

# Decoupling Model Predictive Control of a Reactive Packed Distillation Column

Abdulwahab Giwa<sup>1</sup> and Süleyman Karacan<sup>1</sup>

<sup>1</sup>Department of Chemical Engineering, Faculty of Engineering, Ankara University, Tandoğan, 06100, Ankara, Turkey  
[agiwa@ankara.edu.tr](mailto:agiwa@ankara.edu.tr), [karacan@eng.ankara.edu.tr](mailto:karacan@eng.ankara.edu.tr)

## Abstract

*In this work, the applications of decouplers in the temperature control of a reactive packed distillation column has been carried out using two different types of controller models. The controller models used were neural network model and transfer function model. The production of ethyl acetate (desired product) and water (by-product) from the esterification reaction between acetic acid and ethanol in the presence of Amberlyst 15 solid catalyst was used as the case study process. The neural network and the transfer function models were developed respectively with the aid of Neural Network Toolbox and System Identification Toolbox of MATLAB by using the data generated from the experimental studies carried out in the reactive packed distillation column setup. Top segment temperature, reaction segment temperature and bottom segment temperature were selected as the controlled variables while reflux ratio, feed ratio and reboiler duty were chosen as the manipulated variables of the control system. After the control simulation, the results obtained showed that the performance of the Neural Network Decoupling Model Predictive Controller (NNDMPC) was better than that of the Transfer Function Decoupling Model Predictive Controller (TFDMPC) because the integral squared error values calculated for the top segment and reaction segment temperatures for the NNDMPC were found to be lower than those of the TFDMPC.*

**Keywords:** Reactive distillation, Neural Network, System Identification, Decoupling Model Predictive Control, MATLAB/Simulink, Esterification

## 1. Introduction

In recent years, integrated reactive separation processes have attracted considerable attentions in both academic research and industrial applications (Völker et al., 2007). One of these processes, known as reactive distillation, is potentially attractive whenever conversion is limited by reaction equilibrium (Giwa and Karacan, 2012a). Reactive distillation is a process that combines both separation and chemical reaction in a single unit. It combines the benefits of equilibrium reaction with distillation to enhance conversion provided that the product of interest has the highest or the lowest boiling point (Giwa and Karacan, 2012b). It has a lot of advantages especially for those reactions occurring at temperatures and pressures suitable for the distillation of the resulting components (Giwa and Karacan, 2012c). Its advantages include: a) shift of chemical equilibrium and an increase of reaction conversion by simultaneous reaction and separation of products, b) suppression of side reactions and c) utilization of heat of reaction for mass transfer operation. These synergistic effects may result in significant economic benefits of reactive distillation compared to a conventional design. These economic benefits include: a) lower capital investment, b) lower energy cost and c) higher product yields (Moritz and Hasse, 1999). Though there are many economic benefits of reactive distillation, the combination of both reaction and separation in a single unit which has made the design and modelling of the process very challenging (Giwa and Karacan, 2012d) has also made the control of the process very tasking.

The control of reactive distillation has received some attentions only recently. Sneesby et al. (1997) worked on the dynamic simulation and control aspects of reactive distillation for the synthesis of ethyl tert-butyl ether and presented general recommendations for the control of the reactive column of this type including the need for addressing the control issues early in the design process. Bock et al. (1997) developed a control structure for a reactive column with a recovery column by analysing the reaction column's steady state and dynamic sensitivity of possible disturbances and manipulated variables. Sneesby et al. (1999) used an ethyl tert-butyl ether reactive distillation column as a case study to show how a two-point control configuration, which recognized the importance of both composition and

conversion, can be developed and implemented for a reactive distillation process. Kumar and Daoutidis (1999) studied the dynamic behaviour and control of an ethylene glycol reactive distillation column by deriving a detailed tray-by-tray model that explicitly included the vapor-phase balances. They developed a nonlinear controller that yielded good performance with stability in the high-purity region with the aid of a physical insight into the nonminimum phase behaviour, and the superior performance of the developed controller over linear PI controllers was demonstrated through simulations. Monroy-Loperena et al. (2000) also studied the control problem of an ethylene glycol reactive distillation column with the control objective of regulating the ethylene glycol composition in the product by manipulating the reboiler boil-up ratio. They proposed a new idea for robust stabilization based on an analysis of the underlying input/output bifurcation diagram and on modelling error compensation techniques. Al-Arfaj and Luyben (2000) explored the closed-loop control of a reactive distillation column with two products and discovered that single-end temperature control could keep both products at or above specified purity values, even for large disturbances, if reactive-zone holdup was sufficiently large. Vora and Daoutidis (2001) studied the dynamics and control of an ethyl acetate reactive distillation system and designed model-based linear and nonlinear state feedback controllers, along with conventional SISO PI controllers. They demonstrated the superior performance of the nonlinear controller over both the linear controller and the conventional PI controller. Grüner et al. (2003) applied asymptotically exact input/output-linearization to an industrial reactive distillation column and found through simulation studies that, in comparison with a well-tuned linear controller, the controller showed a superior performance with respect to set-point changes and disturbances, even in the presence of unknown input delays. Khaledi and Young (2005) investigated the nonlinearity of an ethyl tert-butyl ether reactive distillation column and developed a 2 x 2 unconstrained model predictive control scheme for product purity and reactant conversion control by using the process dynamics approximated by a first-order plus dead time model to estimate the process model for the model predictive controller. They found that the controller was very efficient for disturbance rejection and set-point tracking. Völker et al. (2007) designed a multivariable controller for a medium-scale semi-batch reactive distillation column and showed experimentally that the controller performed well for large set-point changes and in the face of process disturbances.

