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System Identification of Extractive Distillation Process

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Abstract **- Extractive distillation is one of the enhanced distillation processes whereby another substance which is relatively non-volatile compared to the components to be separated is added to aid the process in achieving the desired separation level. Due to cascade nature of the process, modeling the process from first principle can lead to high dimensional model which may constitute serious computational challenges for real-time application. This work thereforeused black box modeling approach to identify dynamic model for extractive distillation process using system identification toolboxin MATLAB software.**

The recovery of methylcyclohexane (MCH) from its mixture with toluene using phenol as the solvent was simulated in ASPEN TECH flow-sheeting software in order to generate data for model identification. The steady state simulation was carried out using ASPEN PLUS to measure the effect of the input variables on the output variables. The input variablesconsidered arereflux flow rate and condenser heat dutywhile the output variablesconsidered aremethylcyclohexane (MCH) mole fraction (top product) and toluene mole fraction (bottom product) was considered. ASPEN DYAMICS was then used to generate the dynamic input-output data which was later used to formulate the dynamic model using System identification toolbox in MATLAB environment. The black box models considered areDiscrete-time AutoRegressive Moving Average with eXternal input (ARMAX) model and Box-Jenkins (BJ) model.

TheARMAX model developed gave a data fit of 90.26% for the first output and 89.66% for the second output while that of BJ gave a data fit of 78.08% for the first output and 92.18% for the second output . The residual analysis carried out on the two MIMO models using autocorrelation function for the residuals as well as cross-correlation function between the inputs and outputs for the MIMO models with confidential interval set to 99% shows that the models are acceptable one.

Keywords: Extractive Distillation,ARMAX, BJ,Aspen Tech, Matlab.

1. INTRODUCTION

Separation of a mixture system into its respective constituents is of great importance in chemical and petrochemical process industries and many techniques have been introduced, developed, tested and used over the years. Among these techniques is distillation. However, because of the complex nature of many real mixtures which have close boiling components, conventional distillation methods are been enhanced to handle the complexity. Examples of these enhanced distillation methods are extractive and azeotropic distillation, in both cases, a third component (solvent) is added to alter the relative volatility by a wide margin for a successful result and traditionally a second column is used to recover the solvent [1]. The solvent introduced will have strong affinity for one of the key components and should be easily separable from the bottom product.Although, both azeotropic and extractive method of distillation involve the introduction of third component (solvent) but azeotropic distillation will only be considered when there is higher tendency that the addition of the solvent will lead to the formation of *azeotropes*.

Modeling of processes in chemical engineering practice is majorly carried out either by first principle approach or by black-box approach and it plays an important role in operations such as process optimization and process control.Distillation process is a multi-stage system, therefore modeling it using first principle approach leads to formulation of numerous sets of differential algebraic equations (DAE) consisting of thousands of variables depending on the number of stages used and the type of components on each stage. Solving these sets of equations consumes much of both time and computational resources though this type of approach is very useful in offline optimization, verification of simplified model but not applicable in online optimization [2]. Black box modeling approach provides easier means of modeling multi stage systems taking care of all forms computational irregularities within a shorter time. [3]used ARMAX Structure to model steam distillation essential oil extraction system by considering different model order criteria. [4]worked on nonlinear modeling of a reactive distillation process to compare sigmoid network based NARX model and tree-partition based NARX model and found out that the sigmoid network based NARX outperformedtree-partition based NARX.

ASPEN TECH is one of many commercial Chemical Engineering simulation softwares which has been tested and used in various capacities in chemical and petrochemical industries.[5]usedAspen plus to simulate distillation process for excess methanol recovery in continuous biodiesel production and achieved between 95-98% of excess methanol recovery.[6]carried out the simulation of atmospheric crude unit using Aspen plus and concluded that the result were satisfactory and that the unit can be used for different crude oil. [7] carried out the modeling and simulation of ethyl Acetate Reactive Distillation Column Using Aspen Plus.

