temperature and molecular weight than the catalyst flow rate, but both of these inputs have a large effect on the system. The central control system for NMPC can be control of each input variable to the system. This system is affected by four disturbances, namely concentration of ethylene ( $C_{\text{ethylene}}$ ), concentration of butane ( $C_{\text{butene}}$ ), concentration of hydrogen ( $C_{\text{hydrogen}}$ ) and input temperature,  $T_{\text{in}}$ . This configuration is adopted in this study. The detail of the model formulation and its solution and validation are described in detail in the same reference.

MATLAB mathematical software was utilised to code the training algorithm using the Neural Networks toolbox. The Levenberg-Marquardt back-propagation optimisation algorithm (LMBP) was used for network training. This algorithm gives good performance with an average prediction error for the two networks ( $u_o$ - $T_e$ ) and ( $Q_c$ -MW) of  $1 \times 10^{-8}$ . The achieved networks then were validated and tested using the data subsets previously generated from the model. A comparison of both modelled and network-predicted outputs for both phases is shown in the form of error profiles in Figures (4), (5) and (6). These indicate low prediction errors even under severe process excitations.

The SQP approach utilising the Quasi-Newton method with a conjugate gradient algorithm was used for the non-linear constrained optimisation in NLMPC as explained previously. For the case of constrained control, the MPC was able to drive the system dynamics to the desired values effectively without violating the limitations assigned for the manipulated variables. While there were some small differences between the two controllers in terms of set-point tracking time and damping of response, in terms of control criteria, the constrained case was acceptable and does not deviate significantly from the unconstrained one. The characteristics of the dynamic responses are calculated and given in Table (2). The missing values in the table indicate no value or an inapplicable measure.

The integral absolute errors (IAE) of the process responses are shown in Tables (3) and (4). From the response characteristics of the different tuning algorithms, the effects of disturbances on the two outputs, shown in Tables (2 to 4), can be seen, and, thus, a clearer picture of the performance of the MPC controller can be gained.

Figures (7) and (8) show the neural network-based predictive controller performance for set-point tracking without any oscillations in both cases. The results show that a fast rise time was achieved, with a very small overshoot for both loops.



**Table 1:** Summary of control studies for polymerization processes from 1990 to 2008.

No	Researcher	Year	Control system	Control strategy	Product
1	Elnashaie, Gonzales Velasco and Abdel-Hakim	1990	Deadbeat method	Set point (Temperature) effect of batch reactor	Polyethylene
2	G. Ravi, Y. Arkun and F. Joseph	1994	NLMPC	Set point (Temperature and Concentration) effect of batch reactor	Polyethylene
4	Wei and Danial	1996	IMC	Control relevant reduction of volterra series models	Polymerization process
6	Thomas and Francis	1997	IMC	An anti-windup scheme for multivariable nonlinear systems	Polymerization process
7	Tian,y.J.Zhang and A.J.Morris	1999	Neural Net Work	Set point (Temperature) effect of batch reactor	Polyethylene
8	A.Bolsoni,E.L.Lima and J.C.Pinto	1999	Predictive control	Set point (Concentration) effect of batch reactor	Polystyrene
9	Morimasa, Masahiro, Kouji and Fuminao	1999	Predictive control	Control melt index	Polyethylene
10	Gangadhar and Evangelhos	1999	Optimal controller	Set point (Temperature) effect of batch reactor	Polystyrene
11	Janos, Lagos and Ferenc	2000	Fuzzy control	Set point (Temperature) effect for batch reactor	Polystyrene
12	Yaohui and Yaman	2000	Predictive control	Set point (Concentration) effect of batch reactor	Emulsion Polymerization system of polystyrene
13	Janson, Lajos and Ferenc	2000	Fuzzy	Distributed (Temperature) effect for batch reactor	Emulsion Polymerization system
14	Boong, Goon, Kee and Hyun	2001	Predictive control	Distributed (Temperature) effect for batch reactor	Methyl Methacrylate
15	W.C.Chen, Ni-Bin. Chang and Jenj	2001	Fuzzy neural control	Distributed (Temperature) effect for batch reactor	polypropylene
16	Boong, Kee and Hyu	2001	MPC	Set point (Temperature and Concentration) effect of batch reactor	Polystyrene
17	O. Abel and W. Marquardt	2001	Predictive control	Set point (Temperature and Concentration) effect of batch reactor	Polystyrene
18	Joachim Horn	2001	Neural net work	Set point (Temperature and Concentration) effect of batch reactor	Polypropylene
19	Hiroya, Morimasa, Satoshi, Kouji, Masahiro and Wang	2001	Predictive control	Set point Temperature effect of batch reactor	Polyethylene
20	Robert, Douglas, Ronald and Babatund	2001	Volterra series model	Identification of nonlinear empirical models for chemical dynamic processes	Polystyrene
21	C.W.Ng and M.A.Hussain	2002	Hybrid Neural Net Work	Distributed (Temperature) effect for batch reactor	Polymerization process
22	Charles and Francis	2002	Open Loop Optimal	Control of particle size distributaries	Emulsion Polymerization system
23	Yuan, Jie and Julian	2002	Optimal control	Control of particle size distributaries and composition	Emulsion Polymerization system
24	Dulce and Nuno	2002	MPC	Control of particle size distributaries and composition of batch polymerization system	Vinyl chloride and methyl methacrylate
25	Sang and Hyun	2002	Auto-regressive moving average model	Set point (Temperature and Concentration) effect of continuous system	Polystyrene
26	Chiaki and Jinyoung	2002	Neural network	Set point (Temperature effect of batch reactor system	Emulsion Polymerization system
27	Nayef Mohamed Ghasem	2005	Optimal control	Distributed (Temperature) effect for batch reactor	Emulsion Polymerization system
28	Zhihua and Jie	2004	Optimal control	Batch-to –Batch control	Poly Methyl methacrylate
29	Nido, Gilles and Timothy	2003	MPC	Set point (Concentration) effect of batch reactor linear system	Polystyrene

