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Application of model predictive control and dynamic analysis to a pilot distillation column and experimental verification

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Abstract

The steady-state and dynamic behaviour of a binary packed distillation column have been simulated using a stagewise approach. The model solutions have been obtained employing modified equilibrium including efficiency and non-equilibrium transfer unit. This work compares an experimental and a theoretical analysis of the steady-state and dynamic behaviour of a packed distillation column using a 0.08 m ID pilot-scale tower distilling a mixture of methanol–water. The packed distillation column was divided into four stages based on McCabe–Thiele method. For control studies, reflux ratio was chosen as a manipulated variable, so the effect of the perturbation on reflux ratio to the overhead temperature was examined. Theoretical and experimental results were compared in order to see the validity of the stagewise approximation. The application of two types of model based control system was considered theoretically, viz PID and dynamic matrix control (DMC). First-order plus dead time model and convolution model were used for step test in the control applications. Performance of these control systems were tested using control performance criterion. These control systems were also compared with open-loop dynamic behaviour and each other.

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1. Introuction

Packed columns are modelled normally by employing one of the two alternative approaches. The first one consists of dividing the packing into various mass transfer sections, each being treated as equivalent to a theoretical stage in a plate column. The corresponding algorithms for stagewise systems can then be applied. This method is of course only as convenient as the ability to obtain an independent characterization of the height equivalent of a theoretical plate (HETP). This is a widely used approach, principally due to its ease of application and the considerable quantity of relevant data available in the literature [1].

The second technique involves the use of the average vapour-phase mass fluxes of each component and solving the resulting sets of differential equations directly [2,4]. The

latter may be achieved by using a finite difference approach, polynomial estimation techniques or orthogonal collocation on finite element methodologies. Karacan et al. [22,23] investigated the steady-state and dynamic properties of a pilot plant packed distillation column experimentally and theoretically. In the theoretical work, a back-mixing model was adapted to simulate the dynamic properties of the continuous packed distillation column with a thermosiphon reboiler and solved by orthogonal collocation on finite element. These all involve a discretization of the basic continuum problem in which the infinite set of numbers describing the unknown functions is replaced by a finite number of unknown parameters, and this process, in general, necessitates some form of approximation. The finite difference method is generally the simplest to apply and thus is favoured by many workers.

In this work, the models are described as a set of ordinary differential equations in which the height of the column is divided into a number of stages. Peters [10] first suggested the use of the concept of the HETP and Chilton and Colburn [11] proposed the height of transfer unit (HTU) approach in the investigation of the mass transfer operations.

Rubac et al. [12] suggested the use of vaporization efficiencies in the modelling of packed columns. These vaporization efficiencies involve an integrating concept which

Abbreviations: DMC, dynamic matrix control; ID, internal diameter; IV, vapour flow; IMC, internal model control; ISE, integral of the square of the error; LF, feed flow; LI, liquid flow; LO, liquid out; LOK, liquid flow from the small reboiler to the big reboiler; LOB, liquid flow from the big reboiler to the small reboiler; MPC, model predictive control; NP, prediction horizon; NC, control horizon

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Tomenciature							
$a_{\rm L}, b_{\rm L}$	the coefficients of specific heat						
A_i, B_i, C_i	<i>i</i> th component Antoine coefficient						
В	bottom flow rate (mol min $^{-1}$)						
D	top product flow rate (mol min $^{-1}$)						
$E_n^{\rm L}$	Murphree liquid phase efficiency						
F	feed flow rate (mol min $^{-1}$)						
$h_{ m L}$	liquid phase enthalpy (cal min $^{-1}$)						
$H_{ m V}$	vapour phase enthalpy (cal mol ⁻¹)						
k	component number						
$K_{n,i}$	equilibrium K values						
L	liquid flow rate (mol min ^{-1})						
Μ	molar holdup (mol)						
Ν	number of stages in column						
p_{T}	total pressure (Pa)						
Q_{R}	reboiler heat duty (cal min $^{-1}$)						
R	reflux ratio						
S	Laplace operator						
t	time (min)						
t_0	dead time (min)						
Т	temperature (°C)						
$T_{\rm D}$	top product temperature (°C)						
и	controller output						
V	vapour phase flow rate (mol min $^{-1}$)						
<i>x</i> _D	top product mole fraction						
x_i	<i>i</i> th component liquid mole fraction						
У	system output						
Уі	<i>i</i> th component vapour mole fraction						

