

ARTIFICIAL NEURAL NETWORK APPROACH TO MODELING OF POLYPROPYLENE REACTOR

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ABSTRACT

This paper shows modeling of highly nonlinear polymerization process using the artificial neural network approach for the model predictive purposes. Polymerization occurs in a fluidized bed polypropylene reactor using Ziegler - Natta catalyst and the main objective was modeling of the reactor production rate. The data set used for an identification of the model is a real process data received from an existing polypropylene plant and the identified model is a nonlinear autoregressive neural network with the exogenous input. Performance of a trained network has been verified using the real process data and the ability of the production rate prediction is shown in the conclusion.

KEYWORDS

Identification, model predictive control, neural networks, polypropylene, fluidized bed reactor

1. INTRODUCTION

Intelligent control methods belongs to the control techniques that use various artificial intelligence computing approaches like fuzzy logic, machine learning, evolutionary computation, neural networks and genetic algorithms. General description could be that intelligent control achieves the control engineering via emulation of a biological intelligence [22]. For better understanding of the neural networks, imagination of a multi-dimensional input-output space is needed. Suppose this multi-dimensional space as a two input and one output space.

1.1 Neural Networks

Definition

Artificial neural network simulates main behavioral functions of biological neurons by collection of multiple signals - inputs, the threshold switching function - activation function and adaptation of the transmission rate of inputs - adaptation of the weights of particular inputs.

In Figure 1 an artificial neuron is showed with n inputs and n weights to produce a single output using sigmoid characteristic - the activation function.

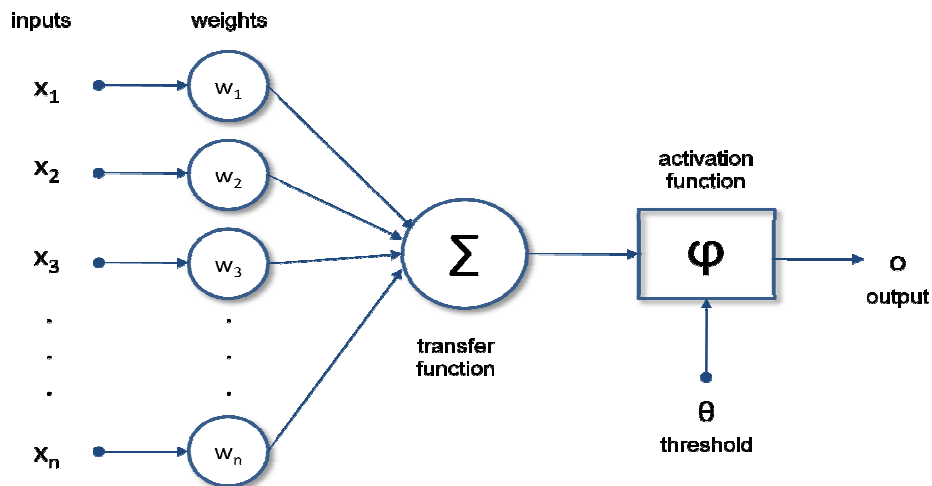


Figure 1. Block scheme of artificial neuron

Typical Neural Network (NN) structures include feed-back and feed-forward NNs. The feed-back networks can have signals travelling in both directions (from input to output and from output to input) by introducing loops in the network [4]. Feed-back networks can get extremely complicated. Feed-back NNs are dynamic - their state is changing continuously until they reach an equilibrium point [3]. They remain at the equilibrium point until the input signals change and a new equilibrium needs to be found. Due to feedback there is no guarantee that the networks become stable. Feed-back networks can converge to one stable point, limit-cycle or divergent. Another type of NN is a multilayer feed-forward NN.

The basic element of a neural network is a simple computational or processing unit that is characterized by

1. $\theta_w \in \mathbb{R}^{n\theta_w}$ - a vector of weights
2. $\theta_b \in \mathbb{R}$ - a bias or offset
3. $s: \mathbb{R} \rightarrow \mathbb{R}$ - an activation function

If $z \in \mathbb{R}^{n_z}$ is an input vector, fed to the processing unit, the activation function computes $s(\theta_w^T z + \theta_b)$ and this value is then taken as an output of the unit. If we connect a finite number of such units in parallel into a layer and subsequently connect a finite number of such unit-layers in series only by feed forward connection we create an architecture called multilayer feed forward neural network of a multilayer perceptron (MLP), shown in Figure 2.

