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Control of Totally Refluxed Reactive Distillation Column Using Model Predictive Controller

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Abstract: ***The reactive distillation combines both chemical reaction and multi component separation into a single unit. According to the mechanism of the reaction operation involved, reactive distillation columns are often designed to work in a totally refluxed operation mode. Since there is no rectifying section in the reactive distillation column, the reflux drum is directly connected to the reactive section and this leads to an intimate interaction between them. Such interaction affects considerably the reaction operation involved and can eventually present a strong impact to the dynamics and controllability of the totally refluxed reactive distillation columns. The paper discusses about the application of PID controller and MPC controller in reactive distillation column. A generic mathematical model of reactive distillation has been taken for simulation. The PID and MPC controllers are designed for the process and then the overall process is controlled by using conventional (PID) and MPC controllers separately. Conventional PID controller is used to control the bottom composition of the column and then it is replaced with MPC controller and then the results from both the controllers are compared.***

Keywords: Reactive distillation column, Modelling, PID controller, MPC controller

1. Introduction

Distillation Column is the most popular and important process studied in the Instrumentation & Control Engineering literature. It is used in many chemical processes for separating feed streams and for purification of final and intermediate product streams. Reactive distillation is attractive in those systems where certain chemical and phase equilibrium conditions exist because there are many types of reactions, there are many types of reactive distillation columns. According to the mechanism of the reaction operation involved, reactive distillation columns are often designed to work in a totally refluxed operation mode. For example, in case of carrying out a reaction, A+B→C, in a reactive distillation column, the desired product C should be with drawn from the bottom of the process because it is the heaviest component. At the top of the reactive distillation column, the reactants A and B, are usually accumulated and they should be recycled back to the reactive section through a totally refluxed operation mode in reflux drum. Since there is no rectifying section in the reactive distillation column, the reflux drum is directly connected to the reactive section and this leads to an intimate interaction between them. Such interaction affects considerably the reaction operation involved and can eventually present a strong impact on the dynamics and controllability of the totally refluxed reactive distillation columns.

Recent years have seen increasingly more studies conducted on the dynamics and operation of reactive distillation columns [1–6]. For the totally refluxed reactive distillation columns, there have also appeared a number of papers dealing with their operation.

In this paper, totally refluxed reactive distillation is provided with PID and MPC controller to control the bottom composition of totally refluxed reactive distillation column and the results are compared.

The structure of this paper is as follows. Section 2 describes about the basic concept of totally refluxed reactive distillation colnmn. The modelling of reactive distillation column is explained in section 3. Section 4 discuses about the system with conventional PID controller. Section 5 discusses about the system with MPC controller. Simulation results is given in section 6. Conclusion is discussed in section 7.

2. Reactive Distillation Column

Reactive distillation is a process of separating reactants, to give products in the common chamber. It is nonlinear and complex process. The chemical industry has already acknowledged its significance due to its high gain and compact nature. Pre-installation optimal design of this process is of great concern because it is an installation of one time, but it requires constant supply of materials like fuel and reactants, out of which fuel is very costly. A saving in the design of an ideal reactive distillation column (Ideal RDC) without compromising any of the desired features would indeed be a great profit to the industry. In the chemical process industries, chemical reaction and purification of the desired products of distillation are usually carried out sequentially. In many cases, the performance of this classic chemical process can be significantly improved by integration of reaction and distillation in a single multifunctional process unit. This integration concept is called 'reactive distillation'. Fig.1 represents a scheme of high purity ethylene glycol reactive distillation column.

2.1 Process Description

Ethylene glycol ($C_2H_6O_2$) is produced from the reaction of ethylene oxide (C_2H_4O) and water, i.e., the main reaction:

$$C_2H_4O + H_2O \rightarrow C_2H_6O_2 \quad \ldots(1)$$

However, the ethylene glycol produced can further react with ethylene oxide to produce the unwanted by product diethylene glycol ($C_4H_{10}O_3$), i.e., the side reaction:

$$C_2H_6O_2+C_2H_4O \rightarrow C_4H_{10}O_3 \quad \ldots(2)$$

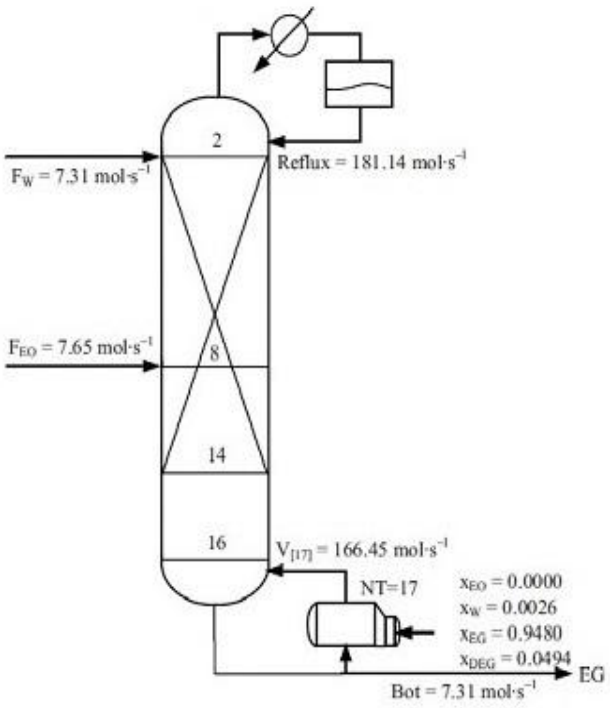

Figure 1: Reactive distillation column for the production of ethylene glycol

Both the reactions are irreversible and highly exothermic. Fig.1 shows a process design with 17 stages including a total condenser at the top and a partial reboiler at the bottom. Since it is totally refluxed reactive distillation column, there is no rectifying section, either and works in a totally refluxed operation mode with water and ethylene oxide fed onto stages 2 and 8, respectively. Table.1 gives the relevant physicochemical properties and nominal steady state operating conditions.

Both the reactions are highly exothermic in nature and occured at temperatures that make feasible the production and separation of ethylene glycol in the same unit. Higher extensions of the first reaction over the second reaction are obtained using a low molar fraction of ethylene oxide in the liquid phase and a high value of the molar fraction of water in the liquid phase. The separation of ethylene glycol from the reactants is favored by the difference in volatility between the product and the reactants, so that the product moves towards the bottom of the column, and the reactants (more volatile) towards the top. This give rise to two different sections: a reaction zone and a striping zone. For this reactive distillation column, the flow rate of distillate is set to zero, contributing to a high molar fraction of water at the top of the column. The steady-state profiles of net reaction rate, temperature, liquid phase composition, vapour and liquid flow rates are calculated and shown in fig. 2, 3, 4 & 5.

