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LINEAR IDENTIFICATION AND CONTROL OF REACTOR FOR PHTHALIC ANHYDRIDE PRODUCTION PROCESS - CASE STUDY

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ABSTRACT

Phthalic anhydride is one of the most essential and rare chemicals used in manufacturing of paints, pigments, dyes and esters. Now a day, the demand for the purest form of Phthalic anhydride is increasing but the production is low to meet the demand. Phthalic anhydride is produced by maintaining the constant ratio of air and ortho xylene at 3:1 at very high temperature in mixing column. The mixture is passed through the reactor for reaction with catalyst. Finally, it enters the switch condenser for product separation. The main problem is if the reactor is not maintained below its critical value, leads to explosion. As feed material is a petroleum product, the energy released is enormous, it can endanger the life of employees and to surroundings. For efficient control, linear and nonlinear model identification using AR, ARX and ARMAX is done and conventional controller is included to operate the plant in closed loop.

KEYWORDS: Phthalic Anhydride, Nonlinear model Identification, AR, ARX, ARMAX

INTRODUCTION

Most of the industrial chemical processes are exothermic, it is essential to ensure protection and safety of the operating personnel as well as the environment.As the reaction proceeds, the amount of heat generated will increase.To achieve the desired product, it is necessary to maintain the process temperature at the required value. Properknowledge on type, ratio of the raw materials added, catalysts used, surrounding and reacting conditions is required to carry out process in efficient and controlled manner.Phthalic anhydride is used in manufacture of paints, esters, dies, pigments etc.Production of phthalic anhydride is an exothermic process, where the amount of heat generated is high. The reaction exothermic as the medium in which the reaction is taking place gains heat. When the increased amount of heat is not compensated by the jacket coolant temperature, reactor cracks and thermal explosion occurs. Thermodynamics and kinetics of the chemical reactions determines the design of the reactor. Batch and continuous type reactors are available. *Batch reactors* are mainly used in laboratories where the reactants are placed in a test-tube, beaker. Reactants are mixed together and heated for the reaction to take place. Finally, after reaction the mixture is cooled and purified based on requirements.Alternatively, the reactants are fed continuously into the reactor at one point. The products are withdrawn at another point after the reaction completes.In a continuous reactor, steady state must be attained where the flow rate into the reactor equal the flow rates out of the reactor, or else the tank would be empty or overflow. By dividing the volume of the tank by the average volumetric flow rate the residence time is calculated .Instead of calculating absolute amount of energy, enthalpy change is calculated as it is easier. The work needed to change the volume of the system against ambient pressure plus the change in internal energy of the system calculates the enthalpy change. World demand for PA is expected to start recovering in 2010-2012, largely as a result of improved activity in the construction, automotive and original equipment manufacture (OEM) sectors. US-based consultant orecasts world consumption to grow at an average rate of 2.8%/year during the 2009-2014 period. However, this growth is expected to vary greatly by application and region. Phthalic anhydride is the organic compound with the formula $C_6H_4(CO)_2O$, anhydride of phthalic acid of formula $C_6H_4(CO_2H)_2$ and an isomer of iso-phthalic acid. Commercially, it is anhydride of dicarboxylic acid. Phthalic anhydride is a colorless solid is an important industrial chemical. It is used for the large scale production of plastics. Market survey dictates the maximum usage of pthalic anhydride is in the manufacture of phthalate plasticisers which is used as a plasticiser in polyvinyl chloride (PVC). The major consumption of PA is mainly dependent on the growth of PVC, which is sensitive to general economic

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conditions as it is consumed mainly in the construction and automobile industries. Fig.1. shows the structure of phthalic anhydride.

Figure:

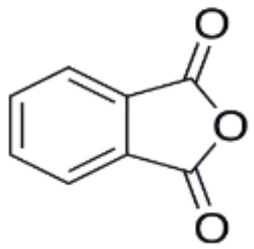

Fig.1.Structure of Phthalic anhydride

The primary preparation for the process starts with mixture of air and ortho-xylene. Air is uncontrolled stream and ortho-xylene is controlled stream. Ortho-xylene is scarce feed material so it must be used efficiently. For initial startup of the reaction air must be preheated to 937ºC. Then air is mixed in a desired ratio with ortho-xylene which is at room temperature.