results in numerical procedures for packed columns which are identical to those for plate columns. Furthermore, the vaporization efficiencies supply relationship between the HTU and the HETP. Holland et al. [13] have suggested unifying computational procedures for packed and plate columns utilizing the concept of vaporization efficiencies. Kisakürek and Sümer (1984) [24] proposed a general dynamic model for packed distillation column which transforms the packed column into its equivalent stagewise representation. They suggested that the problems of transforming a packed distillation column into its plate equivalent are principally one of locating the feed plate, determining the number of mass transfer sections and specifying the set of efficiency coefficients such that the deviation of each calculated overhead product composition from its corresponding experimental value is minimized. These researches found that six mass transfer sections were sufficient for all their runs and that there was good agreement between theory and experiment. Fieg et al. [14] compared an experimental and a theoretical analysis of the steady-state and dynamic behaviour of packed columns using a 0.07 m ID pilot-scale distillation column distilling mixtures of C₁₂, C₁₄, and C₆, C₈, C₁₀, C12 fatty acids. The column was packed with two types of commercial packing obtained from Suzer Chemtech,

Winterthur, Switzerland. The packing was arranged in 0.5 m high sections.

The conventional method of controlling processes is to apply a multiplicity of supposedly independent feedback control loops. Process control systems integrate adjustable controller settings that promote process operation over a wide range of conditions [7]. The simple three term (PID) or two term (PI) controller remains the most generally applied to industrial process controller today. This is mainly due to the ease of operations, the robustness and the lack of specific process knowledge which is required for the initial controller design. Lee [15] formulated a non-linear dynamic model and the resulting non-linear partial differential equations were solved by a finite difference procedure. The design of feedback controllers employing the reaction curve method was carried out in order to control either the distillate or bottom product compositions. Molander and Breitholtz [16] simulated the control of a packed distillation column separating a mixture of benzene and toluene. They used a simplified process model suggested by Breitholtz and Quarnström [17]. The resulting partial differential equations were integrated using orthogonal collocation in which all the functions of the concentration variables were approximated by polynomials. Since the past decade, model predictive control (MPC) has found a wide range of industrial applications, including fluid catalytic crackers, non-linear batch reactors, hydrocracker reactors, distillation columns, evaporators and other chemical processes, Patwardhan and Edgar [18] developed a strategy for the feedback control of constrained non-linear processes called non-linear MPC. Ganguly and Saraf [19] discussed the application of non-linear analytical MPC to distillation column startup between the time when the trays are hydraulically sealed and the time when steady-state operation is reached. In a novel startup method the liquid feed is initially used as reflux to seal the trays by establishing the plate holdups. Zheng and Morari [20] demonstrated how a practical control problem with multiple control/optimization objectives and various operating constraints is formulated in the theoretical framework of state estimation based on MPC. They use the shell control problem of a heavy oil fractionator as a case study. Karacan et al. [8,22] carried out studies on the experimental and theoretical application of generalized predictive control to a packed distillation column.

Cutler and Ramaker [21] described the dynamic matrix control (DMC) which permit the on-line computer solution of multivariable control problems. The general development of DMC algorithm to incorporate feed forward and multivariable control is covered in that paper.

In the present work, some studies were made on the dynamic properties of a packed distillation column. This work compared an experimental and a theoretical analysis of the steady-state and dynamic behaviour of packed columns using a pilot-scale tower distilling a mixture of methanol– water. To use reflux ratio as a manipulated variable and design modern control algorithm, system dynamics were investigated while step changes are given to reflux ratio at steady-state condition. DMC system was applied to control the top temperature. Comparison between performance of DMC and PID system was realized.

2. Mathematical model based on stagewise approach

The general mathematical model for unsteady-state binary packed distillation columns consists of a large set of simultaneous non-linear equations which should be solved to determine the phase flow rates, the liquid and vapour composition, and the temperature profiles. A simplified representation was considered to be sufficient for the present work to serve as a basis for the development of suitable controller design strategies. In establishing the model, the following assumptions have been made: (i) mixture is ideal; (ii) efficiencies in the stripping and enriching sections are constant and they include only the terms for liquid; (iii) vapour accumulation is ignored; (iv) total condenser is used; (v) column operates adiabatically; (vi) molar flooding velocity is not constant; (vii) liquid accumulation in the plates depends on time and there is perfect mixing; (viii) hydraulics of plate delay in liquid flow are simulated by using first-order differential equations; (ix) equilibrium constants used in the estimation depend on Antoine coefficients.