2. PROCESS DESCRIPTION

The recovery of methylcyclohexanefrom its mixture with toluene cannot be achieved by the use of conventional distillation methods and it therefore requires the use of extractive distillation which is an example of an *enhanced-type*of distillation. The separation of the mixturecannot be achieved with conventional distillation because of the closeness in boiling point of the two components with methylcyclohexane having a boiling of 101^0C and toluene with a boiling point of 110.6^0C.The separation can be enhanced by the addition of phenol (boiling point of 181.7 °C)which serves as an extractant to improve the relative volatility of methylcyclohexane over toluene, leaving almost allthe methylcyclohexane to leave through the top product of the distillation column and the other leaving through the bottom product. The nominal operating conditions and column parameters for the process is shown in Table 1 and the phase equilibrium calculations made use of Universal QUAsiChemical (UINQUAC) activity coefficient is shown in Table 2.

Table1.Nominal operating conditions and the column parameters for Methylcyclohexane Recovery by Extractive Distillation

Total no. of trays (*NT*)	22
MCH mixture feed tray	14
Phenol feed tray	7
Flow rate of MCH mixture solution (lbmol/hr)	400
Composition of MCH mixture	(0.5 mol fraction)
Flow rate of Phenol (lbmol/hr)	1200
Composition of Phenol	1 (pure solvent)
Pressure: (psi)	20
Temperature (F)	220
Reflux Ratio	8
Tray type Tray Column diameter (ft) Tray spacing (ft)	Bubble cap 1 2

Table 2: UNIQUAC model parameters

Component i	TOLUENE	TOLUENE	PHENOL
Component j	PHENOL	MCH	MCH
Temperature units	F	F	F
Source	VLE-IG	VLE-IG	VLE-IG
aij	-4.522600000	0.0	0.0
aji	3.641100000	0.0	0.0
bij	3170.523395	-4.161599967	146.9521788
bji	-2737.542398	-45.54737964	-443.8459764
cij	0.0	0.0	0.0
cji	0.0	0.0	0.0
dij	0.0	0.0	0.0
dji	0.0	0.0	0.0
Tlower	230.9000022	213.5300023	213.9800023
Tupper	342.8600013	231.1160022	302.0000016

2.1 Steady and Dynamic State Simulation

The steady state model of process was simulated using ASPEN plus environment as shown in Figure 1. The sensitivity analysis was also carried out to measure the impact of the input variable (phenol flow rate) on the output variables such as methylcyclohexane mole fraction from top product and toluene mole fraction from bottom product..

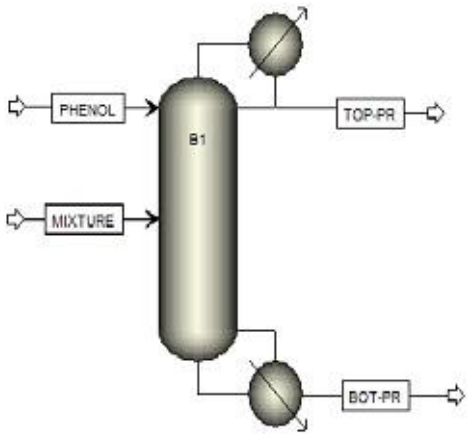

Figure 1: Extractive distillation process simulated with the ASPEN plus environment

The steady state model was later exported to Aspen Dynamics enviroment to generate the input-ouput in the dynamic state. To generate the data, perturbation of phenol flow rate was carried out through the use of PRBS (pseudo random binary signal) control module with the configuration as shown in Table 3.

Table 3: PRBS configuration

Property	Value	Units
Amplitude type	Variable	
Datum	900	lbmol/hr
Amplitude	620	lbmol/hr
Period	5.0	min
Seed	12345	

Multi-input multi-output (MIMO) system using reflux flow rate and condenser heat duty as inputs and Methylcyclohexane mole fraction from the top product and toluene mole fraction from the bottom product was considered.One thousand data set at 1 minute sampling interval was generated. Five hundred data were used for parameters estimation and model orderdetermination models while five hundred data were used for model validation.