The mixture is feed to the reactor for the reaction to take place. Before that the reaction mixture must be preheated because the required temperature for the reaction is very high and it requires more energy and more time for reactor to attain the temperature and the efficiency also reduces. The reaction temperature is 535ºC. So the jacket heat flow must be regulated in the way to maintain the reaction temperature. After that it has to pass through switch condenser for separation of immiscible solid particles in product. Then it must pass through the distillation column for separation of low temperature and high temperature products. The purity of the material is an important factor in this reaction. For that temperature has to be maintained. Along with the coolant temperature also measured for more efficient control in the phthalic anhydride process.There is difficulty in maintaining the reaction because this reaction highly exothermic. The reaction must be triggered for quick formation of phthalic acid. For that a solid catalyst Vanadium Pentoxide (V_2O_5) is added. At 535ºC only the catalyst reacts with the mixture to form phthalic acid. But when the time when the catalyst and mixture starts to react then the reaction turns into highly exothermic reaction and becomes difficult to control. The control action is taken but with large delay in time. The product which are formed between the temperature range 534ºC and 537ºC are considered as the best quality raw material. But the quantity at that range of temperature is very low but the demand for the quality and quantity is increasing day by day.

IDENTIFICATION

Method of identifying the mathematical model of a system from measurements of the process inputs and outputs is termed as system identification. System identification for nonlinear is developed based on four basic approaches, Volterra Series Models, Block Structured Models, Neural Network Models, and NARMAX Models. Volterra Series Modelis a model defined for non-linear behaviour. The input to the process at all other times defines the output of the non-linear process in volterra series model. Block structured model is nothing but Hammerstein - Wiener model. In Hammerstein model, a linear dynamic element is considered after static single valued non-linear element. In Wiener model, the linear element occurs before the static nonlinear characteristic. Generally,a static linear element sandwiched between two dynamic systems is known as Hammerstein – Wiener model. Nonlinear Auto Regressive Moving Averagewith Exogenousinput model (NARMAX) consists of past inputs, outputs and noise terms. Unbiased estimates of the system model can be obtained because the noise is modelled explicitly in the presence of nonlinear noise and unobserved highly correlated.

Dynamic model that connects the excited inputs with measured outputs is identified by using different model structures. Model structures include unknown parameters inside the model. Set of criteria functions are chosen to determine best model structure. Transfer function model, polynomial models like AR, ARX and ARMAX models are discussed.

Transfer function Model

Transfer function is a function that relates input and output is known as **transfer function.** Reference input operates through transfer **function**. Input operating with the function of the process produces an effect resulting in controlled output or response. Thus, a **transfer function provides cause and effect relationship between input and output.**

$G(S) = \frac{C(S)}{R(S)}$ (1)

A. AR Model

Auto Regressive model is a type of polynomial model. AR model parameters are estimated using variants of the least-squares method where model structure is given by the following equation

$$A(q)y(t) = e(t) \quad (2)$$

B. ARX Model

Auto Regressive with Exogenous input also called as Controlled Autoregressive model. This structure is viewed in linear regression. The ARX model structure is

$$y(t) + a_1 y(t-1) + \cdots + a_{na} y(t-na) = b_1 u(t-nk) + \cdots + b_{nb} u(t-nb-nk+1) + e(t) \quad (3)$$

C. ARMAX Model

Auto Regressive Moving Average with Exogenous input estimates the time domain data model. The model is written explicitly as the difference equation

$$y(t) + a_1 y(t-1) + \cdots + a_{na} y(t-na) = b_1 u(t-1) + \cdots + b_{nb} u(t-nb) + c_1 e(t-1) + \cdots + c_{nc} e(t-nc) \quad (4)$$

CONTROL

Proportional-Integral-Derivative (PID) control is the most commonly used control algorithm in industry and is universally accepted. The difference between a desired setpoint and a measured process variable is continuously calculated to obtain the error value. The error is minimized by adjusting the control variable. The position of a control valve, a damper is altered to reduce the error. The PID controller equation includes the proportional, integral and derivative gains as shown in eqn (4).

$$u(t) = K_p e(t) + K_i \int_0^t e(t)dt + K_d \frac{de(t)}{dt} \quad (5)$$

P accounts for present values of the error, *I* accounts for past values of the error and *D* accounts for possible future values of the error, based on its current rate of change.PID controller can deal with specific process requirements if the three parameters of the controller are tuned.

A. Proportional term

Output of the proportional term is proportional to the current error value. A constant kpis adjusted to change the response of the proportional term. The constant term is called the proportional gain constant.The proportional term is given by

$P_{out} = K_p e(t)$ (6)

For a given change in the error, a large change in the output is obtained if the proportional gain is high. The process becomes unstable if the proportional gain is too high. A small gain results in a small output response to a large input error, and a less sensitive controller. The control action may be too small to process disturbances if the proportional gain is too low.