Two versions of the model based on the stagewise approach have been used to describe the unsteady-state and steady-state behaviour of the column.

2.1. Model I

This model is developed by Heathcock [5]. The dynamic mathematical model of the column was written for n equilibrium plates.

Component mass balance is written as:

$$\frac{\mathrm{d}(M_n x_n)}{\mathrm{d}t} = (Vy)_{n-1} + (Lx)_{n+1} - (Vy)_n - (Lx)_n \tag{1}$$

and

$$\sum_{i=1}^{\kappa} m_{n,i} = M_n \tag{1a}$$

Energy balance for a plate is written as:

$$\frac{\mathrm{d}(Mh_{\rm L})_n}{\mathrm{d}t} = (Lh_{\rm L})_{n+1} + (VH_{\rm V})_{n-1} - (Lh_{\rm L})_n - (VH_{\rm V})_n \qquad (2)$$

In the liquid phase, Murphree efficiency is described with the following equation:

$$E_{n,i}^{\rm L} = \frac{x_{n,i} - x_{n+1,i}}{x_{n,i}^* - x_{n+1,i}}$$
(3)

The full derivation of the vapour flow rate equation is shown in Eq. (4)

$$V_n(H_n - h_n - \beta_3) = L_{n+1}(h_{n+1} - h_n - \beta_1) + (V_{n-1} - h_n - \beta_2)$$
(4)

where

$$\beta_{1} = \frac{\sum_{i=1}^{k} x_{n,i} (a_{\mathrm{L},i} + 2b_{\mathrm{L},i}T) \sum_{i=1}^{k} K_{n,i} (x_{n+1,i} - x_{n,i})}{\sum_{i=1}^{k} x_{n,i} K_{n,i} B_{i} / (C_{i} + T_{n})^{2}} + \sum_{i=1}^{k} (a_{\mathrm{L},i} + b_{\mathrm{L},i}T^{2}) (x_{n+1,i} - x_{n,i})$$
(4a)

$$\beta_{2} = \frac{\sum_{i=1}^{k} x_{n,i} (a_{\mathrm{L},i} + 2b_{\mathrm{L},i}T) \sum_{i=1}^{k} K_{n,i} (y_{n-1,i} - x_{n,i})}{\sum_{i=1}^{k} x_{n,i} K_{n,i} B_{i} / (C_{i} + T_{n})^{2}} + \sum_{i=1}^{k} (a_{\mathrm{L},i} + b_{\mathrm{L},i}T^{2}) (y_{n-1,i} - x_{n,i})$$
(4b)

$$\beta_{3} = \frac{\sum_{i=1}^{k} x_{n,i} (a_{\mathrm{L},i} + 2b_{\mathrm{L},i}T) \sum_{i=1}^{k} K_{n,i} (y_{n,i} - x_{n,i})}{\sum_{i=1}^{k} x_{n,i} K_{n,i} B_{i} / (C_{i} + T_{n})^{2}} + \sum_{i=1}^{k} (a_{\mathrm{L},i} + b_{\mathrm{L},i}T^{2}) (y_{n,i} - x_{n,i})$$
(4c)

Equilibrium relationship is written using Dalton and Raoult rules and then Antoine equation was given as:

$$y_{n,i} = K_{n,i} x_{n,i}^* \tag{5}$$

$$y_{n,i} = \frac{p_{n,i}}{p_{\rm T}} = \frac{x_{n,i}}{p_{\rm T}} p_i^0$$
(6)

$$p_i^0 = \exp\left[\frac{A_i + B_i}{C_i + T_n}\right] \tag{7}$$

Last four equations are rearranged and vapour compositions are expressed as:

$$y_{n,i} = \frac{\exp[A_i + B_i / (C_i + T_n)] E_{n,i}^{L} x_{n,i}^2}{p_{T}[x_{n+1,i}]}$$
(8)

The calculations begin with the determination of the liquid compositions for all stages using Eqs. (1) and (1a). Then the vapour compositions and stage temperatures are obtained from the bubble-point equation using the well-known Newton–Raphson technique. Summary of the sequence of calculations is presented in Fig. 1.