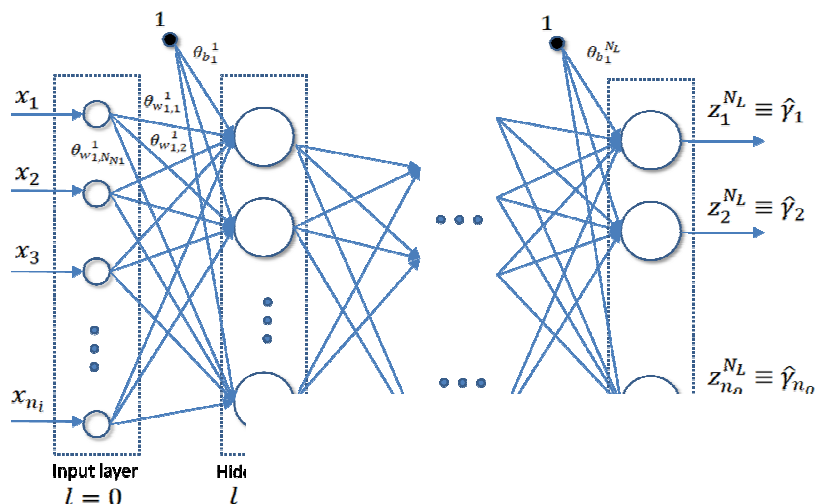


Figure 2. Block scheme of multilayer perceptron (MLP)

The i th node in the l th layer of the network compute its output z_i^l according to

$$u_i^l = \sum_{j=1}^{N_{N_{l-1}}} \theta_{w_{ij}}^l z_j^{l-1} + \theta_{b_i}^l$$

$$z_i^l = s(u_i^l)$$

where $l = 1, 2, \dots, N_L$ is the hidden layer number, $i = 1, 2, \dots, N_{N_l}$ is the node index in the l th layer, $\theta_{w_{ij}}^l$ is weighting factor of the connection between j th node of the $(l-1)$ th layer and i th node of the l th layer and $\theta_{b_i}^l$ is the bias of the i th node in the l th layer. The processing function of the i th node in the l th layer is denoted by u_i^l and the corresponding output is then denoted by z_i^l . The input layer, $l = 0$, is a special layer because it provides the distribution of inputs x_i , for $i = 1, 2, \dots, n_i$, among the nodes of the first hidden layer. It can be seen as

$$z_i^0 = x_i, \quad \text{for } i = 1, 2, \dots, n_i,$$

The variable u_i^l is sometimes called an activation of the node and serves as an input to an activation function $s(u)$. This function is usually chosen as

$$s(u) = \frac{1}{1 + e^{-u}}$$

Or

$$s(u) = \tanh(u) = \frac{1 - e^{-2u}}{1 + e^{-2u}}$$

For the last hidden layer we often chose a linear processing function

$$s(u) = u$$

To make possible any range for the MLP outputs $z_i^{N_L}$. [49] Overall family of functions \mathcal{F} that can be realized by an MLP is characterized by

1. The number of inputs and outputs n_i, n_o ;
2. The number of layers N_L , including the output layer
3. The number of nodes in hidden layers $N_{N_l}, l = 1, 2, \dots, N_L - 1$
4. The set of weights $\theta_{w_{ij}}^l$ and biases $\theta_{b_i}^l$
5. The processing function $s(u)$.

The process of iterative tuning of weights and biases is called learning.

Hebian learning algorithm increases a weight w_i between a neuron and an input x_i , if the neuron y fires.

$$\Delta w_i = a y x_i$$

where a is learning speed. Weights are strengthened if units connected with the weights are activated. Weights are normalized to avoid an infinite increase of weight value.

Levenberg - Marquadt algorithm is the most used and most effective supervised learning algorithm for majority of tasks. It is a back-propagation algorithm which iteratively determines weights of the feed-forward NN.