Reactive distillation is a multi-input multi-output (MIMO) system and, based on that, the system is expected to be controlled as a MIMO type or using one of the early approaches to multivariable control which is "loop decoupling". Loop decoupling can be realized by adding additional controllers called decouplers to a conventional multi-loop configuration. In principle, decoupling control schemes can provide two important benefits (Seborg et al., 2004):

- (i) Elimination of control loop interactions which result in the stability of the closed-loop system being determined solely by the stability characteristics of the individual feedback control loops.
- (ii) A set-point change for one controlled variable having no effect on the other controlled variables.

Considering the two points highlighted above, it is expected that decoupling control should provide good performance in the control of chemical systems especially in the case of MIMO systems like the reactive packed distillation process being considered in this work. Therefore, the aim of this work is to apply decoupling model predictive control for set-point tracking control of top segment, reaction segment and bottom segment temperatures of reactive packed distillation column. The production of ethyl acetate and water (by-product) from the esterification reaction between acetic acid and ethanol was used as the case study process. Temperatures of the segments were controlled in this work because temperature control in a reactive distillation system is an indirect way of controlling composition and the fact is that composition is a function of temperature and vice-versa. Any change in temperature is always accompanied with a corresponding change in composition. Due to the fact that composition is always difficult to control directly online, owing to the large delay time involved in chromatographic analysis of the components, it is normally inferentially controlled by controlling the temperature.

## **2. Procedures**

The procedures used to accomplish this work are as outlined below.

### **2.1. Experimental procedure**

The process involved in this work was an esterification reaction occurring simultaneously with distillation operation that were carried out in the reactive packed distillation column (RPDC) set up as shown pictorially in Figure 1a and schematically in Figure 1b. The column, excluding the condenser

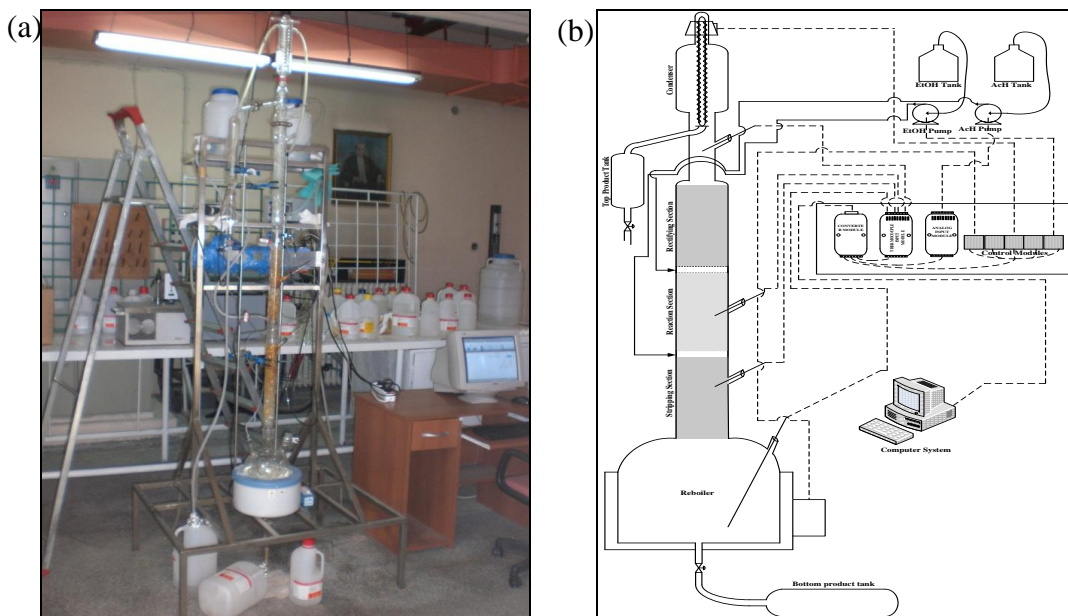
and the reboiler, had a height of 1.5 m and a diameter of 0.05 m. It consisted of a cylindrical condenser with a diameter and a height of 5 and 22.5 cm respectively. The main column section of the plant was divided into three subsections of 0.5 m each. The upper, middle and lower sections were the rectifying, the reaction and the stripping sections respectively. The rectifying and the stripping sections were packed with raschig rings while the reaction section was filled with Amberlyst 15 solid catalyst that had a surface area of 5300 m<sup>2</sup>/kg, a total pore volume of 0.4 cc/g and a density of 610 kg/m<sup>3</sup>. The reboiler was spherical in shape with a volume of 3 Liter. The column was fed with acetic acid at the top (between the rectifying and the reaction sections) while ethanol was fed at the bottom (between the reaction and the stripping sections) with the aid of peristaltic pumps which were operated with the aid of a computer via MATLAB/Simulink program. All the signal inputs (reflux ratio (R), feed ratio (F) and reboiler duty (Q)) to the column and the measured outputs (top segment temperature (T<sub>top</sub>), reaction segment temperature (T<sub>rxn</sub>) and bottom segment temperature (T<sub>bot</sub>)) from the column were sent and recorded respectively on-line with the aid of MATLAB/Simulink computer program and electronic input-output (I/O) modules that were connected to the equipment and the computer system. The esterification reaction occurring in the column was an equilibrium type given as:



Two different types of experiments were carried out to generate two different sets of data. The first data set was used for the development of MIMO transfer functions which were used as the process models while the second one was used for the development of neural network models and SISO transfer function models that were used as the controller models. The conditions used in carrying out the experiments are as shown in Table 1.