2.2. Model II

This model was developed by Luyben [6] and modified by Cabbar [9]. In addition, some other suitable modifications were made on the model for the experimental system according to the same assumptions given in model I. Model equations are obtained for plates and top of the column separately. The equations for the reboiler are the same as in model I.

$$L_n = L_{n-1} + \frac{M_n - M_{n-1}}{\beta}$$
(9)

Stage efficiency for plate n is

$$y_n = y_{n-1} + E_{n,i}^L(y_{n-1}^* - y_{n-1})$$
(10)



Fig. 1. Flowchart of the calculation procedure for model I distillation column.

Total energy balance is

$$V_n = \frac{V_{n-1}H_{V,n-1} + L_{n+1}h_{L,n+1} - L_nh_{L,n}}{H_{V,n}}$$
(11)

Total mass balance is

$$\frac{\mathrm{d}M_n}{\mathrm{d}t} = L_{n+1} + V_{n-1} - L_n - V_n \tag{12}$$

Component mass balance is

$$\frac{\mathrm{d}(Mx)_n}{\mathrm{d}t} = (Vy)_{n-1} + (Lx)_{n+1} - (Vy)_n - (Lx)_n \tag{13}$$

The vapour compositions and stage temperatures are obtained from the bubble-point equation using the well-known Newton–Raphson technique.

The bubble-point equation is

$$\sum (K_{n,i}x_{n,i}) = 1.0 \tag{14}$$

In the liquid phase, Murphree efficiency is described with the following equation:

$$E_{n,i}^{\rm L} = \frac{x_{n,i} - x_{n+1,i}}{x_{n,i}^* - x_{n+1,i}}$$
(15)

from Eq. (15)

$$x_{n,i}^* = \frac{x_{n+1,i}(E_{n,i}^{\rm L}-1) + x_{n,i}}{E_{n,i}^{\rm L}}$$
(16)

Substituting (16) into the $(y_{n,i} = K_{n,i}x_{n,i})$

$$y_{n,i} = \frac{K_{n,i}}{E_{n,i}^{\rm L}} [x_{n,i} + x_{n+1,i} (E_{n,i}^{\rm L} - 1)]$$
(17)

but

$$y_{n,i} = \frac{p_{n,i}}{p_{\rm T}} = \frac{x_{n,i} p_i^0}{p_{\rm T}}$$
 (18)

$$\frac{x_{n,i} p_i^0}{p_{\rm T}} = \frac{K_{n,i}}{E_{n,i}^{\rm L}} [x_{n,i} + x_{n+1,i} (E_{n,i}^{\rm L} - 1)]$$
(19)

or

$$K_{n,i} = \frac{p_i^0 x_{n,i} E_{n,i}^{\rm L}}{p_{\rm T}[x_{n,i} + x_{n+1,i}(E_{n,i}^{\rm L} - 1)]}$$
(20)

Hence

$$y_{n,i} = \frac{\exp[A_i + B_i/(C_i + T_n)]E_{n,i}^{\rm L}x_{n,i}^2}{p_{\rm T}[x_{n,i} + x_{n+1,i}(E_{n,i}^{\rm L} - 1)]}$$
(21)

2.3. Reboiler plate equations

Mathematical models are developed for the thermosiphon reboiler as shown in Fig. 2 and used in the experimental system. A u connection element between the big and small reboilers is available. In this case, liquid in the u element moves into different directions between the big and small reboiler. Thus different mass component balance equations are written as follows:

a) Mass balance for the small reboiler:

When the flow direction is from the small to the big reboiler, component mass balance is

$$\frac{\mathrm{d}x_{\mathrm{LOK}}}{\mathrm{d}t} = \frac{L_{\mathrm{F}}x_{\mathrm{F}} - L_{\mathrm{LOK}}x_{\mathrm{LOK}} - V_{n-1}y_{n-1}}{HLK}$$
(22)

Mass equation for which the flow rate is from the opposite direction and then in Eq. (22)

$$\frac{\mathrm{d}x_{\mathrm{LOK}}}{\mathrm{d}t} = \frac{L_{\mathrm{LOK}}x_{\mathrm{LOK}} - L_{\mathrm{F}}x_{\mathrm{F}} - V_{n-1}y_{n-1}}{HLK}$$
(23)

b) Model equations for the big reboiler:

Mass balance where the flow direction is from the big reboiler to the small one is

$$\frac{\mathrm{d}x_{\mathrm{LOB}}}{\mathrm{d}t} = \frac{L_n x_n - L_{\mathrm{LOK}} x_{\mathrm{LOK}} - L_{\mathrm{LO}} x_{\mathrm{LO}}}{HLB}$$
(24)



Fig. 2. Reboiler section.