**Table 1:** Continue

30	Kenneth and Ahmet	2003	IMC	Control for nonlinear process change in set point concentration	Polystyrene
31	Francis, Christopher and Timothy	2003	MPC	Control of particle size distribution in batch reactor	Emulsion Polymerization
32	R.A.M. Vieira, M. Embirucu, C. Sayer and Lima	2003	MPC	Control of particle size distribution in batch reactor set point concentration	Polystyrene
33	C.Chatziduksa, J. D Perkins and C. Kiparissides	2003	Optimal control	Set point (Concentration) effect of fluidized bed reactor	Polyethylene
34	D. Del Vecchio and N. Petit	2005	Optimal control	Control for tubular chemical reactor	Polystyrene
35	Antonio and Lorenz	2005	Optimal control	Control for unstable polymerization reactors	Polystyrene
36	G. Mourue, D. Dochain, V.Wertz and D. Descamps	2004	MPC	Distributed concentration effect for nonlinear chemical processes	Polystyrene
37	Z. Zeybek, S. Yuce, H.Hapoglu and M. Alpbaz	2004	Adaptive controller	Control heuristic temperature of batch reactor	Polystyrene
38	Dennis and Okko	2005	Predictive control	Distributed (Temperature and concentration) effect for continuous nonlinear chemical processes	Polyethylene
39	Costas Kiparissides	2005	Optimal control	Control on molecular weight distribution	Polyethylene
40	Simant, Baranitharan and Ali	2005	Optimal control	Control for determination of MMA polymerized in non-isothermal batch reactor	Poly Methyl methacrylate
41	Ch. Vekates and K. Venkat	2005	Neural network	Control of unstable nonlinear processes	Poly Methyl methacrylate
42	Jesus, Cerrillo and John	2005	MPC	Distributed (Temperature and Pressure) effect for autoclave process	Nylon polymerization autoclave process
43	Babatunde, Ogunnaike and Kapil	2006	MPC	Control of nonlinear processes	Polystyrene
44	Bassam and Jose	2006	Optimal control	Control of nonlinear processes	Polystyrene
45	Bassam and Jose	2006	Optimal control	Control on emulsion copolymerization of styrene	Poly Styrene
46	B.Ahmad, R. Willis, J. A. Romagnoli and Gomes	2006	Optimal control	Control on molecular weight distribution	Poly Styrene
47	Felix, Masound and Michael	2006	Optimal control	Control of high temperature semi batch reactor	Poly butyl acrylate
48	Ahmed s ibrehem, Mohamed Azlan Hussain and Nayef Mohamed Ghasem	2007	NMPC	Control of emulsion temperature and molecular weight	Poly ethylene
49	Sebastian Terrazas-Moreno, Antonio Flores-Tlacuahuac, and Ignacio E. Grossmann	2008	Optimal control	Control of temperature	Poly Methyl methacrylate

**Table 2:** dynamic response characteristics for a set point of emulsion temperature

Control study	LOOP	Rise Time(min)	Settling Time (min)
MPC	$U_o, T_e$	1.23	1.255
	$Q_c-MW$	-	
PID	$U_o, T_e$	1.7	1.555
	$Q_c-MW$		

**Table 3:** Integrated absolute error for set point and disturbance rejection of the emulsion temperature closed loop using the NN-MPC as compared to the PID controller.

Controller	Set point IAE	Disturbance in hydrogen concentration IAE	Disturbance in ethylene concentration IAE	Disturbance in butane concentration IAE	Disturbance in inlet temperature IAE
MPC	0.045	0.0087	0.0106	0.096	0.0128
PID	0.15	0.091	0.109	0.103	0.130

**Table 4:** Integrated absolute error for set point and disturbance rejection of the molecular weight closed loop using the NN-MPC as compared to the PID controller.

Controller	Set point IAE	Disturbance in hydrogen concentration IAE	Disturbance in ethylene concentration IAE	Disturbance in butane concentration IAE	Disturbance in inlet temperature IAE
MPC	0.1926	0.383	0.2788	0.4382	0.2042
PID	2.255	3.056	2.386	3.755	2.401

The disturbances introduced are changes in the initial hydrogen, butene or ethylene concentrations and inlet temperature; as shown in Figures (9) to (12), the behaviour of the MPC is very active and smooth without any oscillations.