**Table 1.** Experimental conditions

Parameter	Experiment 1			Experiment 2		
	Signal Type	Initial	Final	Signal Type	Initial	Final
Reflux ratio (R)	Step	3	5	PRBS	1	5
Feed ratio (F <sub>a</sub> /F <sub>e</sub> )	PRBS	0.5	2	PRBS	1	2
Reboiler duty (Q, kJ/s)	PRBS	0.595	0.63	PRBS	0.49	0.63



**Figure 1.** Reactive packed distillation column: (a) Pictorial view; (b) Sketch view

## 2.2. System identification procedure

With the three (3) inputs (reflux ratio, feed ratio and reboiler duty) and three (3) outputs (top segment temperature, reaction segment temperature and bottom segment temperature) chosen as the variables of this process, the results obtained from the experimental studies (experiment 1) were used to develop the MIMO transfer function models of the process with the aid of System Identification Toolbox of MATLAB (Mathworks, 2011). The forms of the MIMO process models developed are as given in Equations (2 - 4) below.

$$T_{top}(s) = \frac{k_{p_{1,1}} e^{(-T_{d_{1,1}}s)}}{\tau_{1,1}s + 1} R(s) + \frac{k_{p_{1,2}} e^{(-T_{d_{1,2}}s)}}{\tau_{1,2}s + 1} F(s) + \frac{k_{p_{1,3}} e^{(-T_{d_{1,3}}s)}}{\tau_{1,3}s + 1} Q(s) \quad (2)$$

$$T_{rxn}(s) = \frac{k_{p_{2,1}} e^{(-T_{d_{2,1}}s)}}{\tau_{2,1}s + 1} R(s) + \frac{k_{p_{2,2}} e^{(-T_{d_{2,2}}s)}}{\tau_{2,2}s + 1} F(s) + \frac{k_{p_{2,3}} e^{(-T_{d_{2,3}}s)}}{\tau_{2,3}s + 1} Q(s) \quad (3)$$

$$T_{bot}(s) = \frac{k_{p_{3,1}} e^{(-T_{d_{3,1}}s)}}{\tau_{3,1}s + 1} R(s) + \frac{k_{p_{3,2}} e^{(-T_{d_{3,2}}s)}}{\tau_{3,2}s + 1} F(s) + \frac{k_{p_{3,3}} e^{(-T_{d_{3,3}}s)}}{\tau_{3,3}s + 1} Q(s) \quad (4)$$

Furthermore, the forms of the three SISO transfer function models, which were used as the controller models, also developed using the System Identification Toolbox, between the individual input and the corresponding output are as outlined in Equations 5, 6 and 7 below respectively for the top segment temperature and reflux ratio, the reaction segment temperature and feed ratio and the bottom segment temperature and reboiler duty.

$$T_{top}(s) = \frac{k_{p_1} e^{(-T_{d_1}s)}}{\tau_1s + 1} R(s) \quad (5)$$

$$T_{rxn}(s) = \frac{k_{p_2} e^{(-T_{d_2}s)}}{\tau_2s + 1} F(s) \quad (6)$$

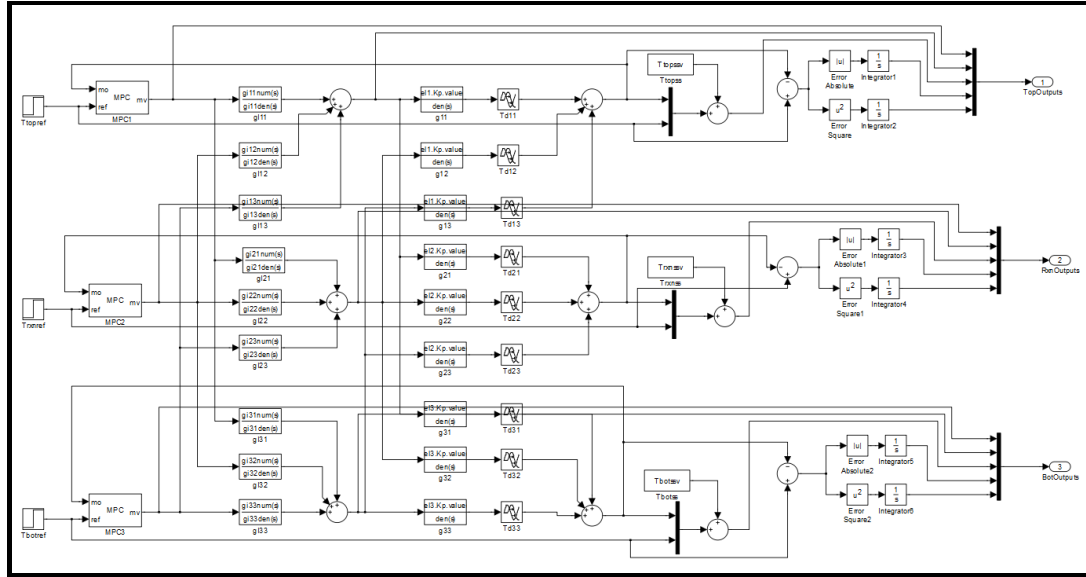
$$T_{bot}(s) = \frac{k_{p_3} e^{(-T_{d_3}s)}}{\tau_3s + 1} Q(s) \quad (7)$$

The formulation of the neural network models for the controllers can be found in Giwa and Karacan (2012a).

## 2.3. Control configuration and simulation procedure

In the control aspect of this work, the top segment temperature, the reaction segment temperature and the bottom temperature were selected as the controlled variables while the reflux ratio, the feed

ratio and the reboiler duty were chosen as the manipulated variables of the MIMO system. Decoupling the MIMO system by applying the decouplers estimated from the process models, the system was controlled like three different SISO systems. After the decoupling, for the control study, the reflux ratio, the feed ratio and the reboiler duty were used as the manipulated variables of the top segment temperature, the reaction segment temperature and the bottom segment temperature respectively. The control study was accomplished with the aid of MATLAB/Simulink (Mathworks, 2011). The Simulink algorithm used for this study is as shown in Figure 2.