3.MODEL STRUCTURE

The ARMAX (AutoRegressive Moving Average with eXternal input) model is defined, as follows:

$$A(q)y(t) = B(q)u(t) + C(q)e(t) \quad (1)$$

Where

$$A(q) = 1 + a_1 q^{-1} + \cdots + a_{n_a} q^{-n_a} \quad (2)$$

$$B(q) = b_1 + b_2 q^{-1} + \cdots + b_{n_b} q^{-n_b+1} \quad (3)$$

$$C(q) = 1 + c_1 q^{-1} + \cdots + a_{n_c} q^{-n_c} \quad (4)$$

And $q^{-1}$is the backward shift operator defined by $q^{-1}u(t) = u(t-1)$ 5

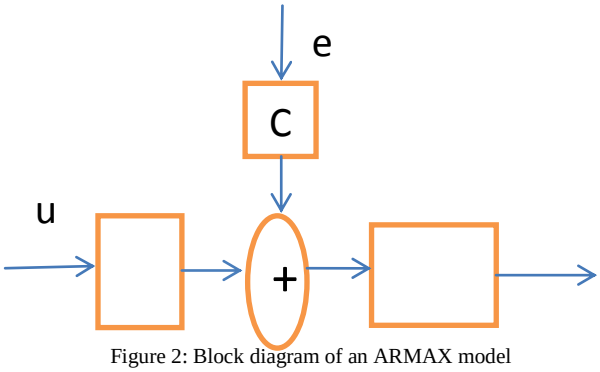

Figure 2: Block diagram of an ARMAX model

The general Box-Jenkins model structure is

$$y(t) = \sum_{i=1}^{nu} \frac{B_i(q)}{F_i(q)} U_i(t - nk_i) + \frac{C(q)}{D(q)} e(t) \quad 6$$

Where*nu*is the number of input channels

The orders of Box-Jenkins model are defined as follows:

$$nb: \quad B(q) = b_1 + b_2 q^{-1} + \cdots + b_{nb}\, q^{-nb+1} \quad 7$$

$$nc: \quad C(q) = 1 + c_1 q^{-1} + \cdots + c_{nc}\, q^{-nc} \quad 8$$

$$nd: \quad D(q) = 1 + d_1 q^{-1} + \cdots + d_{nd}\, q^{-nd} \quad 9$$

$$nf: \quad F(q) = 1 + f_1 q^{-1} + \cdots + f_{nf}\, q^{-nf} \quad 10$$

n_b is the order of the B polynomial plus 1 (Ny-by-Nu matrix)

n_c is the order of the C polynomial plus 1 (Ny-by–1 matrix)

n_d is the order of the D polynomial plus 1 (Ny-by-1 matrix)

n_f is the order of the F polynomial plus 1 (Ny-by-Nu matrix)

n_k is the input delay (in number of samples, Ny-by-Nu matrix)

where Nu is the number of inputs and Ny is the number of outputs.

3.1 Model Order Selection

Selecting the order of the model to get the best prediction for the outputs is very important. To avoid over-fitting or under-fitting of the model, optimal values of the order was determined by Akaike Final Prediction Error for estimated model (FPE).

Akaike's Final Prediction Error (FPE) is defined by the following equation:

$$FPE = V\left[\frac{1 + \frac{d}{N}}{1 - \frac{d}{N}}\right] \quad 11$$

where V is the loss function, d is the number of estimated parameters, and N is the number of values in the estimation data set.