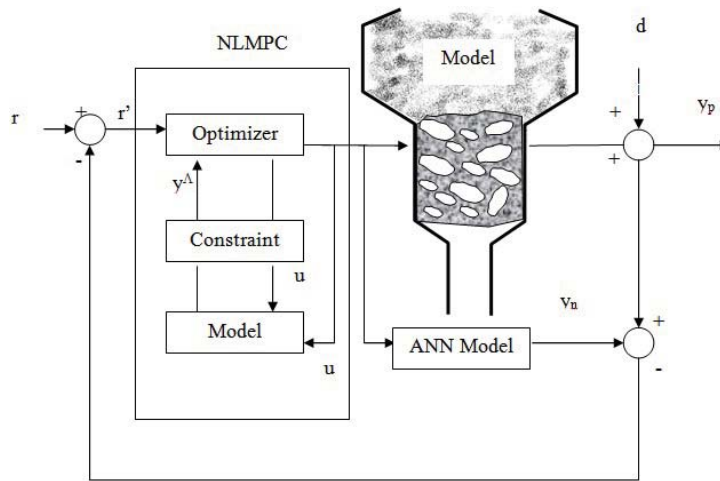


Fig. 1: The general structure of a nonlinear MPC

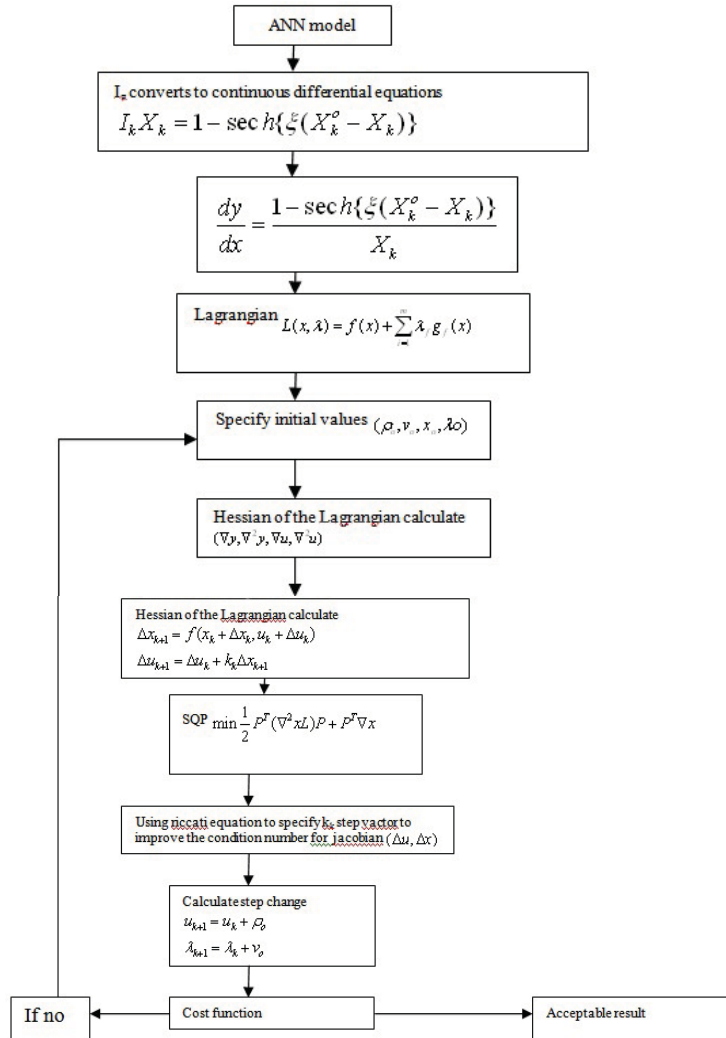
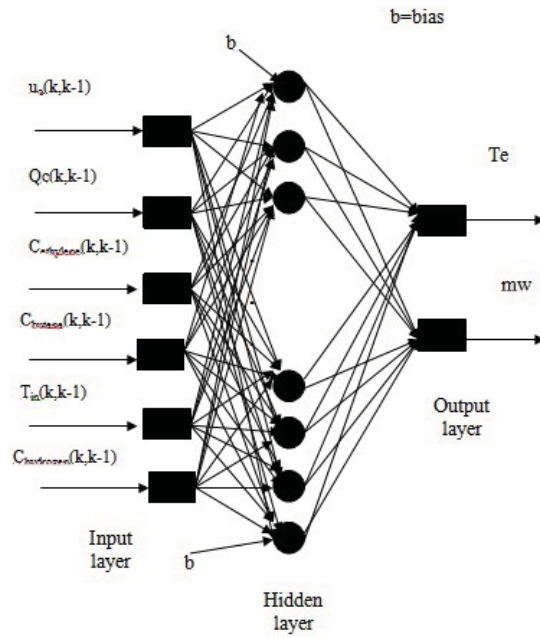
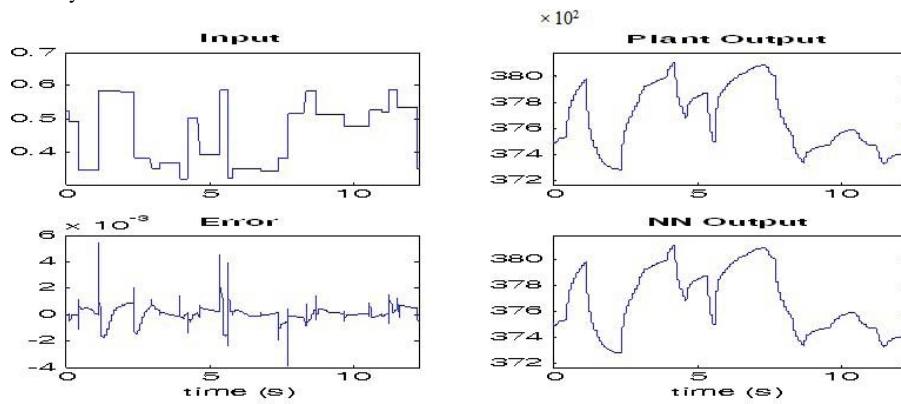