B. Integral term

Output of the integral term is proportional to magnitude and the duration of the error. Sum of the instantaneous error over time is provided by the integral term and provides the accumulated offset to be corrected previously.The integral gain Kiis multiplied with the accumulated error and added to the controller output. The integral term is given by

$$I_{out} = K_i \int_0^t e(t)dt \quad (7)$$

Residual steady-state error is eliminated with the integral part of PID controller. Residual steady-state error occurs with a pure proportional controller. Present value overshoots from the setpoint value as the integral term response depends on accumulated errors from the past.

C. Derivative term

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Slope of the error over time is calculated to obtain the derivative of the process error. The error is multiplied with the derivative gain Kd. The derivative term is given by:

$$D_{out} = K_d \frac{de(t)}{dt} \quad (8)$$

System behavior can be predicted from the derivative action thus settling time and stability of the process is improved. Fig.2. shows the basic block diagram of the closed loop system used in the production of phthalic anhydride process.

Figure:

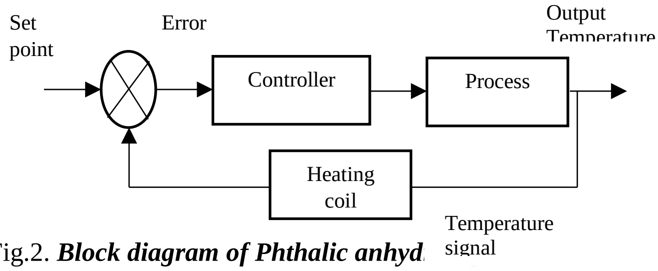

Fig.2. ***Block diagram of Phthalic anhyd***

RESULTS AND DISCUSSION

A. Model Identification

Transfer function Model

The transfer function of the process is estimated as the mathematical model for the process is not available. The experimental data are collected and the transfer function for the process is determined by transfer function estimation method in MATLAB. The input/output data is loaded in and object and then iddata object is created. The initial conditions for the transfer function estimation are given. Then it is loaded in tfest function to give the final Transfer function for the process. Fig.3. shows the step by step procedure to obtain the transfer function of the process. Fig.4. shows the open loop response of the process obtained from the transfer function model. The transfer function for the process is

$$G(s) = \frac{5.5s + 45.7}{s^2 + 23s + 126.5} \quad (9)$$

Figure:

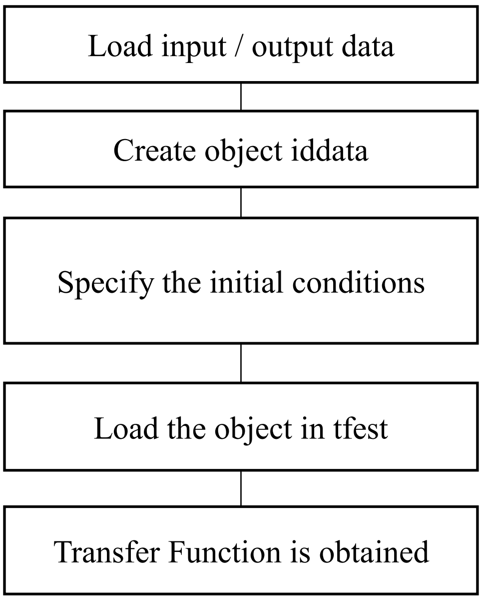

Fig.3. ***Procedure to identify transfer function model***

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Figure:

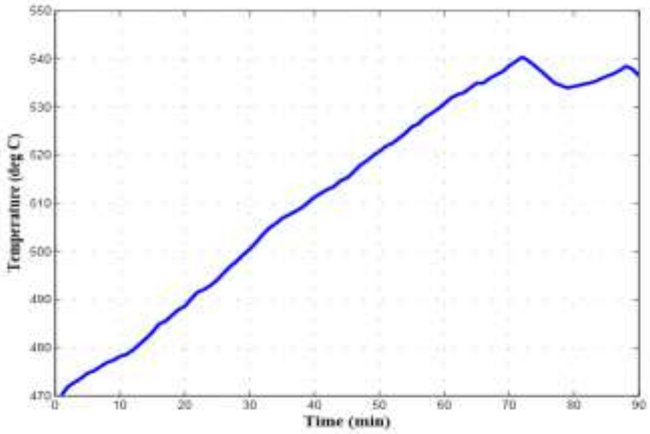

Fig.4.***Response of the obtained transfer function***

AR Model

Once the transfer function is obtained then with the aid of experimental data the AR model identification is done by creating the iddata object. Then the model order specification is provided. Then by least square approach the AR model is obtained with the defined polynomial order. Fig.5. shows the step by step procedure to obtain AR model.