The final prediction error is asymptotic ford<<N and uses the following approximation to compute FPE:

$$FPE = V\left(1 + \frac{2d}{N}\right) \quad 12$$

The loss function V is defined by the following equation:

$$V = det\left[\frac{1}{N}\sum_{1}^{N} \varepsilon(t, \theta_N)(\varepsilon(t, \theta_N))^T\right] \quad 13$$

Where Θ_N represents the estimated parameters

The optimal order structure for the ARMAX model isn_a = [2 2; 2 2], n_b = [2 2; 2 2] , n_c = [2;2] n_k= [1 1; 1 1] while that of BJ (Box-Jenkins) model is n_b= [2 2;2 2] n_c = [2;2] n_d= [2;2] n_f = [2 2 ; 2 2] n_k = [1 1; 1 1].

3.2 Parameter Estimation

The estimation of the model parameters as described in Equations 1 to 10 was carried out in MATLAB Environment to find out the optimum values. An iterative search algorithm which minimizes robustified quadratic prediction error criterion was used for the estimation where the iterations were terminated when the specified tolerance wasgreater than the expected improvement Levenberg-Marquardt was used to effect the minimization [8]..

4. RESULTS AND DISCUSSION

4.1 Model Identification

Inputs – Reflux Flow rate and Condenser Heat Duty

Outputs – MCH (Top product) mole fraction and Toluene mole fraction (Bottom Product)

Discrete-time AutoRegressive Moving Average with eXternal input (ARMAX) model resultsinto the following:

Model for Output y_1:

$$A(z)y_1(t) = -A_{i(z)y_{i(t)}} + B(z)U(t) + C(z)e_{1(t)} \quad 14$$

$$A(z) = 1 - 0.2566z^{-1} - 0.2549z^{-2} \quad 15$$

$$A_{2(z)} = 0.2451z^{-1} + 0.243z^{-2} \quad 16$$

$$B1(z) = -0.01078z^{-1} + 0.0111z^{-2} \quad 17$$

$$B1(z) = 3.365e^{-9}z^{-1} + 1.275e^{-9}z^{-2} \quad 18$$

$$C(z) = 1 + 1.014z^{-1} + 0.5609z^{-2} \quad 19$$

Model for Output y2:

$$A(z)y_1(t) = -A_{i(z)y_{i(t)}} + B(z)U(t) + C(z)e_{2(t)} \quad 20$$

$$A(z) = 1 - 0.2302z^{-1} - 0.2284z^{-2} \quad 21$$

$$A1(z) = -0.2407z^{-1} - 0.2391z^{-2} \quad 22$$

$$B1(z) = 0.01113z^{-1} - 0.0109e^{-9}z^{-2} \quad 23$$

$$B2(z) = -0.3.311e^{-9}z^{-1} - 0.5726z^{-2} \quad 24$$

$$C(z) = 1 + 1.027z^{-1} + 0.5726z^{-2} \quad 25$$

n_a = [2 2; 2 2], n_b = [2 2; 2 2] , n_c = [2;2] n_k= [1 1; 1 1]

Also, Box-Jenkins (BJ) polynomial model results into the following:

Model for Output y_1:

$$y_1(t) = \left[\frac{B(z)}{F(z)}\right]u(t) + \left[\frac{C(z)}{D(z)}\right]e_1(t) \quad 26$$

$$B1(z) = -0.009174z^{-1} + 0.009177z^{-2} \quad 27$$

$$B2 = 2.65e^{-9}z^{-1} + 2.154e^{-9}z^{-2} \quad 28$$

$$C(z) = 1 + 0.3096z^{-1} - 0.2761z^{-2} \quad 29$$

$$D(z) = 1 - 1.684z^{-1} + 0.7263z^{-2} \quad 30$$

$$F1(z) = 1 - 0.7486z^{-1} - 0.2482z^{-2} \quad 31$$

$$F2(z) = 1 - 0.07124z^{-1} - 0.7927z^{-2} \quad 32$$

Model for Output y_2:

$$y_2(t) = \left[\frac{B(z)}{F(z)}\right]u(t) + \left[\frac{C(z)}{D(z)}\right]e_2(t) \quad 33$$