Mass equation for which the flow is from the opposite direction than in Eq. (24)

$$\frac{\mathrm{d}x_{\mathrm{LOB}}}{\mathrm{d}t} = \frac{L_n x_n + L_{\mathrm{LOK}} x_{\mathrm{LOK}} - L_{\mathrm{LO}} x_{\mathrm{LO}}}{HLB}$$
(25)

c) Energy equations for two reboilers can be obtained as:

$$HL\frac{dh_{\rm L}}{dt} + h_{\rm L}\frac{d(HL)}{dt} = Q_{\rm R} + L_{\rm F}h_{\rm F} + L_{\rm LI}h_{\rm L}$$
$$-L_{\rm LO}h_{\rm L} - V_{\rm IV}H_{\rm IV}$$
(26)

Packed distillation column was divided into four theoretical stages based on McCabe–Thiele method.

3. Model identification and DMC control algorithm

Several types of model representation have been used for MPC purposes. The pioneering implementation of MPC uses linear impulse response or step response model (1) and (2). These types of models are termed non-parametric models (3). The most common type of non-parametric model for MPC has been the step response model. The simplest and most intuitive way to generate this type of model is to apply a step test to the manipulated variable and compute a filtered step response model directly from the measured response data.

3.1. Model identification

The process model can be expressed as a first-order process with dead time:

$$G(s) = \frac{K_{\rm m} \,\mathrm{e}^{-t_{\rm m}s}}{\tau_{\rm m}s + 1} \tag{27}$$

where $K_{\rm m}$ represents model gain, $\tau_{\rm m}$ the process model time constant and $t_{\rm m}$ the model dead time. To obtain relevant model, the same parameters must be determined. To determine these parameters, one of the most utilized methods is the step test application. From the reaction curve obtained at the end of this test, the parameters are easily evaluated.

In the relevant method, a block diagram for open-loop step test is shown in Fig. 3. In the step test, a step change is given to the manipulated variable u(t) and then the reaction curve is obtained by observing output variable y(t) change with time. Transfer function and Laplace transform of set point, output and manipulated variables are shown below:

$$G(s) = \frac{y(s)}{u(s)} = \frac{K_{\rm m} \,{\rm e}^{-t_{\rm m} s}}{\tau_{\rm m} s + 1} \tag{28}$$

$$y(s) = \frac{K_{\rm m} \,\mathrm{e}^{-\iota_{\rm m} s}}{\tau_{\rm m} s + 1} \frac{\Delta m}{s} \tag{29}$$

Inverse Laplace transform is

$$y(t) = K_{\rm m} \Delta m \, u(t - t_{\rm m}) [1 - e^{-(t - t_{\rm m})/\tau}]$$
(30)

where $u(t - t_m)$ presents step function and system parameters of dead time t_m and time constant τ which are system parameters and are evaluated by using Smith [3] method.

In this method, to evaluate values of $t_{\rm m}$ and τ , it is necessary to select two points where the change of reaction curve is the fastest (Fig. 4). This point can be determined as follows $(t_{\rm m} + 1/3\tau_{\rm m})$ and $(t_{\rm m} + \tau_{\rm m})$. From these points

$$\tau_{\rm m} = \frac{3}{2}(t_2 - t_1)$$
 and $t_{\rm m} = t_2 - \tau_{\rm m}$ (31)

 $\tau_{\rm m}$ and $t_{\rm m}$ can be calculated using Eq. (31).

3.2. DMC

DMC is a powerful control algorithm that has been used for the design of industrial controllers. In DMC, the manipulated variable is adjusted previously and the controlled variable is influenced by these adjustments as well as by



Fig. 3. Block diagram for open-loop step response [3].