Tables:

Table.1. Polynomial model - AR

$A(s)$		$s^2 + 23s + 129$
Polynomial order	na	2

Figure:

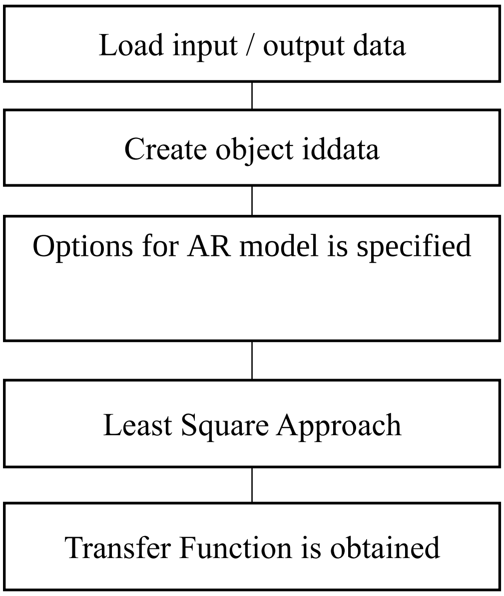

Fig.5***Procedure to identify AR Model***

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Table.1.

Table.1. shows the polynomial equation of the AR model. Then the output response is obtained by applying the polynomial orders using System Identification tool box.Fig.6. compares the response of the experimental data and AR model. The best fit that it fits with the estimated transfer function is 63.5%.

Figure:

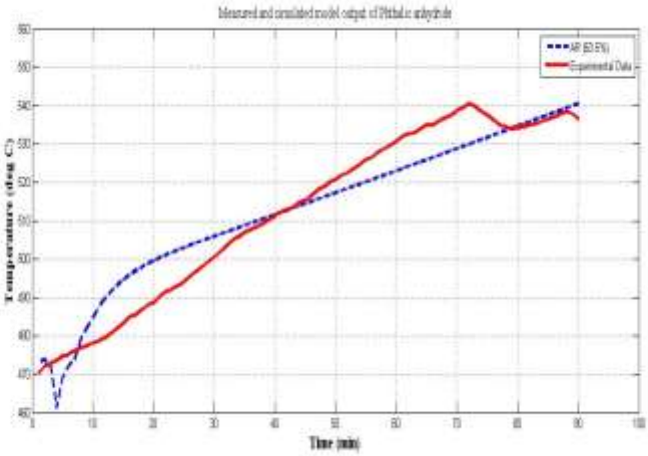

Fig.6.***Response of AR model***

ARX model

ARX model identification is done by creating the iddata object. Then the model order specification is provided. Then by specifying initial conditions ARX model transfer function is obtained along with the polynomial order.

Tables:

Table.2. Polynomial model - ARX

$A(s)$		$s^2 + 25.35s + 142.6$
$B(s)$		$7.42s + 137.7$
Polynomial order	na	2
	nb	1

Figure:

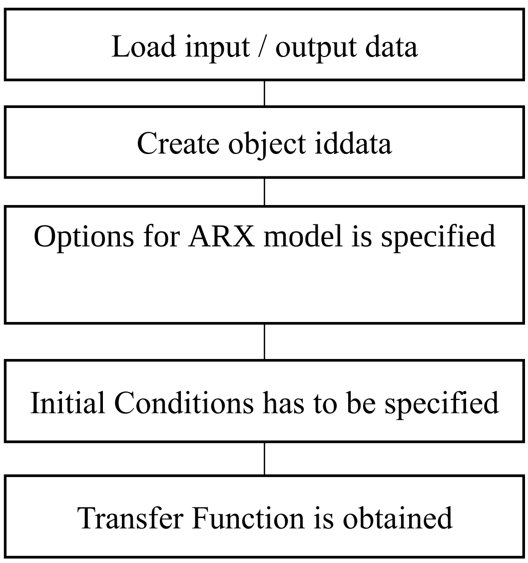

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Fig.4 ***Procedure to identidy ARX model***

Figure

Fig.7. shows the procedure for obtaining the ARX model of the process. TABLE.2. shows the polynomial equation of the ARX model. Then the output response is obtained by applying the polynomial orders using System Identification tool box. The best fit that it fits with the estimated transfer function is 69.8%. Fig..8. compares the response of ARX model and the experimental data of the process.