**Figure 2.** Simulink algorithm of decoupling MPC of RPDC

In this work, two different control algorithms were simulated. The first one used neural network models as the controller models and it was referred to as Neural Network Decoupling Model Predictive Control (NNDMPC) while the other one used transfer function models as the controller models and it was referred to as Transfer Function Decoupling Model Predictive Control (TFDMPC). In designing the model predictive controllers, the number of prediction horizons and the number of control horizons used were 25 and 5 respectively.

## 2.4. Decoupling procedure

The decouplers used in this work for the decoupling control of reactive packed distillation column were estimated using the relationship shown in Equation (8) below and with reference to Equations 2, 3 and 4.

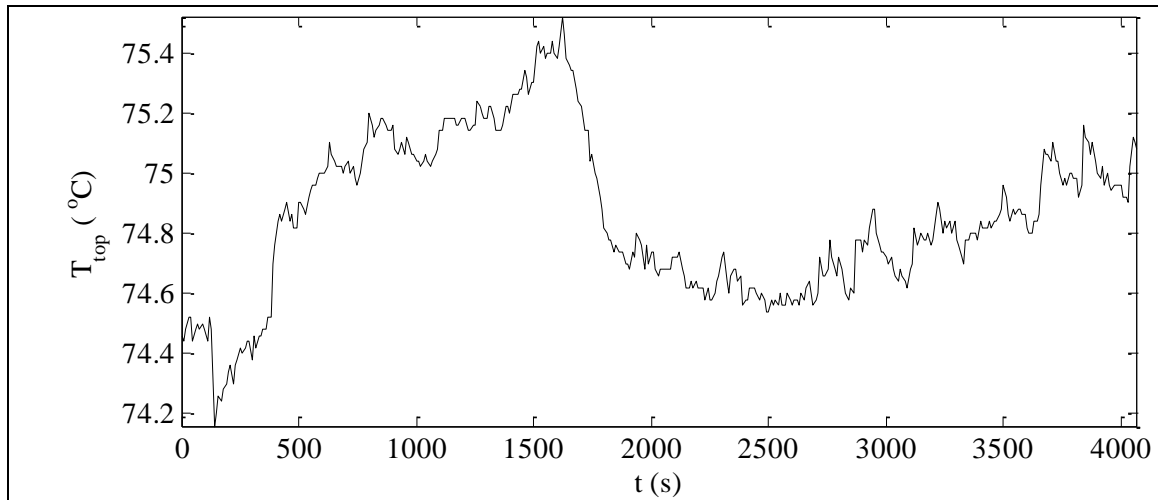
$$D = \begin{bmatrix} k_{p11} & k_{p12} & k_{p13} \\ k_{p21} & k_{p22} & k_{p23} \\ k_{p31} & k_{p32} & k_{p33} \end{bmatrix}^{-1} \quad (8)$$

### 3. Results and discussions

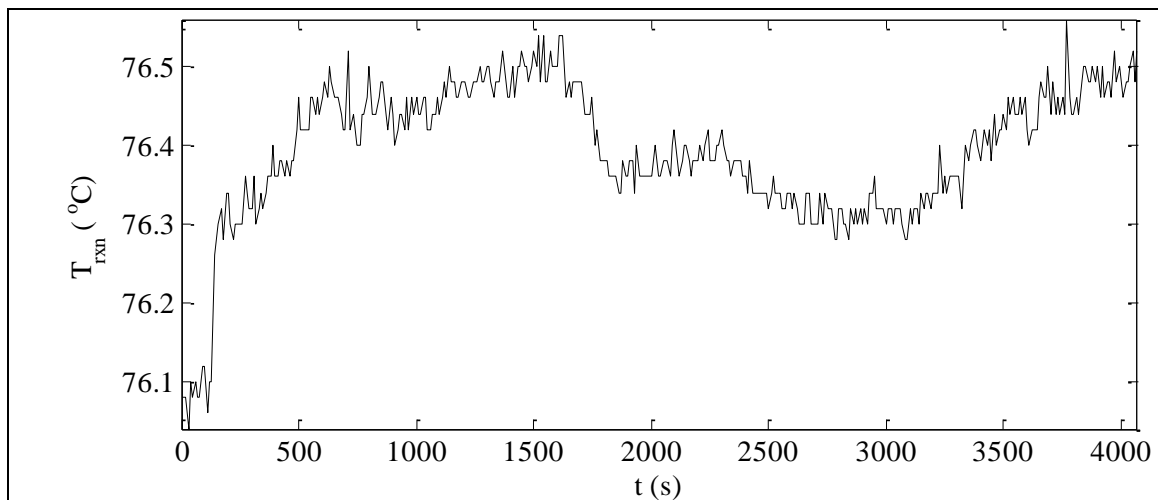
The results obtained from the experimental and the simulation studies of this work are shown and discussed thus.