$$B1(z) = 0.007953z^{-1} - 0.007952z^{-2} \quad 34$$

$$B2(z) = -2.713e^{-9}z^{-1} + 5.879e^{-10}z^{-2} \quad 35$$

$$C(z) = 1 + 0.5503z^{-1} - 0.2912z^{-2} \quad 36$$

$$D(z) = 1 - 1.49z^{-1} + 0.6456z^{-2} \quad 37$$

$$F1(z) = 1 - 0.09z^{-1} - 0.09014z^{-2} \quad 38$$

$$F2(z) = 1 - 1.384z^{-1} - 0.5722z^{-2} \quad 39$$

With orders: n_b=[2 2;2 2] n_c = [2;2] n_d= [2;2] n_f = [2 2 ; 2 2] n_k = [1 1; 1 1]

The MIMO models considered using the combination of reflux flow rate and condenser heat duty as the inputs, having methcyclohexane in top product and toluene in the bottom product as their outputs were ARMAX and BJ model. Thefirst black box model (ARMAX model) represented by Equation 14 to 25 gave data fit of 90.26% for the first output and 89.66% for the second which are represented by Figure 3 and 4 while the second black box model (BJ model) represented by Equation 26 to 39 gave a data fit of 78.08% for the first output and 92.18 for the second output which are represented by Figure 5 and 6.

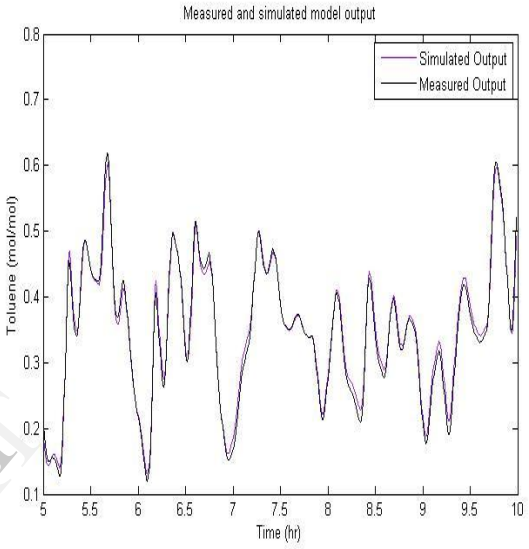

Figure 3. First MIMO model output for Toluene in bottom product when reflux ratio and Condenser heat duty are the inputs

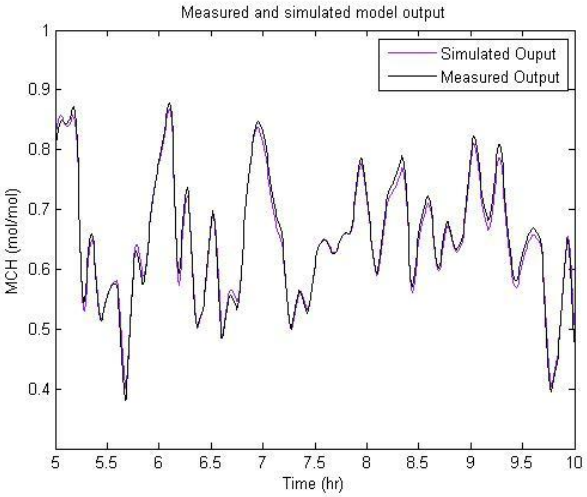

Figure 4.First MIMO model output for MCH in Top product when reflux ratio and Condenser heat duty are the inputs.