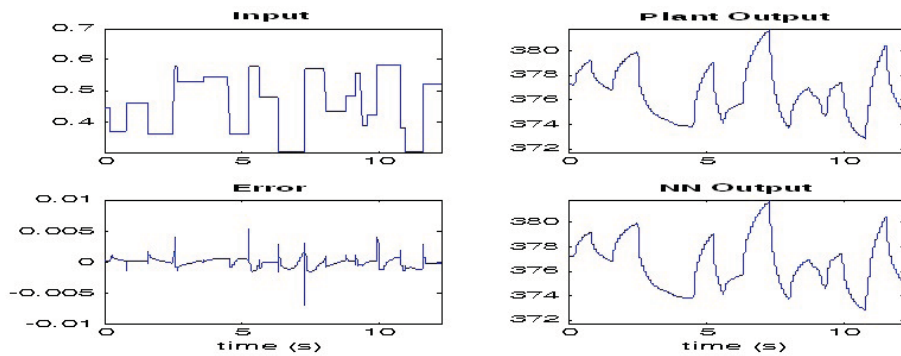
Fig. 2: Represents all optimize control steps



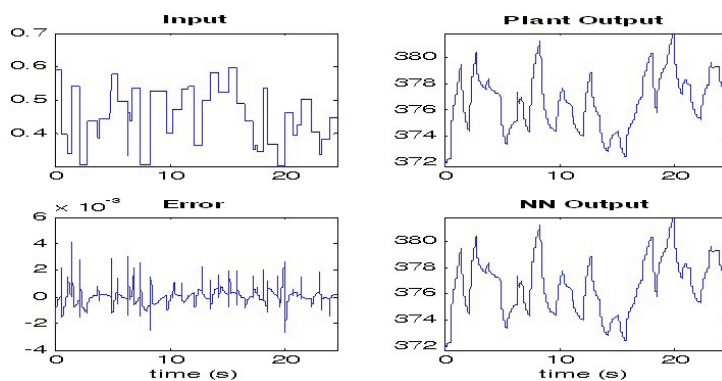
**Fig. 3:** Three layer feed forward neural network



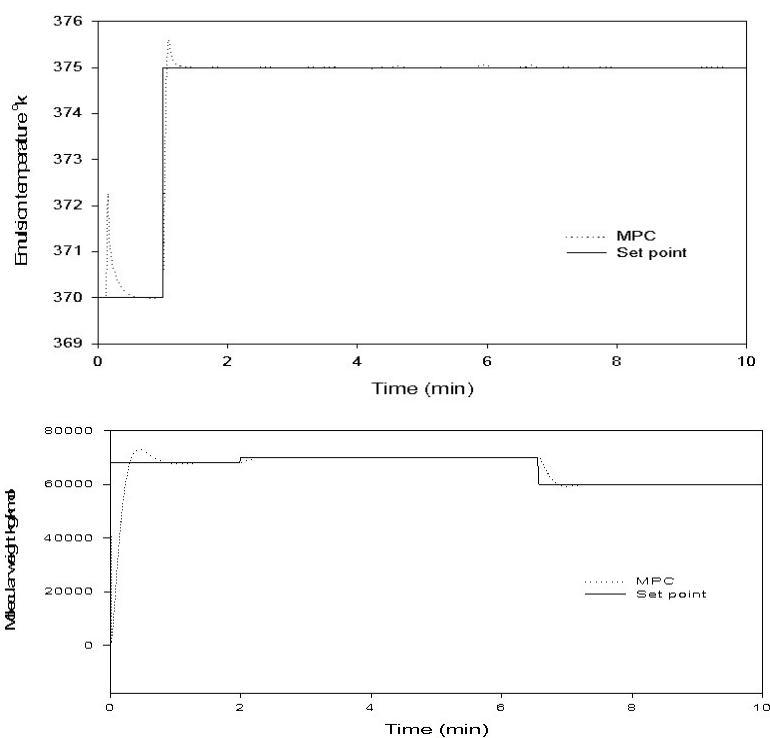
**Fig. 4:** Input-output training set for molecular weight ANN predictions.



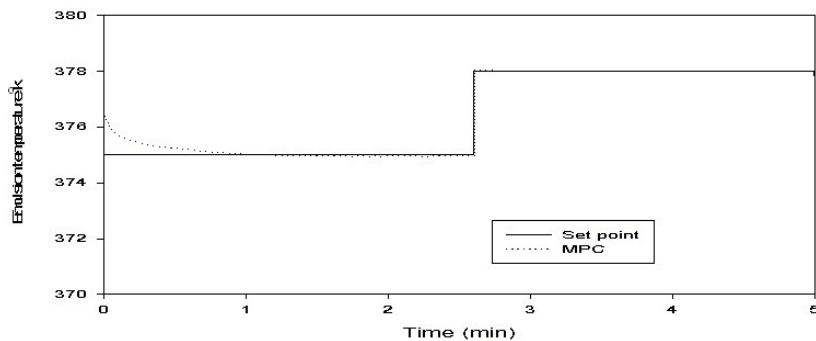
**Fig. 5:** Input-output training set for emulsion temperature ANN predictions.