Let assume that vector \mathbf{E} is an error between the NN output \mathbf{o}^3 and desired - supervisory output data \mathbf{y} . The superscript means a layer number, so \mathbf{o}^3 means an output from output - final layer. The NN outputs depend on synaptic weights so the \mathbf{E} must be a function of weights \mathbf{w} .

$$E(\mathbf{w}) = \frac{1}{2} \sum_{j=1}^{N_k} (\mathbf{o}_j^3 - \mathbf{y}_j)^2 \quad (7)$$

The searching direction of smaller error is determined by calculating a partial differential. The searching direction is then\

$$\mathbf{g} = - \frac{\partial E(\mathbf{w})}{\partial \mathbf{w}} \quad (8)$$

Weight update rule of LMA is then determined by

$$\mathbf{w}_{k+1} = \mathbf{w}_k - (\mathbf{J}_k^T \mathbf{J}_k + \mu \mathbf{I})^{-1} \mathbf{J}_k \mathbf{e}_k \quad (9)$$

where $(\mathbf{J}_k^T \mathbf{J}_k + \mu \mathbf{I})$ is the Hessian matrix in k -th step. In order to make sure that the Hessian matrix is always invertible Levenberg-Marquadt added combination coefficient μ . When combination factor μ is small (almost zero), the equation will result into

$$\mathbf{w}_{k+1} = \mathbf{w}_k - (\mathbf{J}_k^T \mathbf{J}_k)^{-1} \mathbf{J}_k \mathbf{e}_k \quad (10)$$

where Gauss - Newton algorithm will be used. On the other hand, when the combination factor is too large the equation will result into

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \alpha \mathbf{g}_k \quad (11)$$

where the Steepest Descent Algorithm will be used.

Since the calculation is conducted in direction from the output layer to input layer, this algorithm is named the back-propagation algorithm. When a sigmoid function is used for the activation function of neurons,

$$f(x) = \frac{1}{1 + e^{-x+T}} \quad (12)$$

the differential is determined as,

$$\frac{\partial f(x)}{\partial x} = (1 - f(x))f(x) \quad (13)$$

and the calculation of the algorithm becomes simple.

2. NONLINEAR PROCESS IDENTIFICATION

Many studies have been reported focusing on the petrochemical industry, especially the polymerization process. The polymer materials are widely used in many different areas. Due to the high and differentiated market demand of polymers, the polymerization process is continuously in development. Polypropylene is normally tough and flexible, especially when copolymerized with ethylene. Perfectly isotactic polypropylene has a melting point in the range from 160°C to 166°C. The Melt Flow Rate (MFR) or Melt Flow Index (MFI) is a measure of molecular weight of polypropylene. The measure helps to determine how easily the molten raw material will flow through the processing. As the MFI increases, some physical properties like strength will decrease. MFI and MFR polymer properties depend on the polymer production process and the level of control. One of the key properties to observe and control is a production rate. There are three general types of polypropylene:

- homo-polymer
- random copolymer
- block copolymer

The copolymer is usually used with ethylene. Ethylene-propylene rubber (EPDM) added to polypropylene homo-polymer increases its low temperature impact strength. Randomly polymerized ethylene monomer added to the polypropylene homo-polymer decreases the polymer crystallinity, lowers the Melting point and makes the polymer more transparent. Traditionally, three manufacturing processes are the most common ways to produce polypropylene.

1. Hydrocarbon slurry or suspension
2. Bulk (or bulk slurry)
3. Gas phase

Because of the high efficiency and complexity of the process, the gas phase production type is the most used in petrochemical plants [11]. Gas phase production process uses gaseous propylene in contact with the solid catalyst, resulting in a fluidized-bed medium. Due to non-linearity in the process dynamics and difficulties involved in the control of the gas phase propylene polymerization fluidized bed reactor, an efficient process control scheme is vital for stable and efficient operation of the process. Linear MPC algorithms are unable to handle the

complexity of such non-linear process. The non-linear MPC has good capability to improve control and operation of the non-linear processes such as this polymerization process. Successful applications of Non-linear Model Predictive Control (NMPC) with capability of dealing with unanticipated changes in process dynamics through the state estimator, on polymerization reactors have been reported. Summary of relevant studies in olefin polymerization and its control are listed and well summarized by [40]. Mostly implemented polypropylene technology is UNIPOL. The Figure 3 shows an example of olefin polymerization process - industrial gas phase fluidized-bed polypropylene (UNIPOL-type) reaction process. Main functional parts of UNIPOL polypropylene reactor are

- Reactor – fluidized bed gas phase polymerization reaction system
- Cycle gas compressor – continuous flow of cycle gas
- Cycle gas cooler – removes reaction heat

UNIPOL Polypropylene Technology is a simple and delicate processing system, comprising of one or two gas phase fluidized-bed reactors. To produce homo-polymers and random copolymers a single reactor is used. In this work a single reactor is considered for homo-polymerization. The reactor is a gas phase reaction system using Ziegler – Natta catalyst. Simplified block diagram is shown in Figure 4. The cycle gas supplies fresh propylene and fluidizes the reactor bed.