Figure

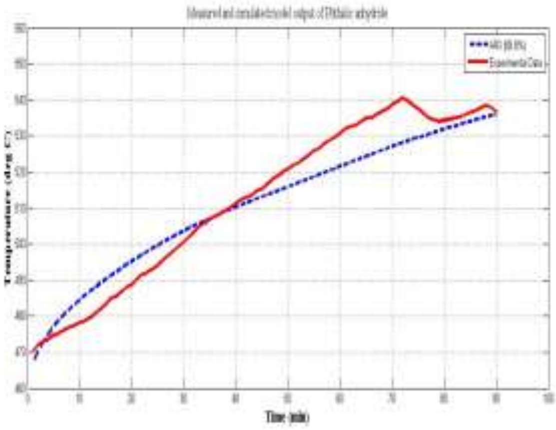

Fig.8. ***Response of ARX model***

ARMAX model

ARX model identification is done by creating the iddata object. Then the model order specification is provided. Then by specifying initial conditions ARX model transfer function is obtained along with the polynomial order. Fig.9. shows the procedure to obtain ARMAX model for the process. TABLE.3. tabulates the polynomial equations of the ARMAX model.

Figure

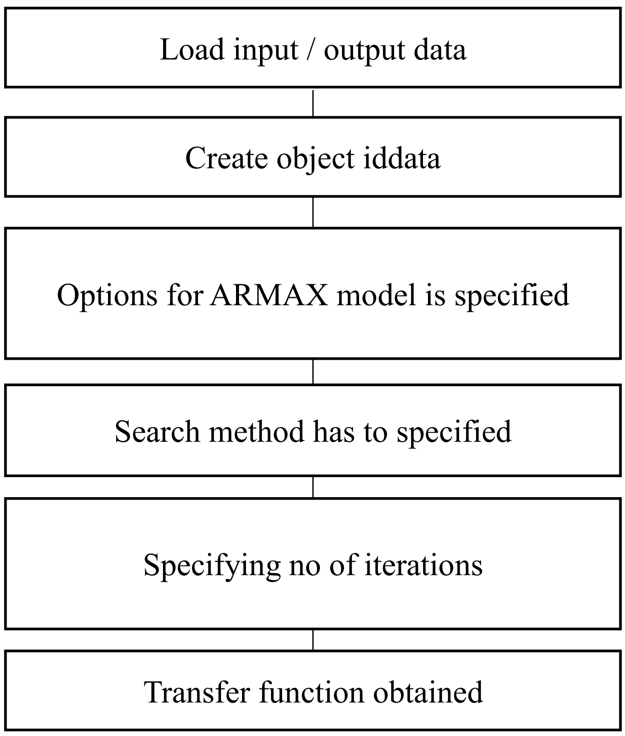

Fig.9. ***procedure to identify ARMAX model***

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Tables:

Table.3. Polynomial ARMAX model

$A(s)$		$s^2 + 25.35s + 142.6$
$B(s)$		$4.41s + 60.2$
$C(s)$		$3.01s + 80.5$
Polynomial order	na	2
	nb	2
	nc	2

Then the output response is obtained by applying the polynomial orders using System Identification tool box. The best fit that it fits well with the estimated transfer function is 73.2%. Fig.10. shows the response of ARMAX model of the process.

Figure

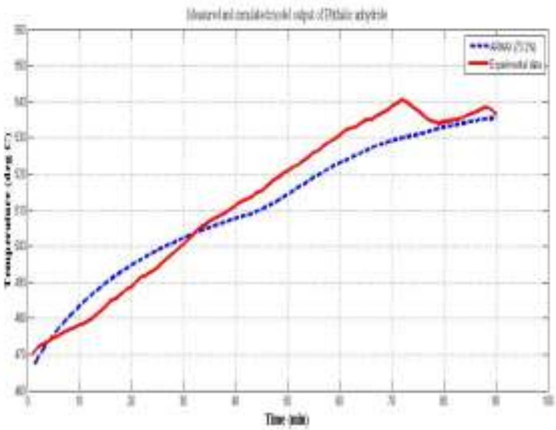

Fig.10. ***Response of ARMAX model***

Table:4
Table.4. shows the various criteria and best fit model for the production of phthalic anhydride. AR, ARX and ARMAX models are polynomial models considered for the Phthalic anhydride process.