**Fig. 6:** analysis for validation data



**Fig. 7:** MPC controller response for set point tracking study of superficial gas velocity on set point



**Fig. 8:** MPC controller for set point tracking study of catalyst flow rate on set point

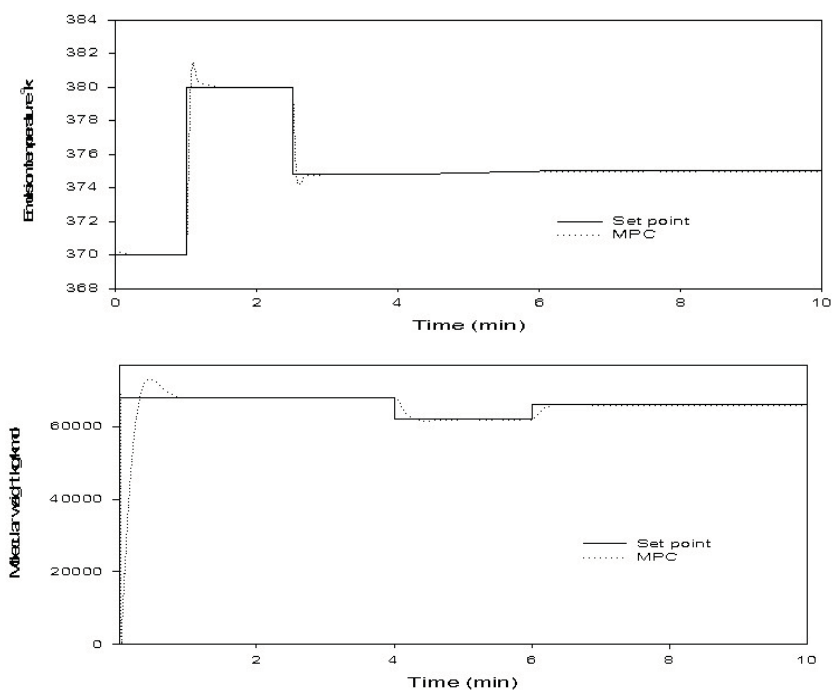


Fig. 9: MPC controller for disturbance hydrogen concentration on set point