#### 3.1. Experimental studies

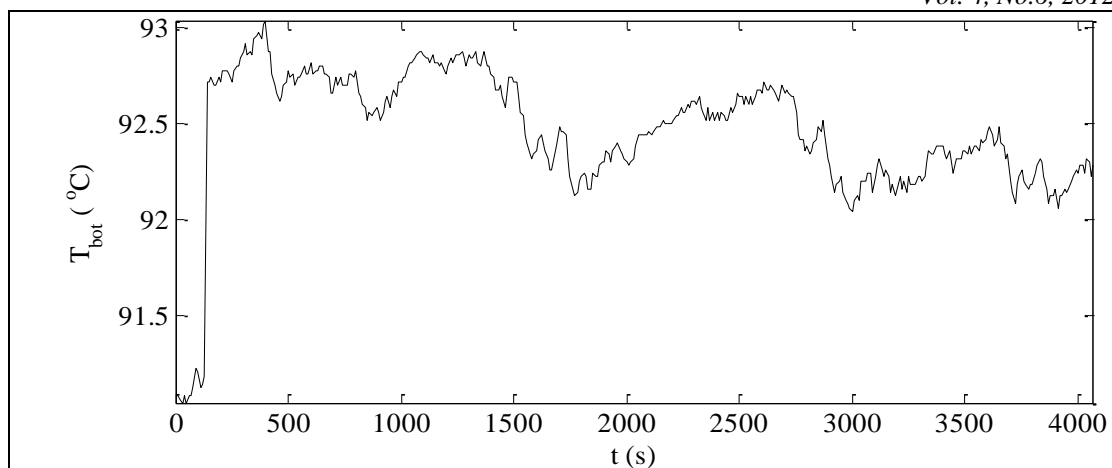
In the experimental studies, after applying the inputs shown in Table 1, the response obtained from experiment 1 are as shown in Figures 3, 4 and 5 below for the top segment temperature, the reaction segment temperature and the bottom segment temperature respectively. As can be observed from the results, the application of the inputs resulted in changes in the dynamic responses of the segment temperatures. This is an indication that the segment temperatures are functions of the inputs. This is, of course, the reason for choosing the inputs as the manipulated variables of the control of this process.