Monomer (propylene), hydrogen, nitrogen and occasionally ethylene is provided by the gas stream to reactor. The cycle gas feed stream fluidizes and agitates at the same time as the reactor bed and removes heat generated by polymerization reaction.

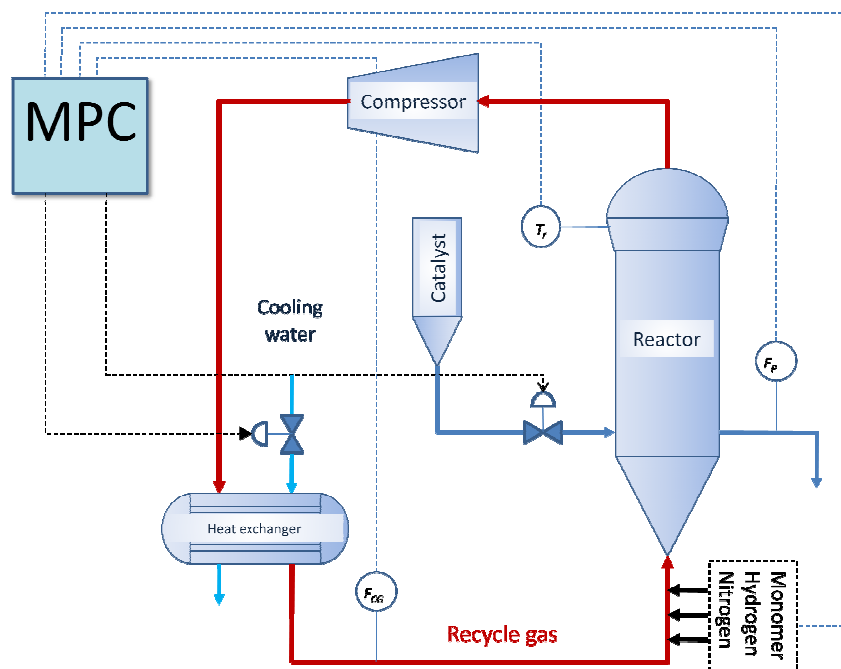


Figure 3. Simplified schematic of an industrial gas-phase fluidized bed polypropylene reactor with model predictive control design

Polymerization occurs in the pores of Ziegler - Natta catalyst and presence of co-catalyst and donor (selectivity control agent). The not reacted gas exits the top of the reactor and is then compressed and cooled before being fed back into the bottom of the fluidized bed.

The polymer production rate in this system also depends on the heat removal from the cycle gas since the polymerization reaction is exothermic. To achieve a stable polymer production rate, which is an important goal for this industry, it is necessary to keep the bed temperature above the dew point of the reactants to avoid the gas condensation and below the melting point of the polymer to prevent particle melting, agglomeration and resulting reactor shutdown. Polypropylene process stabilization is a challenging problem and an important task for the design of the control system of the process.

3. CASE STUDY

Subjected polymerization reaction takes place in a fluidized-bed reactor and basic overview is shown in Figure 4. Prepared catalyst and purified reactants (*propylene, hydrogen, and occasionally ethylene*) are fed continuously to the reactor. Liquid Teal (*tri-ethylaluminium*) and either donor (*SCA - Selectivity Control Agent*) are fed to the reactor inlet gas stream as co-catalysts. An externally cooled cycle gas loop fluidizes the reactor bed, provides fresh reactants, and removes heat from the exothermic polymerization reaction. The product flows intermittently from the reactor through two Product Discharge Systems (PDS), which operate in a sequentially alternating mode. The resin is transported to a receiving vessel by a dense phase conveying system. The reaction system consists of a reactor, a cycle gas cooler and a cycle gas compressor. Gaseous reactants (a mixture of propylene, hydrogen, and occasionally ethylene) and inert gases are continuously recycled by the cycle gas compressor through the reactor bed with fluidized resin containing the catalyst. The heat of polymerization is transferred to the cycle gas and released in the external water-cooled cycle gas cooler.