Fig. 4. Experimental equipment: (1) big vessel; (2) packed column; (3) condenser; (4) temperature converter; (5) A/D converter; (6) refluxer; (7) magnetic valve; (8) computer; (9) D/A converter; (10) transducer; (11) control valve; (12) heat exchanger; (13) rotameter; (14) feed vessel; (15) pump; (16) triyac module; (17) oil tank; (18) cooling tank; (19) small reboiler; (20) bottom product valve.

disturbances. The task of the control algorithm is to determine the future adjustments to the manipulated variable so that the controlled variable can return quickly to the set point.

The difference between the predicted values of the controlled variable and the set point are defined as the performance index J. To minimize J, the sum of the errors squared is calculated [21] as:

$$J = \sum_{i=1}^{NP} [X^{\text{set}}(k+i) - X_{\text{new}}(k+i)]^2 + f_t^2 \sum_{i=1}^{NC} [\underline{\Delta u}(k+i)]^2$$
(32)

where X_{new} is the closed-loop real response for the value at the *i*th step into the future and it is the sum of past response (X_{past}) and the future changes in the manipulated variable are

$$X_{\text{new}} = X_{\text{past}} + \sum_{k=1}^{\text{NC}} a_{ik} (\underline{\Delta u})^{\text{new}} + \underline{d}$$
(33)

or

$$X_{\text{new}} = X_{\text{past}} + \underline{A\Delta u} + \underline{d} \tag{34}$$

Here NP denotes the future time over which the control performance is evaluated and termed the output horizon. NC is the number of adjustments and is given by the input horizon. NC must be less than NP.

 \underline{A} is the dynamic matrix and it is composed of the step response coefficients as:

$$\underline{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1,\text{NC}} \\ a_{21} & \vdots & \dots & \vdots \\ \vdots & \vdots & \dots & \vdots \\ a_{\text{NP},1} & a_{\text{NP},2} & \dots & a_{\text{NP},\text{NC}} \end{bmatrix}$$
(35)

To prevent large swings in the manipulated variables, f_t weighting factor is added into the performance index. Increasing f_t increases the damping coefficient of the closed-loop system.

 X^{set} is the set point and can remain constant at its current value in the future. The goal of perfect controlled-variable performance would be to have zero error for all samples in the future. The solution to this problem is a least-square solution in the form of the following control increments:

$$\underline{\Delta u} = [\underline{A}^{\mathrm{T}}\underline{A} + f_t^2 \underline{I}]\underline{A}^{\mathrm{T}}(X^{\mathrm{set}} - X_{\mathrm{past}} - \underline{d})$$
(36)

where *I* is the identity matrix, the vector Δu is the NC values of the future changes in the manipulated variables that minimize the performance index. NP, NC and f_t are used as tuning parameters by the designer.

In the present work, the steps used in the application of the DMC algorithm may be summarized as:

i) calculate the NP values of X_{past} from the equation below

$$X_{\text{past}} = X_0^{\text{meas}} + \sum_{k=0}^{1-\text{NP}} [b_{i+1-k} - b_{i-k}] (\underline{\Delta u})^{\text{past}}$$
(37)

- ii) calculate the NC values of the future changes in the manipulated variables from Eq. (36) using the dynamic matrix <u>A</u>
- iii) implement the first change $(\Delta u)^{\text{new}}$
- iv) repeat these calculations at the next sampling time to account for changing disturbances and to incorporate feedback.

4. Experimental equipment

To check the mathematical models and solution results, a pilot plant packed column was used to distillate the binary methanol–water mixture. Physical details of the packed column used were demonstrated in Table 1. All experimental equipment were shown in Fig. 4. In the present experimental work, overhead product composition and temperature changes with time were observed at steady-state and dynamic conditions. Experimental procedure was summarised as below.

Table 1 Physical properties of packed distillation column

Packing height (mm)	1400
Inside diameter of packed column (mm)	80
Packing type	Rasching
Packing diameters (mm)	20/15
Feed tank volume (1)	60
Reboiler volume (l)	13
Heater oil volume (l)	25
Total pressure (mmHg)	690

In the initial work, the reboiler was filled with methanolwater mixture at the feed composition. When the reboiler temperature reached the boiling temperature of feed composition, cooling water was sent to the condenser. Column was operated approximately 1 h at the total reflux. In this case, there were no feed and product flows. Temperature profiles observed on the computer were recorded and samples were taken regularly from the top and bottom of the column. Absorbances of the samples were determined by using UV–visible recording spectrophotometer (UV-160A). When the absorbances and temperatures were constant, the system was at steady-state condition for total reflux.