**Figure 3.** Experimental dynamic response of top segment temperature to the inputs of experiment 1

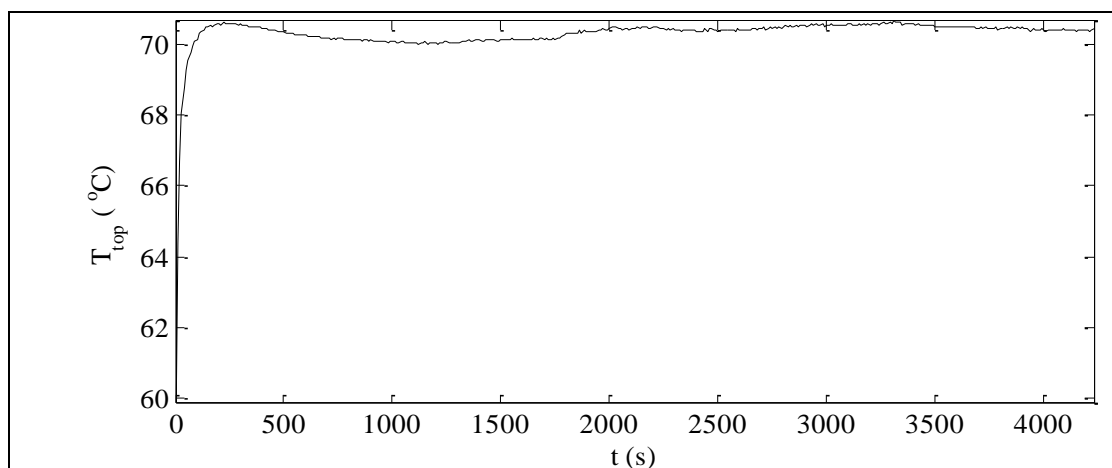


**Figure 4.** Experimental dynamic response of reaction segment temperature to the inputs of experiment 1

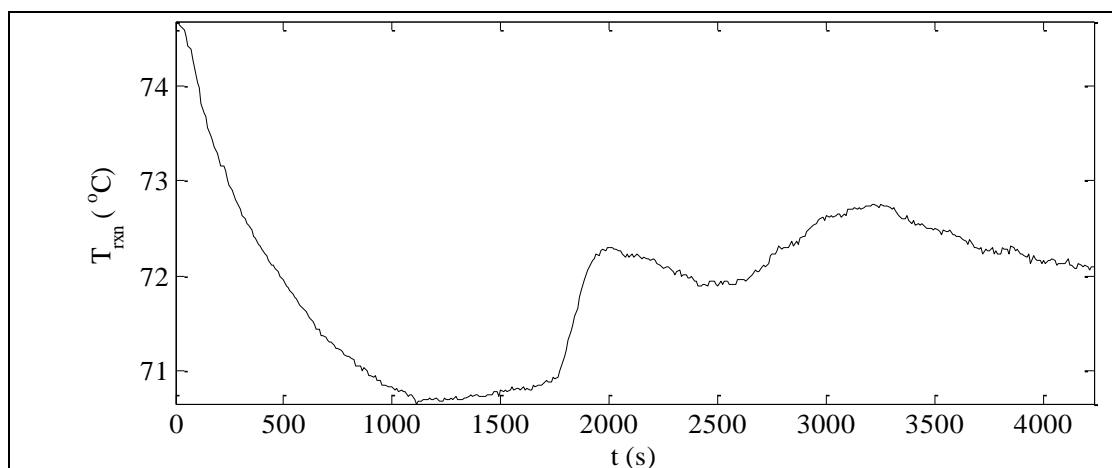


**Figure 5.** Experimental dynamic response of bottom segment temperature to the inputs of experiment 1

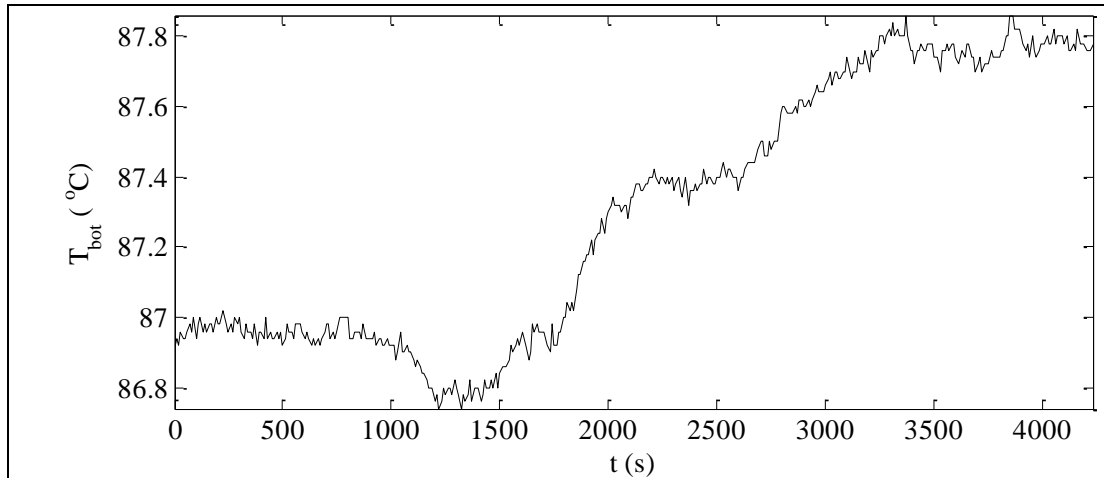
Furthermore, the application of the inputs of experiment 2, also given in Table 1, resulted in the responses given in Figures 6, 7 and 8 respectively for the top segment, the reaction segment and the bottom segment temperatures. As was observed in the case of Experiment 1, there were significant dynamic responses towards the individual inputs for each of the segment temperatures.



**Figure 6.** Experimental dynamic response of top segment temperature to the inputs of experiment 2



**Figure 7.** Experimental dynamic response of reaction segment temperature to inputs of experiment 2



**Figure 8.** Experimental dynamic response of bottom segment temperature to the inputs of experiment 2

### 3.2. System identification studies

The values of the model parameters shown in Equations (2 - 4) above are as given in Table 2. It can be seen from the model parameters that while some static gains ( $K_p$ ) were positive, others were negative. The static-gain sign change observed in the models is one of the phenomena occurring as a result of the complex nature of the reactive packed distillation process. Also, it was observed that the maximum static gain occurred between input 2 and output 2 (that is, between the feed ratio and the reaction segment temperature).

**Table 2.** Process model parameters

Transfer function	$K_p$	$\tau$ (s)	$T_d$ (s)
$g_{11}$	-79.3210	330.2110	0.0552
$g_{12}$	-1.3652	311.0872	29.7532
$g_{13}$	-89.1061	310.1599	0.1070
$g_{21}$	31.9472	507.9150	29.3428
$g_{22}$	427.8996	315.9785	0.5421
$g_{23}$	-18434.8989	317.4466	0.5411
$g_{31}$	-739.4685	2138.5997	0.0005
$g_{32}$	6.7914	60.3371	29.9644
$g_{33}$	-231.1889	47.4288	30.0000

Considering the time constant ( $\tau$ ) of the process, the transfer function of the relationship between the reflux ratio and the bottom segment temperature was found to possess the highest value. This is an indication of the fact that when the same input unit is applied to the process, this part of the process is likely to have the highest effect on the time required for the process to get to the steady state.

As can be seen from the values of the delay time ( $T_d$ ) also shown in Table 2 above, the maximum delay time possessed by the system was found to be 30 s. This means that the output variables of the reactive packed distillation studied in this work were responding quickly to changes in the input variables.

The results of Experiment 2 were similarly used to develop the SISO transfer function models that were used to design the model predictive controllers. The parameters of the SISO transfer functions shown in Equations 5, 6 and 7, calculated with the aid of MATLAB, are as shown in Table 3 below.



**Table 3.** Control model parameters

Transfer function	$K_p$	$\tau$ (s)	$T_d$ (s)
$g_1$	23.6436	9908.6647	20.3652
$g_2$	47.7977	1136.2326	7.6296
$g_3$	173.0116	34771.5505	12.7033

According to the results shown in Table 3, the model with the highest static gain and time constant was discovered to be that of the bottom segment temperature. This is revealing that, especially when this system is simulated as a SISO type, the reboiler must be heated for a long time before the bottom segment temperature can response. That is, the reboiler heat must be applied to the system for a long time before the liquid mixture will be boiled and thereby evaporated to the top segment of the column via the reaction segment. This phenomenon was actually observed during the experimental studies and found to be so.

### 3.3. Decouplers

Using the process models shown in Equations 2, 3 and 4, the decouplers were obtained to be

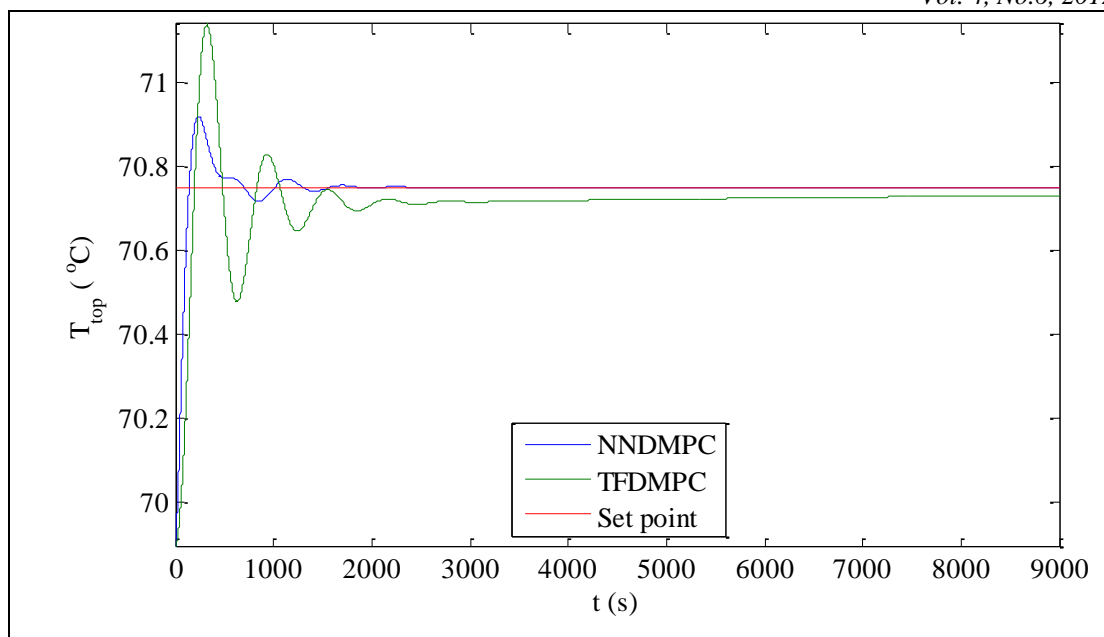
$$D = \begin{bmatrix} -0.00053709 & 1.8823e-005 & -0.0012939 \\ -0.27882 & 0.00097208 & 0.02995 \\ -0.0064727 & -3.1649e-005 & 0.00069294 \end{bmatrix} \quad (9)$$