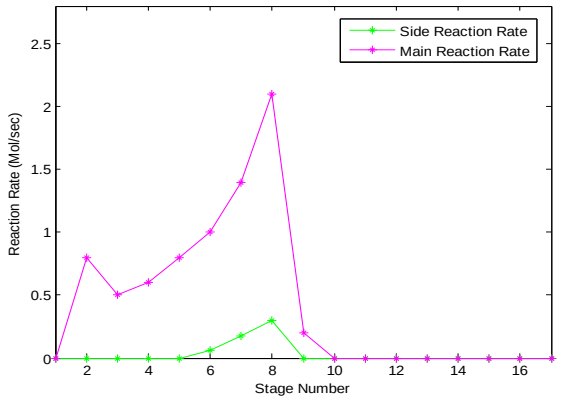

Figure 2: Net Reaction Rate Profile

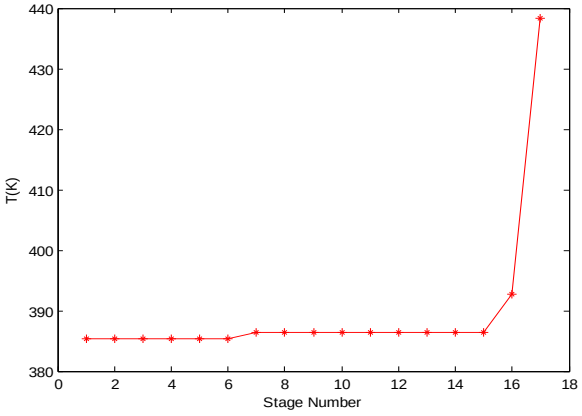

Figure 3: Temperature Profile

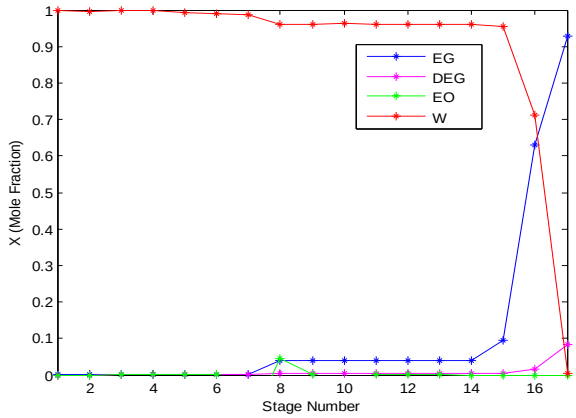

Figure 4: Liquid Composition

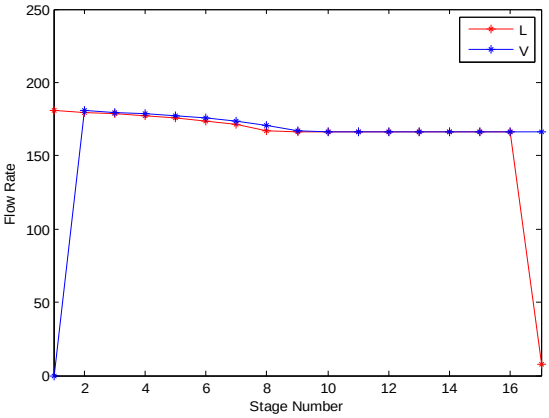

Figure 5: Vapour and Liquid Flow Rate

3. Modelling of the Reactive Distillation Column

The reactive distillation column is modeled as a tray column, using reactive and non reactive stages where appropriate. The vapor and liquid stream leaving a stage are in thermodynamic equilibrium with one another. This is known as equilibrium model for reactive distillation, the condenser and reboiler stage numbered 1 and N, respectively. Figure represents a scheme of high purity ethylene glycol reactive distillation column. The proposed model for reactive distillation column includes the following assumption:

- Steady state.
- Neglect of vapour holdup.
- Column pressure is constant.
- Perfect mixing on all stages and in all vessels (condenser and reboiler).
- Total condensation.
- The streams leaving any particular stage are in equilibrium with each other.
- The condenser and the rebioler are treated as equilibrium stages.
- The stage efficiency is assumed 100% (for simplicity).

The net reaction rate for component j on tray n in the reactive zone is given by

$$R_{n,j} = v_j M_n \left(k_{fn} x_{n,A} - k_{bn} x_{n,C} x_{n,D}\right) \quad \ldots(3)$$

$R_{n,j}$: Rate of reaction on the n^{th} tray
v_j : Stoichiometric coefficient of component j
M_n : Molar holdup on n^{th} tray
k_{fn} : Forward specific reaction rate on n^{th} tray
k_{bn} : Backward specific reaction rate on n^{th} tray
$x_{n,A}$: Mole fraction of component A on n^{th} tray
$x_{n,B}$: Mole fraction of component B on n^{th} tray
$x_{n,C}$: Mole fraction of component C on n^{th} tray
$x_{n,D}$: Mole fraction of component D on n^{th}tray

The steady-state vapor and liquid rates are constant through the stripping and rectifying sections because equimolar overflow is assumed. However, because of the exothermic reaction these rates change through the reactive zone. The heat of reaction vaporizes some liquid on each tray in that section. Therefore, the vapor rate increases up through the reactive trays and the liquid rate decreases down through the reactive trays.

Liquid flow rate is given by

$$L_n = L_{n+1} + \frac{\lambda}{\Delta H_v} R_{n,C} \quad \ldots(4)$$

Vapour flow rate is given by

$$V_n = V_{n-1} - \frac{\lambda}{\Delta H_v} R_{n,C} \quad \ldots(5)$$

V : Vapor flow rate
L : Liquid flow rate
ΔH_v: Heat of vaporization
λ : Heat of reaction

The dynamic components balances for the column are

Reflux drum:

$$\frac{d(x_{i,j}M_i)}{dt} = V_{n+1}y_{n+1,j} - L_n x_{i,j} \quad \ldots(6)$$

n : Tray number
j : Component

Rectifying and Stripping Trays :

$$\frac{d(x_{n,j}M_i)}{dt} = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} - L_n x_{n,j} - V_n y_{n,j} \quad \ldots(7)$$

Reactive Trays :

$$\frac{d(x_{n,j}M_i)}{dt} = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} - L_n x_{n,j} - V_n y_{n,j} + R_{n,j} \quad \ldots(8)$$

Feed Trays :

$$\frac{d(x_{n,j}M_i)}{dt} = L_{n+1}x_{n+1,j} + V_{n-1}y_{n-1,j} - L_n x_{n,j} - V_n y_{n,j} + R_{n,j} + F_n Z_{n,j} \quad \ldots(9)$$

F_n : Input feed flow rate
$Z_{n,j}$: Feed composition

Reboiler :

$$\frac{d(x_{B,j}M_B)}{dt} = L_{N-1}x_{N-1,j} - Bx_{b,j} - V_N y_{b,j} + W_N R_{N,j} \quad \ldots(10)$$

B : Bottom flow rate
W : Steam flow rate

Equilibrium Relationship :
The most commonly used vapour-liquid equilibrium relation is modified Raoult's law, which is valid for low to moderate pressure:

$$y_{i,j}\mathrm{P} = x_{i,j}\gamma_i Pi^{sat} \text{ (i=1 to c)} \quad \ldots(11)$$

$$y_{i,j} = \mathrm{k}x_{i,j} \quad \ldots(12)$$

k : vapour liquid equilibrium constant
Activity coefficients γ_i were calculated from NRTL equation.