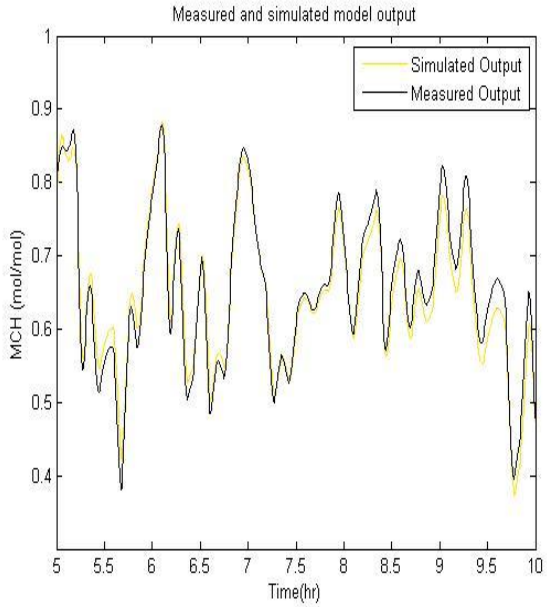

Figure 5. Second MIMO model output for MCH in bottom product when reflux ratio and Condenser heat duty are the inputs

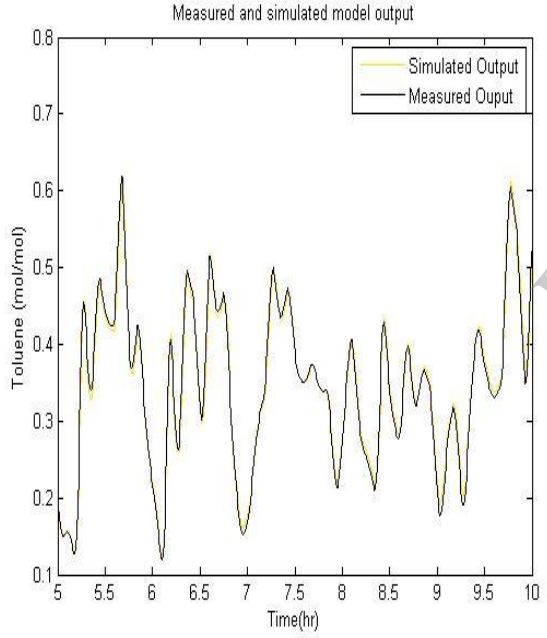

Figure 6. Second MIMO model output for Toluene in bottom product when reflux ratio and Condenser heat duty are the inputs

4.1Residual Analysis

The autocorrelation function for the residuals as well as the cross correlation functions between input and output for the two MIMO models are computed and displayed as shown in figure 7 to figure 14.The confidential interval for this work is set as 99%. The confidential interval for these functions is shown by default as dashed lines. Since the correlation curves lie between these lines, it shows that the model is an acceptable one.

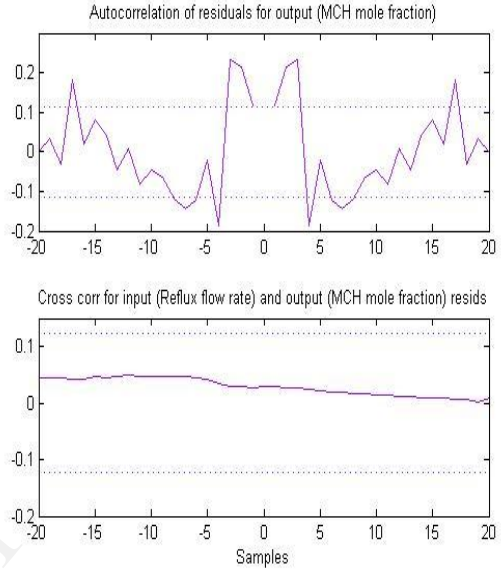

Figure 7. Autocorrelation of Residuals for Output (MCH mole fraction) and Cross Correlation for Input (Reflux flow rate) and Output (MCH mole fraction) residual for the first model.