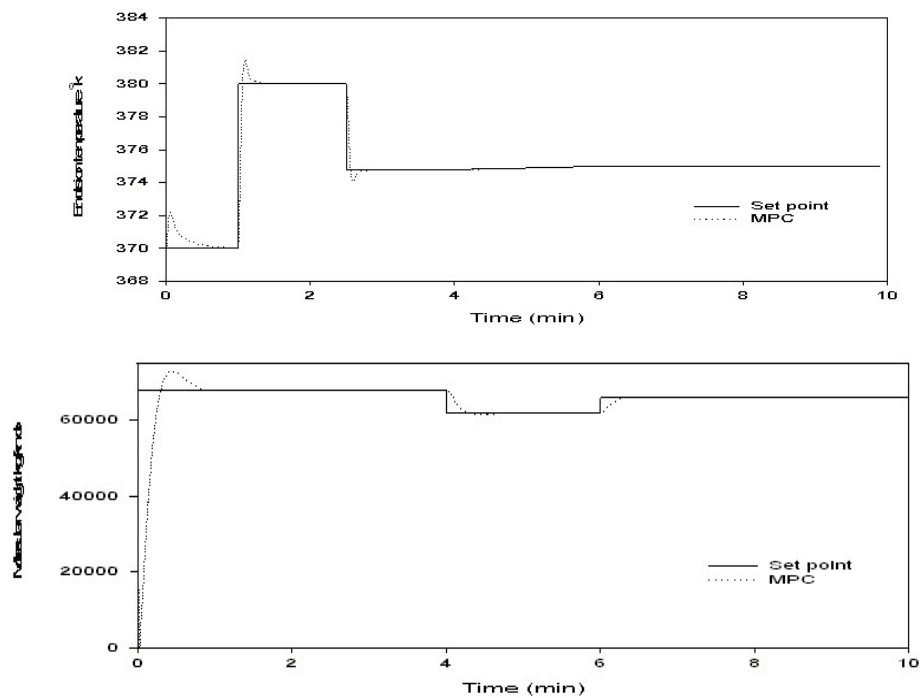
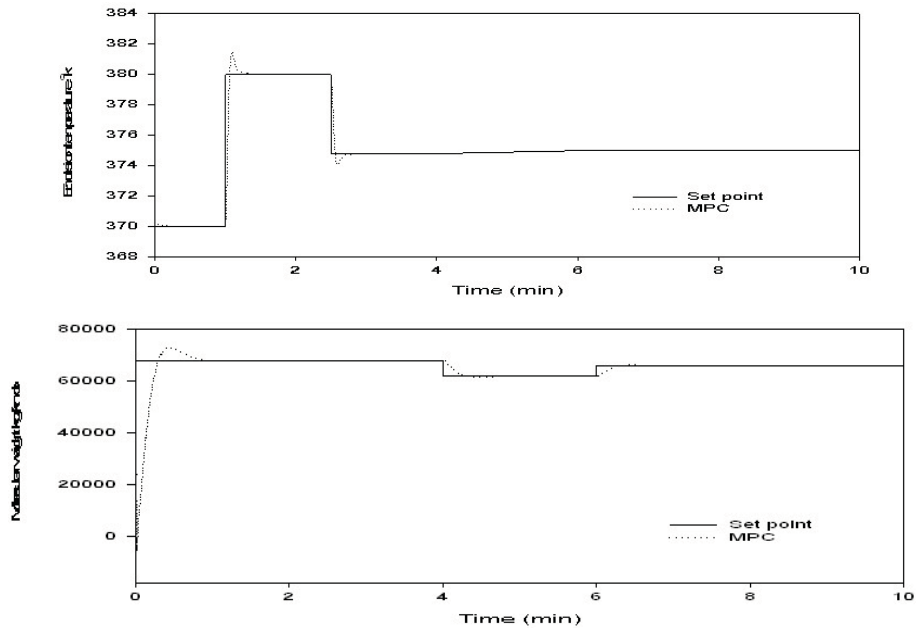
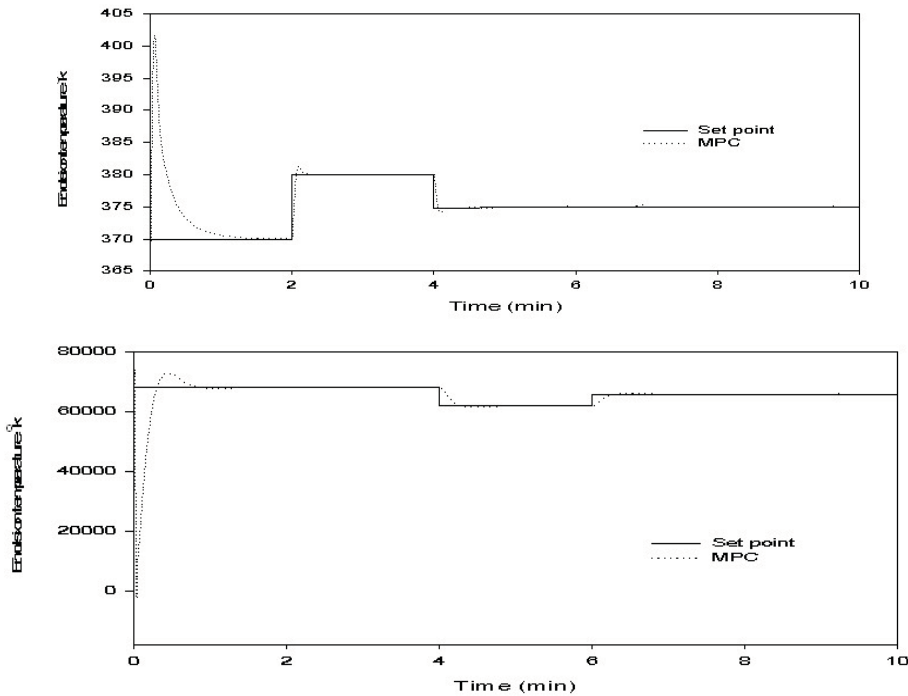


Fig. 10: MPC controller for disturbance of butene concentration disturbance on set point





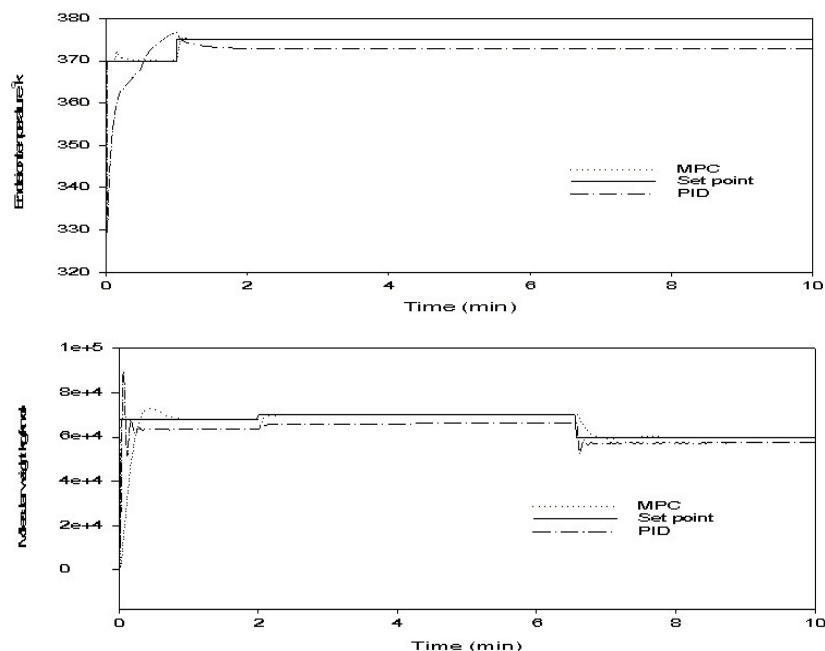
**Fig. 11:** MPC controller for disturbance of ethylene concentration on set point