After the system reached steady-state condition, preheated mixture was fed to the reboiler and a continuous system was obtained. At the same time, reflux ratio was adjusted to get a required value. At short time intervals, product samples were taken and their compositions were recorded. Temperature profiles were recorded by a computer and a data bank was created. When the system reached steady-state condition temperature profiles and compositions achieved constant values. After this steady-state condition was maintained, pulse or step disturbance was given to the input variables. Therefore, the system became unsteady-state again and then the second steady-state condition was observed by checking whether the temperature profiles and compositions were constant.

5. Experimental and theoretical results

In this section, experimental and theoretical results for the relevant research are given. As mentioned in the experimental part that after the system reaches the steady-state condition, a step change is given to the input variable of the system. For control and dynamic work, the magnitude of a step change is chosen as required and it is given to the reflux ratio which is selected as the manipulated variable and then the dynamic behaviour of the system is observed. DMC system properties for overhead product temperature of the column are investigated. Experimental and theoretical control work was realized when the packed column was operated under the effects of various step changes given to the input variables. In control work, reflux ratio is chosen as a manipulated variable. Step test is realized for calculating control system parameters.

5.1. Steady-state results

When the distillation column works under the steady-state condition at total reflux, reflux ratio and feed flow rate are adjusted to 3 and $4.576 \text{ mol min}^{-1}$, respectively, and then 0.153 mol methanol in mixture is fed to the column for continuos operating condition. The system works under this condition and the occurrence of the steady-state condition is waited. This steady-state condition is given in Table 2. Simulation results are compared with the experimental data and shown in the same table. It is concluded that a reasonable agreement is obtained.

5.2. Unsteady-state results

When the distillation column works at continuous steady-state condition, a negative step change from 3 to 2 is given to the reflux ratio, and then the system starts to show dynamic behaviour. After approximately 70 min, the system reaches second steady-state condition. Overhead composition and temperature are measured to determine whether

Table 2

Illustration of steady-state conditions of experimental data and simulation results from models I and II

Input and output variables of distillation column	Experimental data	Simulation results	Simulation results	
		Model I	Model II	
Feed composition, <i>x</i> _F (mole fraction)	0.153	0.153	0.153	
Top product composition, $x_{\rm D}$ (mole fraction)	0.930	0.930	0.931	
Bottom product composition, $x_{\rm B}$ (mole fraction)	0.096	0.120	0.107	
Feed flow rate, $F \pmod{\min^{-1}}$	4.576	4.576	4.53	
Top product flow rate, $D \pmod{\min^{-1}}$	0.130	0.132	0.130	
Bottom flow rate, $B \pmod{\min^{-1}}$	4.466	4.454	4.400	
Reflux ratio, R	3	3	3	
Feed temperature, $T_{\rm F}$ (°C)	62	62	62	
Bottom temperature, $T_{\rm B}$ (°C)	84.2	84.48	84.65	
Top product temperature, $T_{\rm D}$ (°C)	64.15	64.15	64.15	
Reboiler heat duty, $Q_{\rm R}$ (cal min ⁻¹)	21200	21200	21200	



Fig. 5. Response of top product concentration of methanol to a negative step change in reflux ratio from 3 to 2.

the system reaches second steady-state condition. In Figs. 5 and 6 there is a comparison of experimental and theoretical responses of compositions and top product temperature are compared in the face of a negative step change in the reflux ratio. Responses obtained from model I and model II show good agreement with experimental data as shown in Figs. 5 and 6.

The third experimental work is done by giving reflux ratio a positive step change from 3 to 5. Experimental and theoretical overhead composition and temperature profiles are compared with each other in Figs. 7 and 8.

Model identification methods were applied to experimental data from step test. Reflux ratio was used as the manipulated variable to control the top product temperature efficiently. A negative step change was given to the reflux ratio from 3 to 1 and the relevant experimental result is given in Fig. 9 for comparison with identified models. Two model identification methods based on Laplace transform are applied and theoretical results are compared with experimental data. Reaction curve shown in Fig. 9 is used to generate the model parameters and these are found as $t_{\rm m} = 4.5$ min and $\tau = 10.5$ min. Transfer function is as follows:

$$G(s) = \frac{K_{\rm m} \, {\rm e}^{-4.5s}}{10.5s + 1}$$

The result obtained from Eq. (30) is compared with experimental work shown in Fig. 9. Parameters for PID control are calculated from Cohen–Coon tuning method. These values are $K_c = 6$, $\tau_I = 3.2$ min and $\tau_D = 4.6$ min.