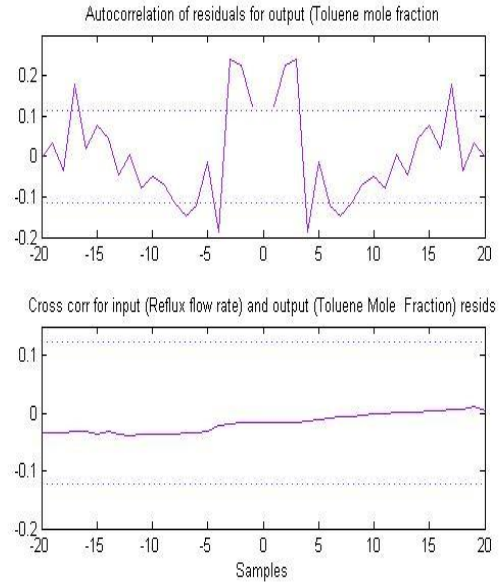

Figure 8. Autocorrelation of Residuals for Output (Toluene mole fraction) and Cross Correlation for Input (Reflux flow rate) and Output (Toluene mole fraction) residual for the first model.

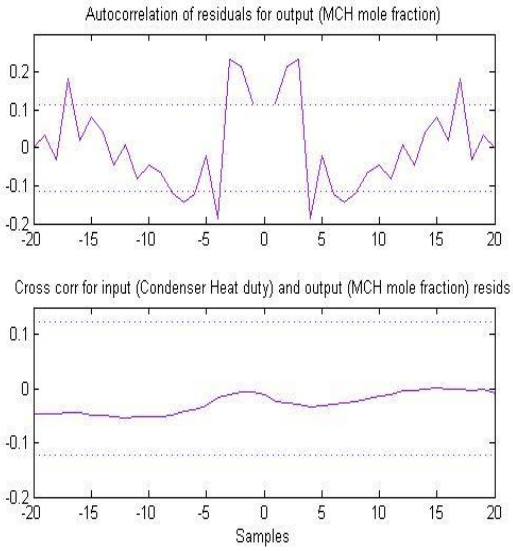

Figure 9. Autocorrelation of Residuals for Output (MCH mole fraction) and Cross Correlation for Input (Condenser Heat Duty) and Output (MCH mole fraction) residual for the first model.

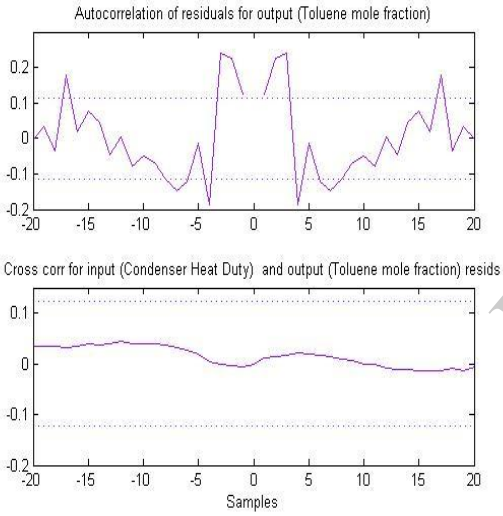

Figure 10. Autocorrelation of Residuals for Output (Toluene mole fraction) and Cross Correlation for Input (Condenser Heat duty) and Output (MCH mole fraction) residual for the first model.

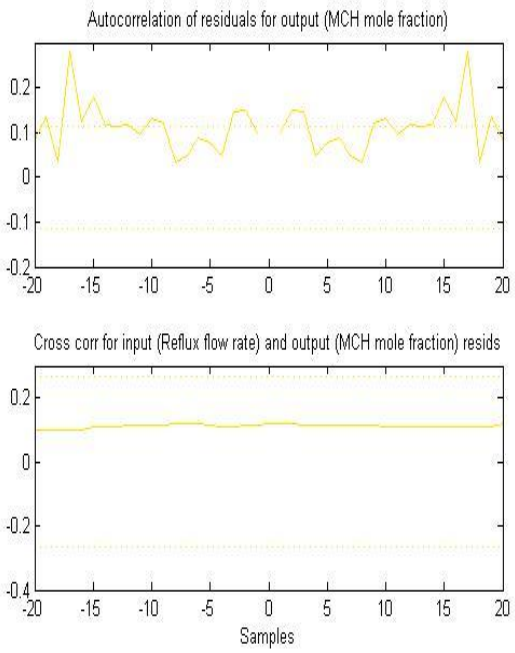

Figure 11. Autocorrelation of Residuals for Output (MCH mole fraction) and Cross Correlation for Input (Reflux flow rate) and Output (MCH mole fraction) residual for the second model.