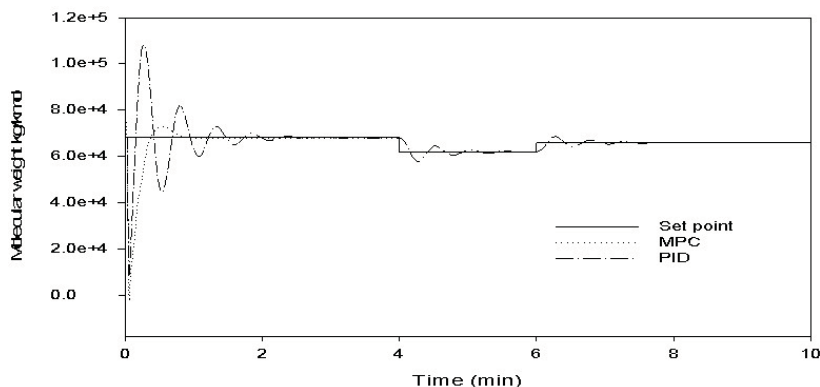
**Fig. 12:** MPC controller for disturbance of inlet temperature on set point

From these results it can be inferred that when comparing the behaviour of the PID and MPC set-point controllers, shown in Figure (13), it is seen that the PID controller is characterised by slightly longer settling times for control action, with oscillations before achieving the set point and with higher overshoot than the MPC controller.

Figures (14) through (18) display the PID and MPC controller response for disturbances in hydrogen, butene and ethylene concentrations and inlet temperature, respectively; the rejection study on the set-point shows that the PID controller is characterised by slightly longer settling times for control, with a digressive action towards oscillations before achieving the set point and with higher overshoots compare to the MPC controller.



**Fig. 13:** Response for set point tracking studies - MPC comparison with PID controllers.



**Fig. 14:** controller response of MPC and PID controllers for disturbance of hydrogen rejection study

**Conclusion:**

The trained neural network was capable of capturing the fluidized-bed process dynamics with high prediction efficiency and thus can be used in control applications where the process exhibits high nonlinear dynamics such as the fluidized bed process. The performance of the NN-MPC for the set-point tracking and disturbance case was excellent in forcing the process output variables to their target values smoothly and within reasonable speed compare to PID because it is optimizer control system depends on SQP one of the best non linear optimization methods. The controller showed stable behavior for the whole spectrum of excitations in the output variable. Therefore, we prefer to use NMPC controller especially for complex industrial processes where controller computing time is important.

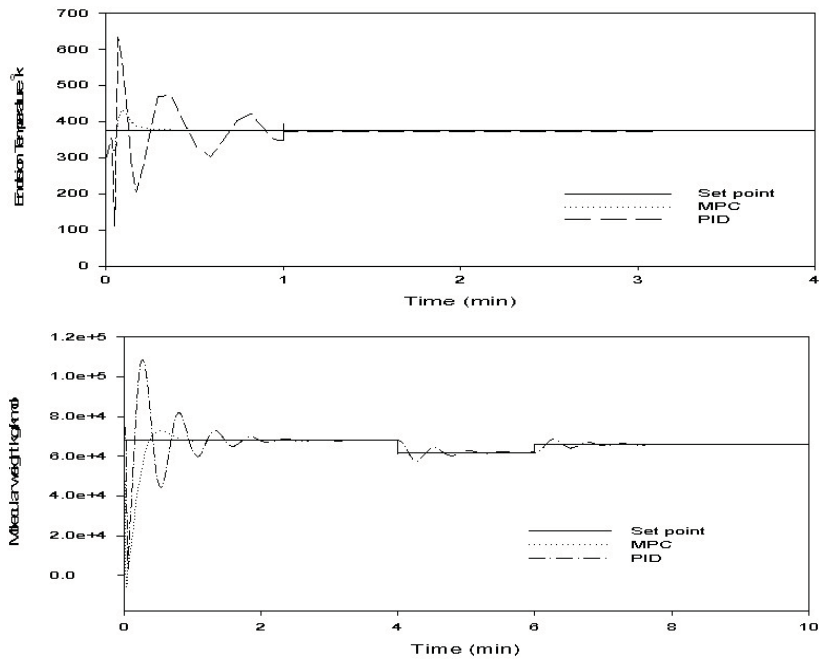


Fig. 15: controller response of MPC and PID controllers for disturbance of butane rejection study