The applications of the decouplers to the system resulted in the elimination of the effects of interactions among the variables involved in the control of the MIMO reactive packed distillation column. Thus, the control of the MIMO system was accomplished like that of SISO systems. This made the control of the column easier and more efficient, as can be seen from the results of the control studies outlined and discussed below.

### 3.4. Control studies

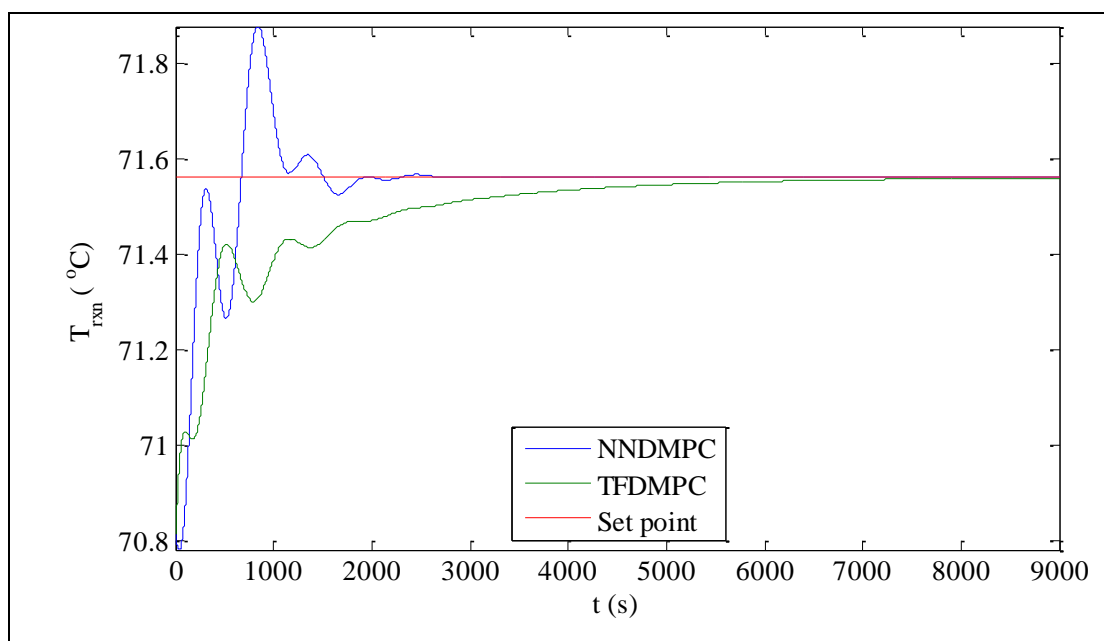
The control system of this study was simulated with the aim of raising the steady state value (69.89 °C) of the top segment temperature to 70.75 °C because that is the temperature at which high composition of ethyl acetate can be obtained from the system. In addition, the reaction segment temperature and bottom segment temperature were simulated by applying 0.75 and 1 step units to their steady state values of 70.81 and 87.97 °C respectively. The results obtained from the simulation of the control system of this work are as shown in Figures 9 – 11.

As can be observed from Figure 9, when neural network model was used as the control model, the response of the top segment temperature was able to get to the set point within 30 minutes. Also seen from the figure (Figure 9), when the transfer function model predictive control system was simulated, the top segment temperature was able to get stabilized but there was an offset. In fact, apart from the fact that there was an offset in the response obtained from the Transfer Function Decoupling Model Predictive Control (TFDMPC), its overshoot was observed to be higher than that of the Neural Network Decoupling Model Predictive Control (NNDMPC). At this point, the better performance of the neural network model for the control of top segment temperature can be clearly seen.