Tables:

Table.4. Comparison of polynomial models

Model	Polynomial Orders				No of free Coefficients	Percentage match
	na	nb	nc	nk		
AR	2	-	-	-	2	63.5%
ARX	2	1	-	1	4	69.8%
ARMAX	2	2	2	0	6	73.2%

Controller
In order to achieve automation, PD controller is employed for the closed loop control technique.Fig.11. shows the block diagram of conventional controller.TABLE.5.The controller parameters for PD controller for conventional transfer function model are tabulated

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Figure

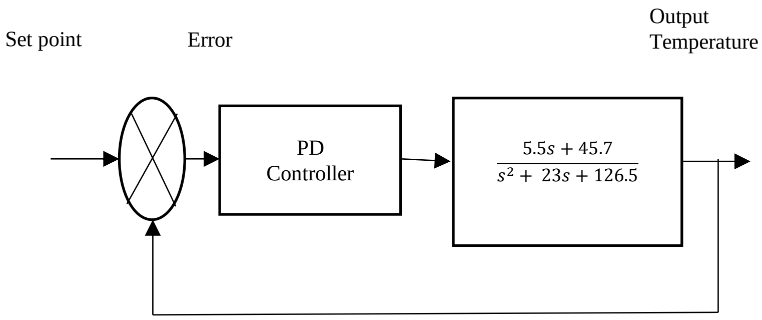


Fig.11.***Block diagram of conventional transfer function model***

Tables:

Table.5. Controller parameters for transfer function model

K_p	τ_d
5.0326	0.893

Figure:

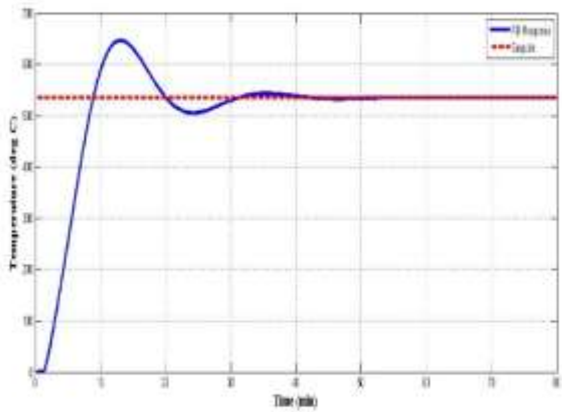


Fig.12.***Response of conventional transfer function model***

Fig.12.shows the response of conventional transfer function model.
Fig.13. shows the block diagram for the ARMAX transfer function control. Table.6. The controller parameters for PD controller for ARMAX model are tabulated

Figure:

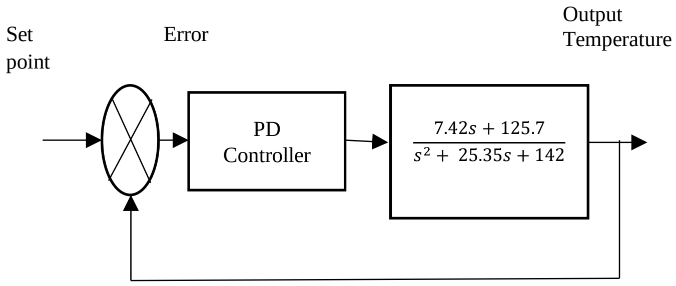


Fig.13. ***Block diagram for ARMAX transfer function model***

Tables:

Table 6. Controller parameters for ARMAX transfer function model

K_p	τ_d
49.564	0.893

Fig.14.shows the response of conventional transfer function model.

Figure:

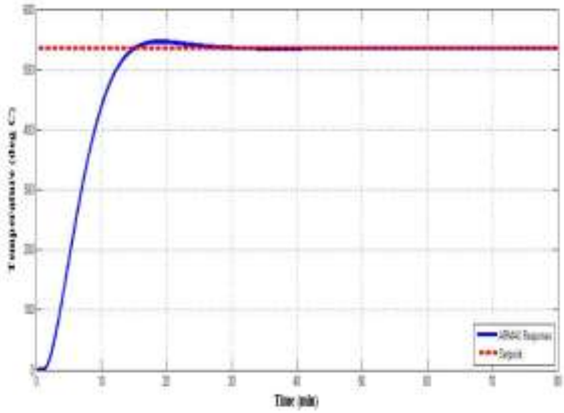
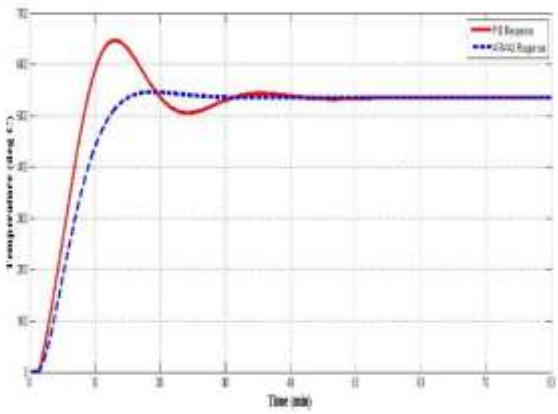


Fig.14.***Response of ARMAX transfer function model***

The response for the conventional transfer function controller and the ARMAX transfer function model controller are shown in Fig.15. In conventional transfer function model, it is observed that high overshoot is present when compared to that of ARMAX transfer function model.