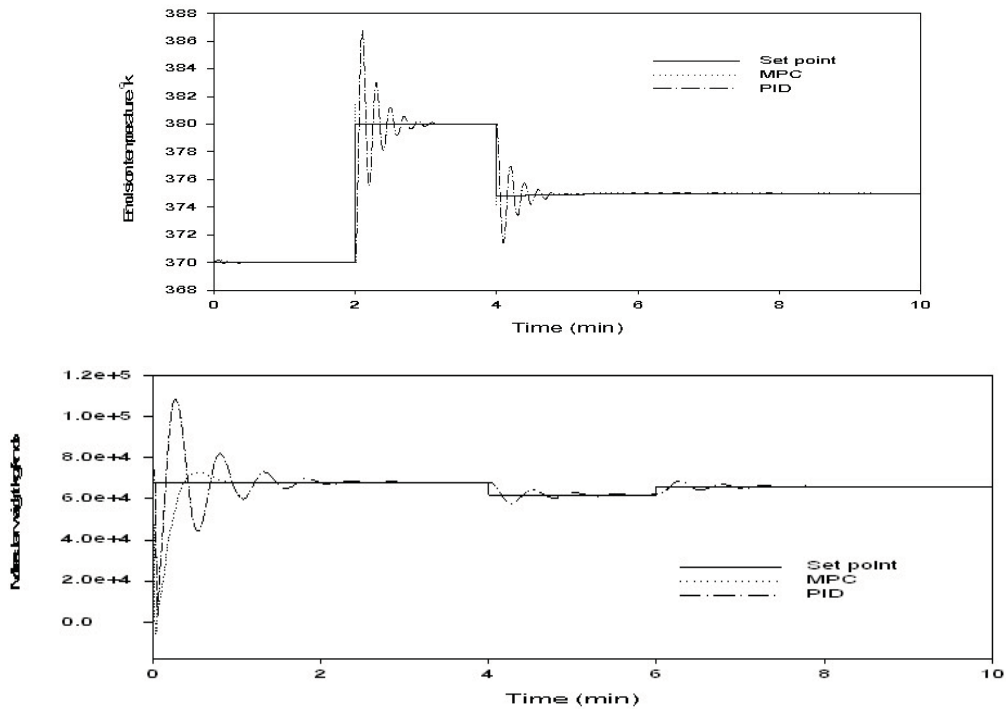


Fig. 16: controller response of MPC and PID controllers for disturbance of ethylene rejection study

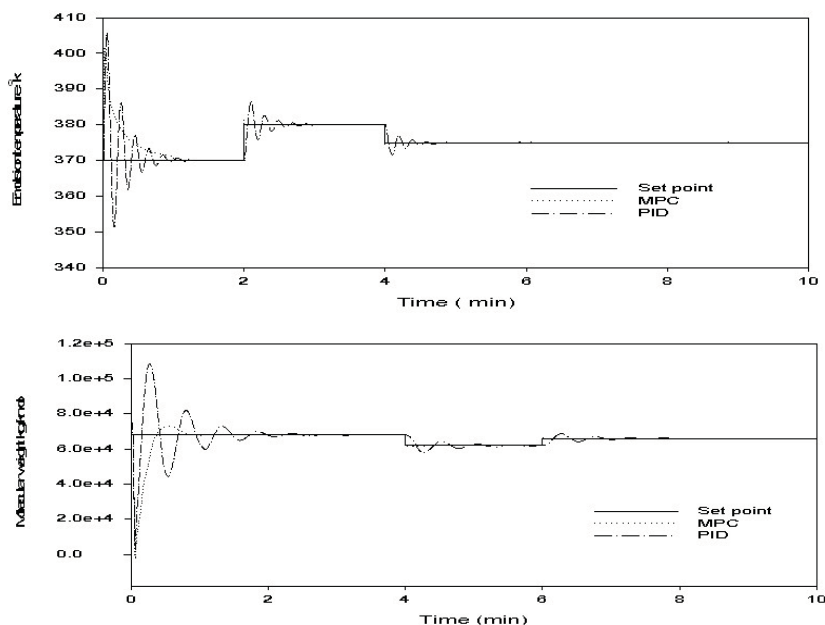


Fig. 17: controller response of MPC and PID controllers for disturbance of inlet temperature rejection study

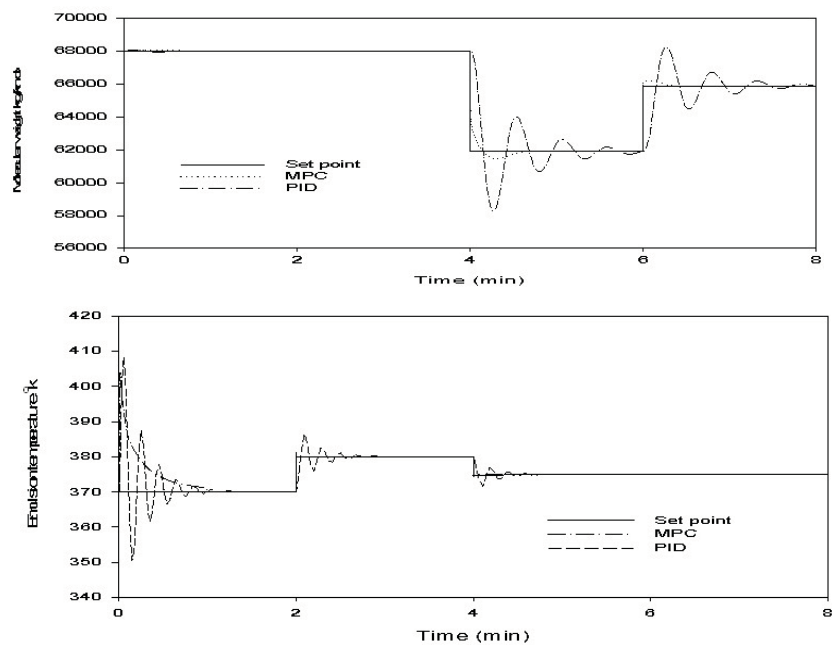


Fig. 18: controller response of MPC and PID controllers for disturbance of catalyst flow rate rejection study

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