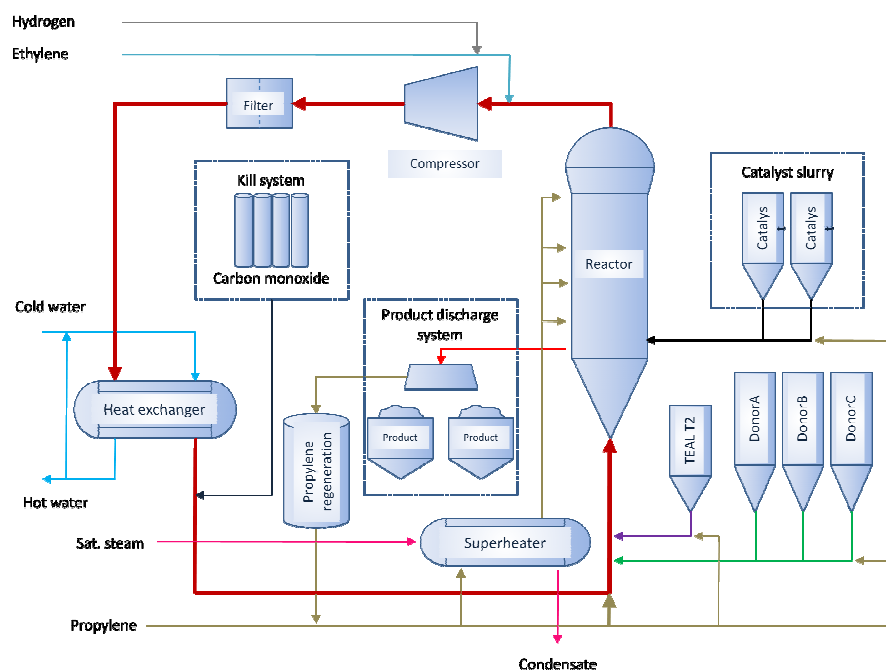


Figure 4. Principal diagram of the main process part of polypropylene reactor

The reactor is a skirt supported cylindrical vessel with a top expanded section for solids disengagement. A perforated distributor plate supports the bed of granular resin and distributes the gas flow into the bottom of the bed. The cycle gas compressor is a single stage, constant speed, centrifugal compressor. The cycle gas circulation flow rate is controlled by discharge throttling and shovel angle of rectifier section of the compressor. The cycle gas cooler is a single-

pass shell and tube heat exchanger. The cycle gas flows through the tubes and the cooling water flows counter-currently through the shell. The temperature is controlled by varying the cooling water makeup/return rate.

Several simplifications have been considered during the analysis and design:

1. Propylene or Nitrogen used for purging and conveying of catalyst/co-catalyst considered as negligible compared to the fresh propylene monomer feed.
2. Single feed of already prepared catalyst slurry (catalyst mixed with mineral oil) considered instead of two standalone, stirred vessels with catalyst and mineral oil feeding systems. These two systems are never used both at the same time.
3. Shell - tube cycle gas cooler make-up/fresh cooling water input system simplified to shell - tube exchanger with cooling water input and output with real flow and temperature values. Only temperature and flow of water considered in this work.
4. Product discharge systems switching are not included because these are not related directly to the polymerization reaction process. Production rate data are downloaded from the control system used as output variable.

Detailed study and analysis of UNIPOL process and technology units were necessary to understand the polypropylene production unit. Several legal steps were required for the proper protection of private property and author rights of license owner and technology operator. Consultancy with people responsible for the polypropylene process operation and maintenance was necessary for understanding of the process control and the operation. Polypropylene production unit is a complex plant consisting of different standalone units. Focusing only on polymerization reaction control, deep technology breakdown was required for the recognition of the process parts/units importance. Several partial tasks recognized during solution development and model identification:

1. Analysis of recorded data and measured values
2. Reactor model
3. Comparison of data measured vs. data simulated

Partial tasks, like catalyst vessels level, concentration and mixing control, are solved by lower-level distributed control system (DCS). Because it is physically impossible to measure real amount of product on-line, mathematical model is used for the product production rate estimation. Model details are unknown and licensed by provider of technology. The main parts of the technology were chosen considering the priority and effect to the control of polypropylene reaction. The accuracy of different measurement instruments was recognized as important factor during analysis of downloaded data. As an example we can take a simple orifice flow meter which is used to measure the cycle gas flow. This flow meter measures the flow with the accuracy of approximately +/- 5% at nominal value of approximately 30000 m³/h approximately.