The vapour compositions and stage temperatures are obtained from the bubble-point calculation using Newton–Raphson technique. The individual value of $y_{i,j}$ and $x_{i,j}$

should satisfy the below equations:

$$\sum_{i=1}^{c} x_{i,j} = 1 \quad \ldots(13)$$

$$\sum_{i=1}^{c} y_{i,j} = 1 \quad \ldots(14)$$

4. Control of Reactive Distillation Column

An automated system is used to maintain its output within desirable limits by means of a control action. The deviation of the output from the reference input is detected by an error detector. The error thus detected is used as an actuating signal for control action of the controller.

4.1 Conventional PID Controller

PID controllers are the most effectively used for controlling the systems. The PID controller calculation involves three separate parts: the proportional, the integral and derivative parts. The PID controller produces the control signal as follows.

$$u(t) = u(t-1)+k_p e(t)+k_i \int_0^t e(t)dt + k_d \frac{d(e(t)}{dt} \quad \ldots(15)$$

where u(t) : Plant input or set point ;
e (t) = r(t) − y(t) : Error between the set point and measured value at time instant ;
k_p: Proportional gain; k_i : Integral gain; k_d : Derivative gain.

A PID controller is adopted to control the composition of the bottom product. The controller gains for PID are designed and optimized with simulation model by using Simulink response optimization library block. It is mainly a numerical time domain optimizer developed under MATLAB/Simulink environment There are three parameters to be optimized in order to have satisfactory control performance. Those are corresponding respectively to k_p, T_i and T_d which are the proportional, integral and derivative gains for the composition control. These parameters are tuned using Ziegler-Nichols tuning method.

4.2 Model Predictive Controller (MPC)

Model predictive control (MPC) is an advanced method of process control that has been in use in the process industries in chemical plants and oil refineries. The main advantage of MPC is the fact that it allows the current timeslot to be optimized, while keeping future timeslots in account. This is achieved by optimizing a finite time-horizon, but only implementing the current timeslot. MPC has the ability to anticipate future events and can take control actions accordingly. PID controller do not have this predictive ability. In the control aspect of this work, single controlled variable (bottom composition) and single manipulated variables (reboiler duty (Q)) were selected for the formulation of the model predictive control. It was simulated with the aid of Model Predictive Control Toolbox of MATLAB. MPC has the ability to anticipate future events and can take control actions accordingly.

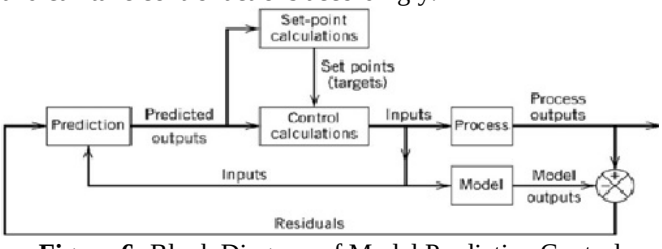

Figure 6: Block Diagram of Model Predictive Control

Basic structure of MPC is given above. Current values of the output variables are calculated using a process model and then difference between predicted and actual outputs are used as a feedback signal to a prediction block. The predicted outputs are used in controlled calculation and setpoint calculation after considering constraints on the input and output variable. MPC configuration is analogues to both internal model control configuration and smith predictor configuration because model and process are parallel acted and difference act as feedback control signal. But coordination of the control and set point calculations makes MPC superior than others. Traditionally economic optimization setpoint for the control calculation, called as target, is calculated from a steady-state model of the process. Economic optimization is depending on maximizing a cost function, or maximizing a production rate. The optimum values of set points are distorted continuously which in turn functions of variations in process conditions, equipment, and instrumentation, as well as economic data such as prices and costs. In MPC, Set points are calculated in each sampling time. Control action is determined based on current measurements and predictions of the future output.