Fig. 6. Response of top product temperature to a negative step change in reflux ratio from 3 to 2.



Fig. 7. Response of top product concentration of methanol to a positive step change in reflux ratio from 3 to 5.

For the convolution model, the result obtained from step test is used to generate matrix A. For this purpose, similar experimental results from Fig. 9 are used. The matrix A obtained is given as:

A =	0.150	0	0	0	0	0 7
	0.235	0.150	0	0	0	0
	1.250	0.235	0.150	0	0	0
	2.350	1.250	0.235	0.150	0	0
	2.800	2.350	1.250	0.235	0.150	0
	3.070	2.800	2.350	1.250	0.235	0.150

and control design is done by using matrix A. Values of tuning parameters of DMC are varied and the best values for these parameters are determined as NP = 4, NC = 1 with using ISE criteria. Using these parameters, efficient DMC control results are obtained.

The time profiles of the controlling variable obtained from DMC system in the face of 30% step decrease and increase in feed composition are shown in Figs. 10 and 11. Control results are compared with each other using ISE criteria that the top temperature reaches to set point in a minimum time and less oscillation and it is concluded that DMC control has better performance than conventional control strategies.



Fig. 8. Response of top product temperature of methanol to a positive step change in reflux ratio from 3 to 5.



Fig. 9. Step test results.



Fig. 10. DMC and PID control of the overhead product temperature in the face of 30% step decrease in feed composition changes from 0.153 to 0.120. (a) Response of controlling variable and (b) response of manipulated variable.



Fig. 11. DMC and PID control of the overhead product temperature in the face of 30% step increase in feed composition changes from 0.153 to 0.20. (a) Response of controlling variable and (b) response of manipulated variable.

6. Discussion

At the beginning of this work, by using necessary data at the steady-state condition, packed distillation column is considered as a plate column. Number of plates is evaluated with graphical method. As a result of this calculation, the number of plates with column and reboiler is found as 5. In the theoretical work, this number is utilized for the model development based on stagewise approach of packed distillation column. When the comparison was made with experimental work, this number of plates was found to be enough for simulation studies.

In the first section of theoretical work, the model developed by Heathcock [5] for plate towers and multicomponent distillation was applied to the packed distillation column by utilizing necessary modifications. These modifications are as follows: Feed mixture is given to the reboiler. For condenser, temperature and composition profiles are calculated according to dew point equilibrium approach. Efficiency and inlet tower accumulations are accepted as the most important parameters. The best determination of these parameters is very important for calculation. In addition, in the relevant model, holdup change with time of the plate is taken as zero for total mass balance. Antoine coefficients are used for equilibrium condition. Second model is developed by Luyben [6] and used for packed distillation column. The same assumptions were made to calculate the system variables.

Both models for packed distillation column were used to design the control system. These calculations have been realized by using process reaction curve obtained from step test. In this control work, the reflux ratio was chosen as the manipulated variable to control the overhead product temperature efficiently. Two different models were developed for the use of DMC and PID control systems. The first model deals with first-order plus dead time type based on Laplace transform. Second type is based on partial model. Using the second model, dynamic matrix <u>A</u> is generated and used to design DMC control system.

Experimental work is performed using a pilot-scale packed distillation column distilling methanol-water mixture. A positive or negative step change is given to the system input under continuous steady-state condition. Overhead and bottom product compositions and temperatures of the column are observed. Measurement of temperature is taken with thermocouples and time profiles are observed graphically on the computer. Composition measurements at certain time intervals are made with refractometer. Dynamic behaviour of the column is observed at various step changes given to the feed composition. Numerical results obtained from theoretical model are compared with experimental data and the results are in good agreement with experimental data. Values of tuning parameters of DMC are varied and the best values for these parameters are determined as NP = 4, NC = 1. Using these parameters, efficient DMC control results are obtained.

This work provides the comparison of DMC and PID control methods applied to a packed distillation column. The simulation results showed that the performance of DMC controller for tracking a temperature set point is better than that of conventional PID controller. Many industrial systems can be represented by the general dynamic matrix model and DMC can be expected to provide adequate control performance.

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