3.1 Reactor model

The neural network training appears unsuccessful using the complete set of data and standard training methods (the neural network toolbox in the Matlab using Levenberg - Marquardt training method). However, separating the data into different sets according to product type and using of combination of two training methods – scaled conjugate gradient and Levenberg - Marquardt, brings better results. The production unit is switching the production between 13 different product types – polymers, sometimes on daily basis. Production rate prediction and control is one of the key performance indicators during the plant operation and provides set points to other control loops.

4. CONCLUSION

In this work we focused mainly on a design and training of a reliable model for the prediction of the reactor production rate. This value is non-linear and difficult to measure on-line as the product is removed from the reactor not periodically and depending on many variables.

Using the classic control methods often resulted into non-optimal set up of regulators and control system to achieve acceptable efficiency of the plant respecting the technology design limits. This approach frequently results into highly operator dependant control. In many cases, including the polypropylene unit described above, there are several constants which are adjusted by skilled operators to reach requested production target. Current high level control system is frequently switched off due to new procedures which are not included in current high level control system.

Identified model is a Non-linear Autoregressive neural network with Exogenous Input (NARX) where $x(t)$ represents vector of input variables which can be obtained from the field sensors and valves and $y(t)$ represents output value - reactor production rate.

$$y(t) = f(x(t-1), x(t-2), y(t-1)) \quad (14)$$

NARX neural network model uses sigmoid activation function in the hidden layer and linear activation function in the output layer. Hidden layer of network has 30 neurons trained on process data. Performance of the model was evaluated using Mean Square Error method

$$\sigma_{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = 0,0143 \quad (15)$$

,for $i = 1,2, \dots, 58000$

and results are shown in Figure 5-13.

The results show that the identification of such a non-linear process like polypropylene reaction using real process data is possible using neural networks.

A system of reactor constraints needs further discussion with plant operations to achieve safe and reliable operation with maximum leverage of input materials and energy. The cycle gas flow variable and high/low pressure hydrogen flow signal we considered as main challenge for the identified neural network model because of high non-linearity. An appropriate filtration of measured data is necessary to achieve desirable results during the model identification.

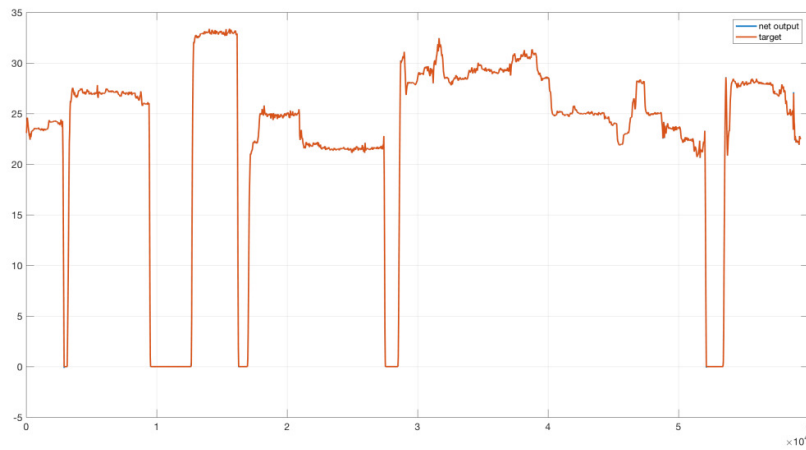


Figure 5. Time response of output variable obtained from open loop simulation

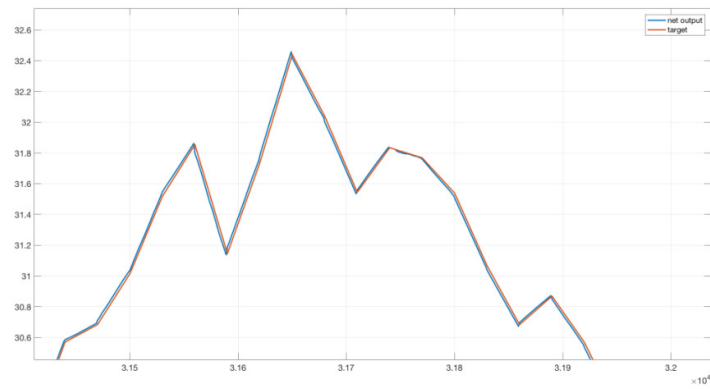


Figure 6. Time response of output variable obtained from open loop simulation - detail view