Table 1: Physicochemical properties and nominal steady state operating conditions

Parameter		Value
Number of stages	Rectifying section Reactive section Stripping section	0 13 2
Liquid holdup (mol)	Condenser Column tray Reboiler	30,000.0 1000.0 30,000.0
Reaction Rate ($molm^{-3}s^{-1}$)	Main reaction Side reaction	$3.15\times10^{15} e^{\frac{-9547}{T}} x_{EO}x_W$ $6.30\times10^{15} e^{\frac{-9547}{T}} x_{EO}x_{EG}$
Feed location	EO W	8 2
Heat of reaction ($Jmol^{-1}$)	Main reaction Side reaction	−80,000.0 −13,100.0
Feed flow rate ($mols^{-1}$)	EO W	7.65 7.31
Latent heat of vaporization ($Jmol^{-1}$)		40,000.0
Bottom product specification (EG, mol %)		94.54

5. Simulation Results

In this project, used ordinary differential equation solver ode23s, Math toolbox and Simulink toolbox of MATLAB software. First lumped parameter model of the RD column is developed and dynamic simulation is done. Simple PID control strategy and the MPC control strategy for bottom composition control by manipulating reboiler steam flow rate are designed and simulated in Simulink. The steady state response shows a stable behaviour in which the bottom product, mole fraction of ethylene glycol reaches a steady state value of 0.945% of purity in composition. The steady state response is shown in fig.7. The system attains steady state response only when no disturbance affects the system. If there is any change occurs in the nominal value of feed flow rate and feed composition the product composition will not attain the steady state value.

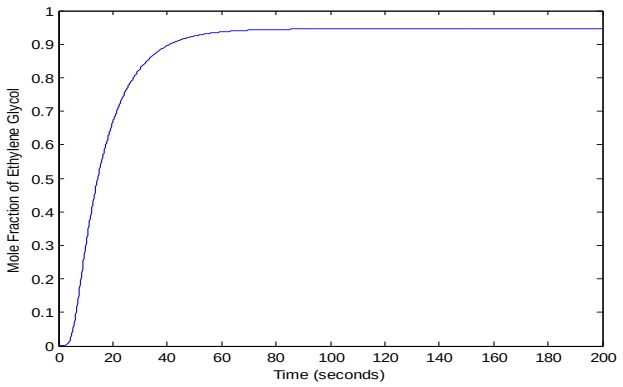

Figure 7: Steady State Response

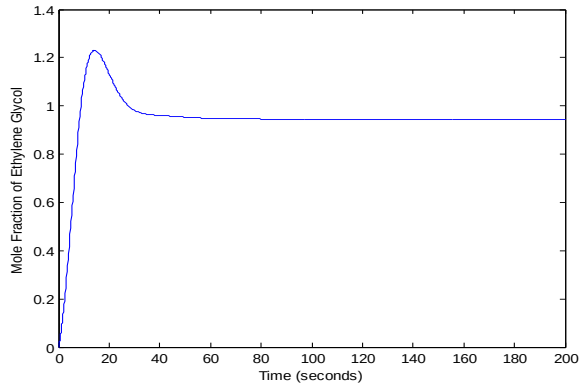

Figure 8: Bottom Composition Control using PID controller

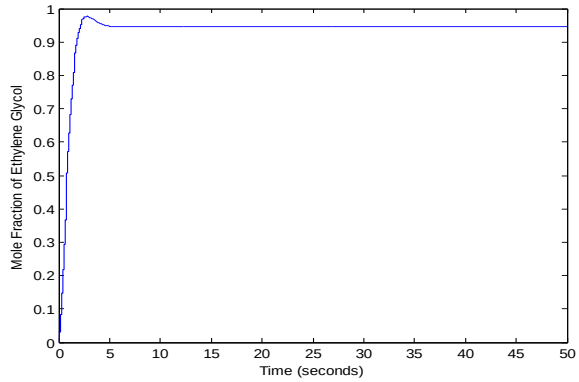

Figure 9: Bottom Composition Control using MPC

Response with two controllers is given in fig.8 & 9 respectively. PID control scheme exhibits large and poor dynamic performance, while MPC control scheme showed perfect dynamic response with the same controller and tuning parameters. The MPC controller shows significant performance improvement with little overshoot and no oscillations.

6. Conclusion

Here in this paper I have presented the modeling and control design of a totally refluxed reactive distillation column without disturbance. Control of the bottom compositions of the column is a difficult task due to presence of process nonlinearities. The structure allows taking into account dynamic variations of the process and adapting the controller parameters to this various conditions. MPC controller achieved a accurate performance in controlling the bottom compositions.

7. Future Scope

From the foregoing analysis, disturbance is not introduced into the system. A Model predictive controller eliminates the disturbance affect into the system. A disturbance is added in the system and compare the response of the system with tuned PID controller.

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