Fig.15. ***Comparison of response of conventional transfer function and ARMAX transfer function model***

Figure:



INTRODUCTION OF MODEL PREDICTIVE CONTROL

MPC is widely adopted in industry as an effective approach to deal with large multivariable constrained control problems. Model Predictive Control is an optimization based procedure. At each time k, an optimization problem is solved. An objective function (least square/quadratic) is minimized by selection of manipulated variable moves over a control horizon of M control moves, based on output predictions over a prediction time horizon of P time steps. After u_k is implemented, measurement at the next time step y_{k+1} is obtained. Correction for model error is performed since the measured output y_{k+1} will not be equal to the model predicted value. Now again a new optimization problem is solved over a prediction horizon of P steps by adjusting M control moves. This approach is called as receding control, this scheme introduces notion of feedback in the control law to compensate for disturbances and modeling errors.Factors to be considered while implementing MPC are the type of objective function used optimization, type of model used to predict the output, initialization of the model to predict future output values, desired set-point trajectory, disturbance compensation and implementation of constraints.The basic concept of MPC is to use a dynamic model to predict system behavior, and optimize the prediction to produce the best decision — the control action at the current time. Based on the past and present values and future control actions, the dynamic model predicts the future plant outputs. Optimizer calculates the control actions based on the constraints presented as well as the objective function. Minimization of objective function is solving of the optimization problem by adjusting control moves M which is subjected to modeling equations and input output constraints.

In general for P prediction horizon & M control horizon,
Objective function is given as,
$\boldsymbol{\varphi} = \sum_{i=1}^{P} |\mathbf{r}_{k+i} - \hat{\mathbf{y}}_{k+i}| + \mathbf{w} \sum_{i=1}^{M-1} |\Delta \mathbf{u}_{k+i}|$ and Optimization is min (φ).
Fig. 16. Shows the structure of Model Predictive control. MPC has the ability to anticipate future events and can take control actions accordingly. PIDand PD controllers do not have this predictive ability. MPC is nearly universally implemented as a digital control, although there is research into achieving faster response times with specially designed analog circuitry. MPC control algorithm is not generally needed to provide adequate control of simple systems, which are often controlled well by generic PID and PD controllers. Common dynamic characteristics that are difficult for PID and PD controllers include large time delays and high-order dynamics.