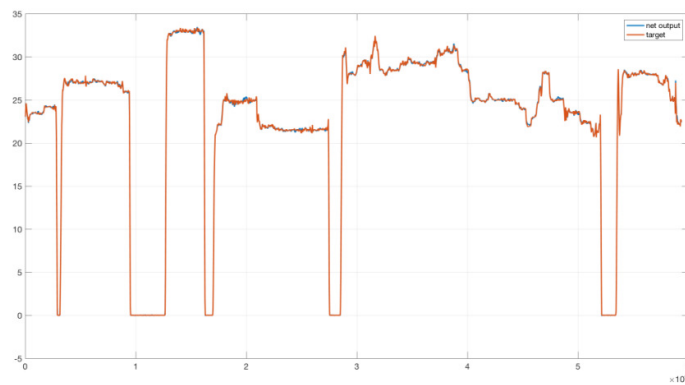


Figure 7. Time response of output variable obtained from closed loop simulation

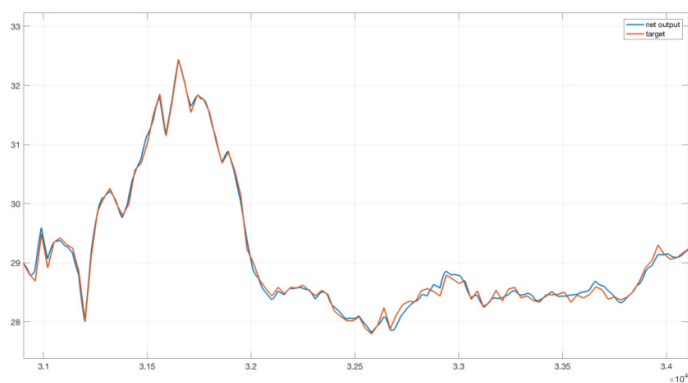


Figure 8. Time response of output variable obtained from closed loop simulation - detail view

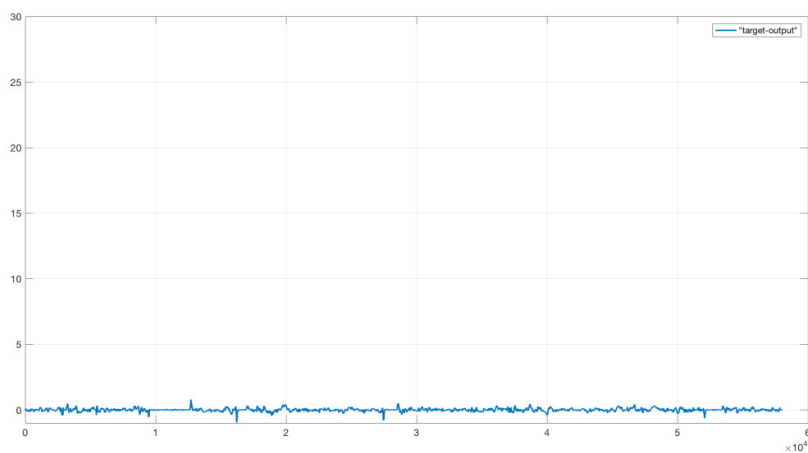


Figure 9. Time response of difference between output variable obtained from closed loop output and target values obtained from process

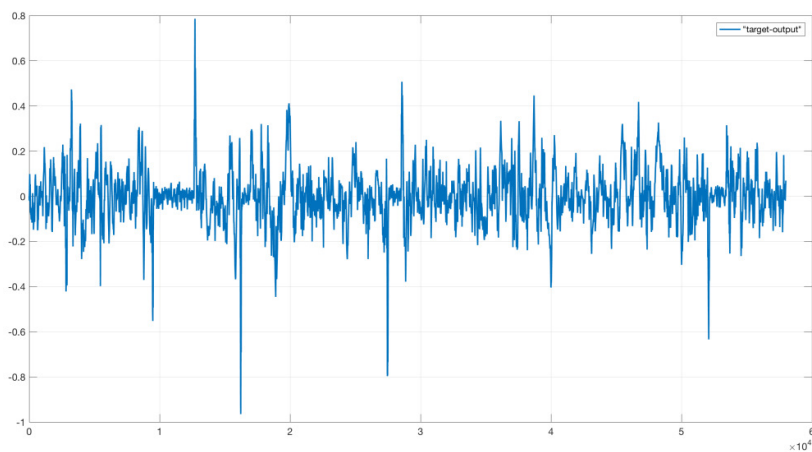


Figure 10. Time response of difference between output variable obtained from closed loop output and target values obtained from process - detail view