**Figure 9.** Dynamic responses of top segment temperature to a set-point change from 69.89 °C to 70.75 °C

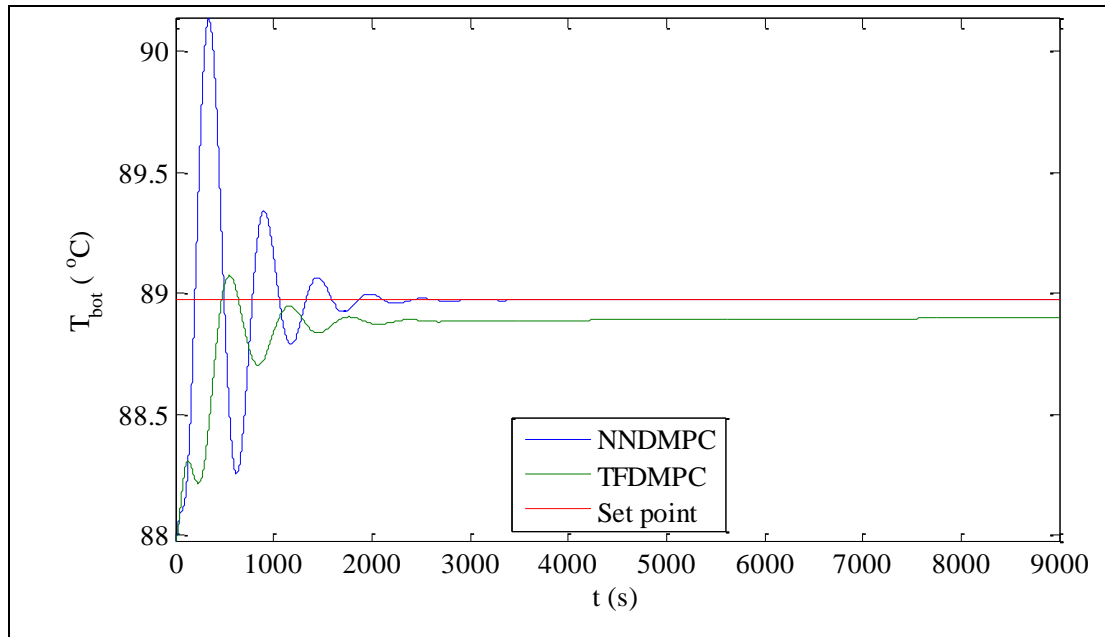
Shown in Figure 10 is the response of the reaction segment temperature for the control systems (NNDMPC and TFD MPC). As can be seen from the figure, even though the two methods were able to take the reaction segment temperature to the desired set point, the response of the TFD MPC was found to be very sluggish as compared to that of the NNDMPC.



**Figure 10.** Dynamic responses of reaction segment temperature to a 0.7 unit set-point change

Figure 11 shows the response of the bottom segment temperature for both the Neural Network Decoupling Model Predictive Control and the Transfer Function Decoupling Model Predictive Control. As can be observed from the figure, while the response of the NNDMPC was able to reach the set point

within 45 minutes, that of the TFDMPMC could not get there. The offset encountered in the case of the TFDMPMC of the bottom segment temperature can be vividly seen in Figure 11.



**Figure 11.** Dynamic responses of bottom segment temperature to a unit (1) set-point change

In order to quantitatively analyse the performances of the controllers, a performance criterion was calculated for each of the responses. The performance criterion used in this study is the Integral Squared Error (ISE). The criterion (ISE) was calculated with the aid of Simulink blocks incorporated into the control system developed in Simulink. The results obtained from the ISE calculations are as shown in Table 4 below.

**Table 4.** Performances of the controllers

Method	ISE Values		
	Top segment	Reaction segment	Bottom segment
NNDMPC	37.97	120.00	404.26
TFDMPMC	109.71	150.29	270.08

As can be seen from the results shown in Table 4, the ISE values of NNDMPC was discovered to be lower than those of the TFDMPMC for the top segment and reaction segment temperatures that are the important variables of the process. This has actually shown the better performance of neural network models over transfer function models in the control of reactive packed distillation column.

## 4. Conclusion

The results obtained from the simulations of Neural Network Decoupling Model Predictive Control and Transfer Function Decoupling Model Predictive Control of the reactive packed distillation column for the production of ethyl acetate have revealed that the integral squared error of the top segment and reaction segment temperatures of the NNDMPC were lower than those of the TFDMPMC. Therefore, it has been discovered that the Neural Network Decoupling Model Predictive Controller was able to control the process better than the Transfer Function Decoupling Model Predictive Controller.

## 5. Acknowledgements

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## 6. Nomenclatures

$\tau$	Time constant of the process (s)
AcH	Acetic Acid
EtOH	Ethanol
F	Feed ratio ( $\text{mL s}^{-1}$ of acetic acid feed rate / $\text{mL s}^{-1}$ of ethanol feed rate)
$F_a$	Acetic acid feed rate ( $\text{mL/s}$ )
$F_e$	Ethanol feed rate ( $\text{mL/s}$ )
ISE	Integral Squared Error
$K_p$	Static gain of the process
MIMO	Multi-Input Multi-Output
NNDMPC	Neural Network Decoupling Model Predictive Control
PRBS	Pseudo-Random Binary Sequence
Q	Reboiler duty ( $\text{kJ/s}$ )
R	Reflux ratio
RPDC	Reactive Packed Distillation Column
SISO	Single-Input Single-Output
t	Time (s)
$T_{\text{bot}}$	Bottom segment temperature ( $^{\circ}\text{C}$ )
$T_d$	Time delay of the process (s)
TFDMPC	Transfer Function Decoupling Model Predictive Control
$T_{\text{rxn}}$	Reaction segment temperature ( $^{\circ}\text{C}$ )
$T_{\text{top}}$	Top segment temperature ( $^{\circ}\text{C}$ )

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## Authors Profile



**Abdulwahab Giwa** received his B.Eng. degree from Federal University of Technology, Minna, Nigeria in 2004 with First Class Division. He won the Nigerian Society of Engineers (Minna Branch) award for the Best Student in Chemical Engineering Department and the Vice Chancellor's Prize for the Best Student in School of Engineering and Engineering Technology, Federal University of Technology, Minna, Nigeria in 2004. This author also won the Nigerian Society of Engineers (Minna Branch) for the Best Project in the School of Engineering and Engineering Technology, Federal University of Technology, Minna in 2004. He is, at present, working towards Ph.D. degree in Process Systems Engineering at the Department of Chemical Engineering, Ankara University, Turkey.



**Dr. Süleyman Karacan** received his Ph.D. degree from Ankara University, Turkey in 1997. He is a member of Union of Chambers of Turkish Engineers and Architects. He is currently working as a Professor at the Department of Chemical Engineering, Ankara University, Turkey. He is having overall teaching experience of 12 years. His major research interests are in Reactive Distillation, Modelling, Process Control, and Simulation.