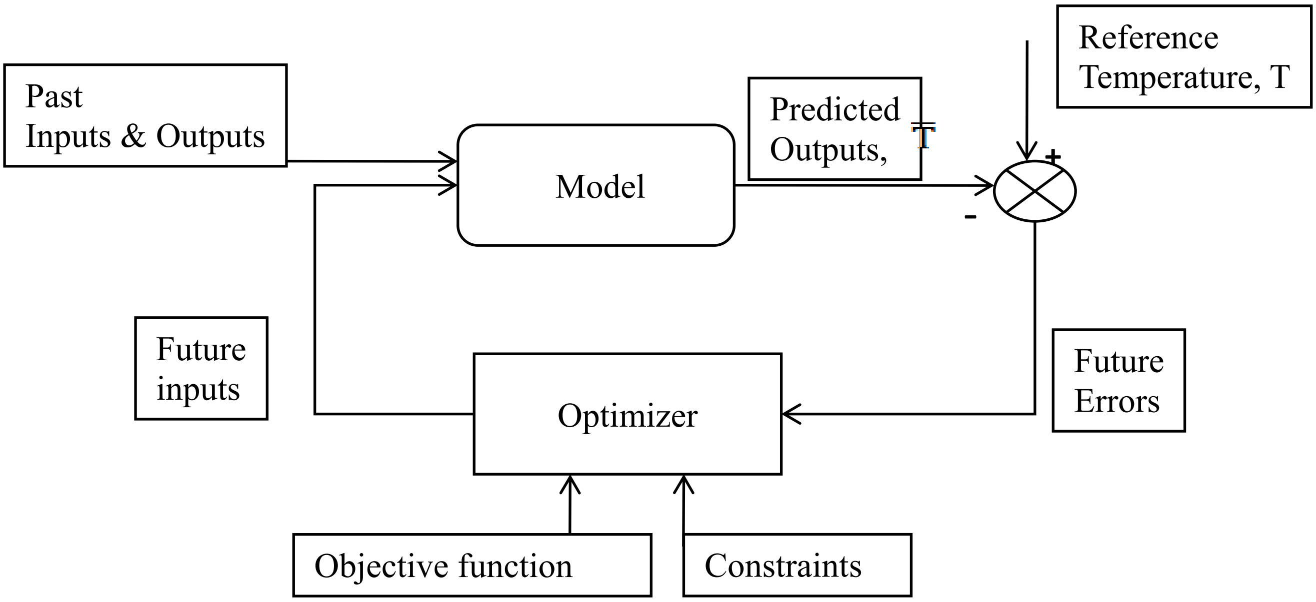


Fig. 16. structure of model predictive control

The controller response is obtained from the ARMAX model transfer function is shown in Fig,18.

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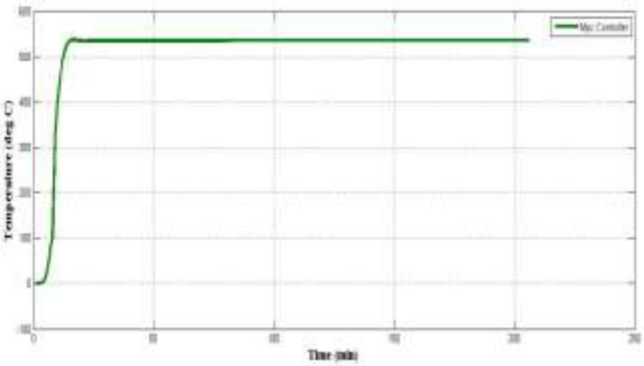

Fig.17. Response of Model Predictive Control for Phthalic anhydride process

COMPARISON OF CONVENTIONAL CONTROL Versus MODEL PREDICTIVECONTROL

The performance is analyzed by comparing Model Predictive Controller with Conventional PD controller for Phthalic anhydride process and shown in Fig.18.

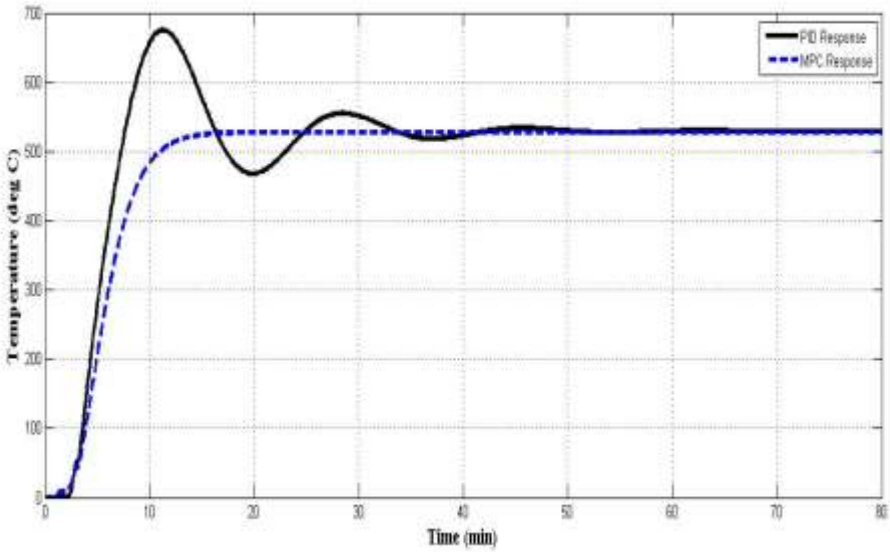

Fig.18. Comparision of the model predictive control and conventional PD control.

CONCLUSION

Production of phthalic anhydride significantly depends on the reactor temperature. From the input-output data of the reactor various model structures like transfer function, AR, ARX and ARMAX models are simulated. ARMAX model provides the best fit for the process. Conventional PD controller is implemented for the transfer function and ARMAX models of the process. It is found that the transfer function model possess high overshoot in closed loop compared to ARMAX model. One of the advanced control strategies called model predictive control is implemented. It is found that MPC shows better performance when compared with conventional PD controller.

NOMENCLATURE

Na	Order of the polynomial A(q)
Nb	Order of the polynomial B(q) + 1
Nk	Input-output delay expressed as fixed leading zeros of the B polynomial (dead time)

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