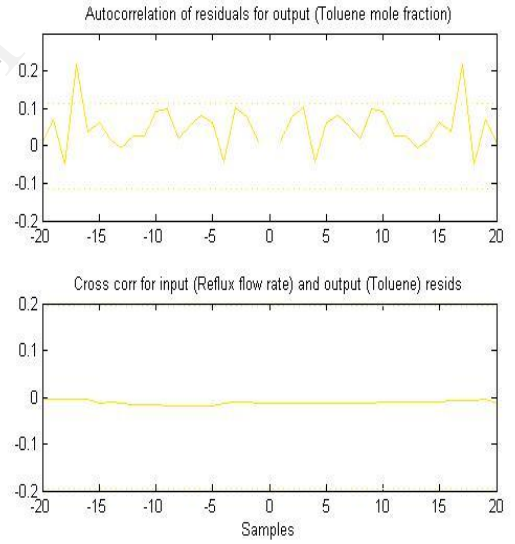

Figure 12. Autocorrelation of Residuals for Output (Toluene mole fraction) and Cross Correlation for Input (Reflux flow rate) and Output (Toluene mole fraction) residual for the second model.

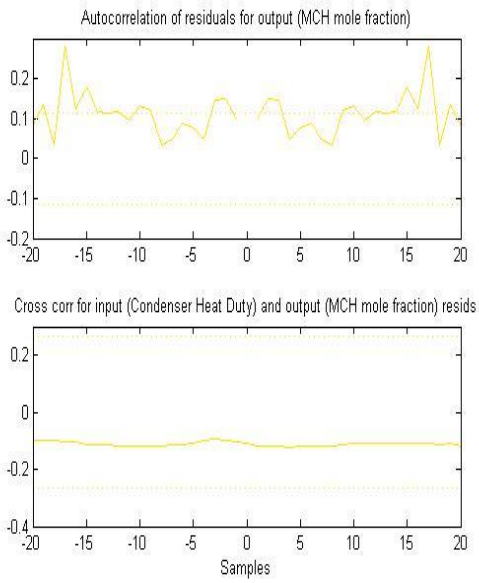

Figure 13. Autocorrelation of Residuals for Output (MCH mole fraction) and Cross Correlation for Input (Condenser Heat Duty) and Output (MCH mole fraction) residual for the second model.

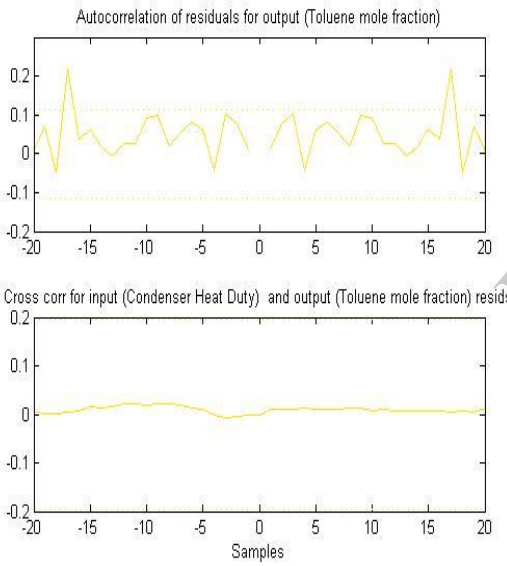

Figure 14. Autocorrelation of Residuals for Output (Toluene mole fraction) and Cross Correlation for Input (Condenser) and Output (Toluene mole fraction) residual for the second model.

5. CONCLUSION

It can be concluded from the obtained results that the model is able to capture the relationship between the mole fractions of methylcyclohexane produced from the top product and toluene from the bottom product and that of the solvent and mixture which are the inputs to the system

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