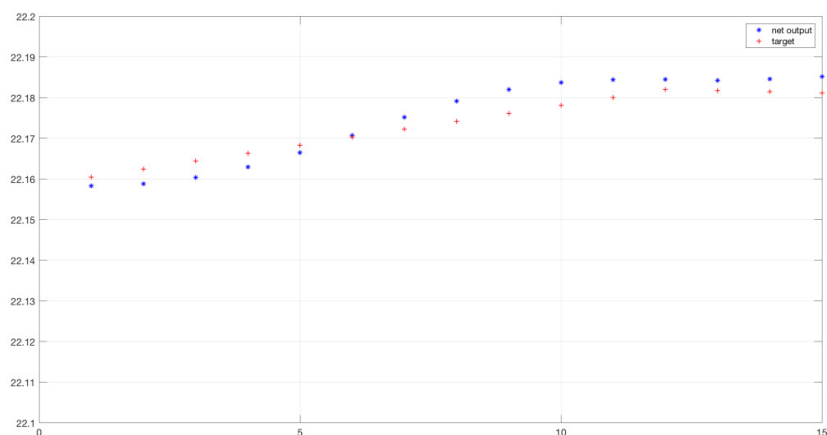


Figure 11. Time response of output variable obtained from closed loop simulation - prediction of 15 steps compared to real values (starting at step 9000)

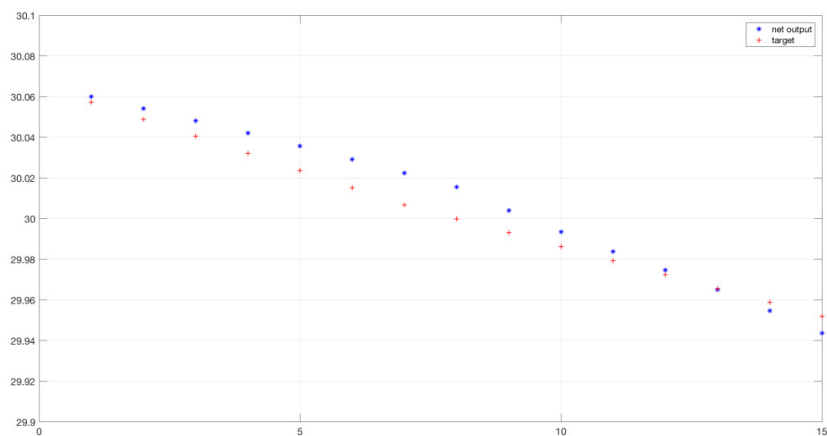


Figure 12. Time response of output variable obtained from closed loop simulation - prediction of 15 steps compared to real values (starting at 28000)

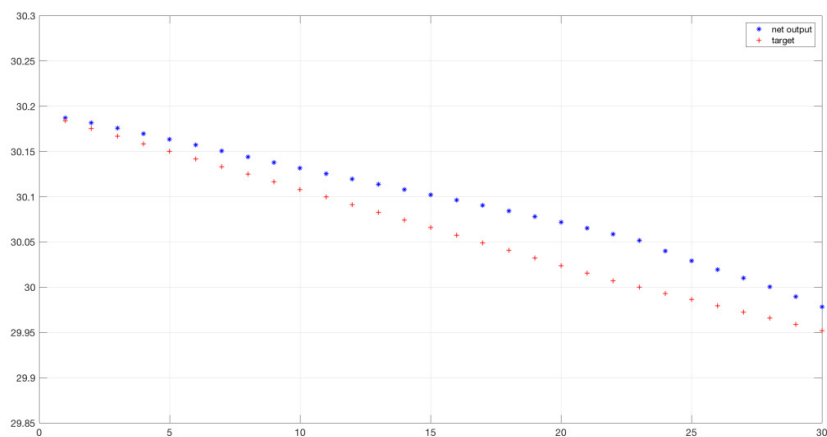


Figure 13. Time response of output variable obtained from closed loop simulation - prediction of 30 steps compared to real values (starting at 37000)

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