DETERMINATION OF CONTROL STRUCTURE OF REACTIVE DISTILLATION CONTROL SYSTEM IN DIMETHYL ETHER SYNTHESIS

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Abstract
Conventionally, dimethyl ether (DME) was synthesized from methanol and purified using two distillation columns, which contributes about 50-70% to the cost of production. Using reactive distillation process, the conversion of methanol can be enhanced greatly and purifying the DME at the same time, thus reducing the cost of production, significantly. The two processes (reaction and separation) occurred in the same column reduce the number of control valves as the actuator for control system. This makes reactive distillation column is very non-linear in terms of controllability, and therefore the design of control system of such column can be quite a challenge. In this research, the optimum PI controller configuration will be obtained. The parameters for this configuration are the choice of manipulated variable (MV) that can be the feed flow rate or steam flow rate in reboiler and the controlled variable (CV) that can be the most sensitive tray temperature or the production rate. The configuration also including the PI controller tuning by using Auto Tuning Variation (ATV) method. The CV-MV pairing choice results two possible control structures, namely CS 1 and CS 2. The result showed that the tray #5 was the most sensitive tray temperature and selected as CV. The dynamic simulation showed that CS 1 failed to handle -5% disturbance change, while CS 2 succesfully handle up to ±25% disturbance change.

Keywords: dimethyl ether, methanol, reactive distillation, nonlinearities, control structure

INTRODUCTION

Nowadays, dimethyl ether is produced by converting natural gas, coal, oil residue or biomass into syngas followed by methanol synthesis and methanol dehydration. This conventional production process uses fixed bed reactor for methanol dehydration process and two distillation columns for dimethyl ether purification up to 99.9% wt (Kiss & Suszwalak, 2012). This process is costly in terms of operating cost, caused by the energy needed by two distillation columns. To reduce the operating cost, a single reactive distillation column can be used instead of one reactor followed by two distillation columns. Reactive distillation is the integration concept of reaction and distillation in a single multifunctional process unit (Sundmacher & Kienle, 2002).

The main difficulty of applying reactive distillation until now is the controllability problem. Reaction and separation process occurred in single column reduce the number of valves available for control purposes, and this makes this column is very non-linear in terms of controllability (Engel and Fernholz, 2003). The non-linearity can lead to steady-state multiplicities. Because of these complexities, reactive distillation control continues to receive much attention in the literature.

The previous works on reactive distillation control were done by many authors. Various kind of study in reactive distillation control has been done by Al-Arfaj and Luyben (2000-2004). Some other authors also focus on the importance of steady-state analysis to the control system design of the reactive distillation column have been assessed. This steady-state analysis is discussed mainly about steady-state multiplicity. Reactive distillation column is very prone to facing steady-state multiplicity problems. Therefore, the design of control system of such column can be quite a challenge (Kumar & Kaistha, 2008).

Steady-state multiplicities can be classified into input and output multiplicity. Input multiplicity is multiple input giving the same output, while output multiplicity is multiple output resulted from the same input. In the control perspective, inputs are manipulated variables and outputs are potential controlled variables. Kumar & Kaistha (2008) stated that there are several articles reporting steady-state multiplicities in reactive distillation systems, like Ciric & Miao (1994), Guttinger & Morari (1997), Mohl, et al.(1999) and Bisowarno & Tade (2000).

These multiplicities can lead to some controllability problem. Input multiplicity can lead to “wrong” control action being taken for large enough disturbances, while output multiplicity can lead to steady state transition in the absence of proper feedback control (Kumar & Kaistha, 2008). So, these problems must be prevented with good control system. Kumar & Kaistha (2009) stated that the reactive distillation control literatures thus propound the application of non-linear or model-based control techniques. Even these literatures stated that advanced or non-linear control techniques can provide effective column regulation, industrial practice still dependent on traditional decentralized control because of the simplicity of PID algorithm.

Kumar & Kaistha (2008) proposed some strategies to overcome these problems. For the output multiplicity problem, Kumar & Kaistha (2008) suggesting constant reflux ratio policy (so the reflux ratio must not be used as the manipulating variable and must be maintained at a constant value) and controlling the most sensitive tray temperature because this temperature tray will be more prone to be drifted from the desired steady-state value. As for the input multiplicity, the strategy is to do a rangeability analysis. Rangeability is defined as the new metric that quantify the severity of input multiplicity. Rangeability is used for the design of robust control structures for the reactive distillation column. In many cases, control structure that controlling the most sensitive output will result low robustness due to low rangeability causing "wrong" control action for large disturbances. Kumar and Kaistha (2008) had apply these strategies in controlling reactive distillation column for methyl acetate synthesis and these strategies give good control performance and robustness. The control structure can handle up to 25% disturbance without any steady state transition and wrong control action occurred.

Based on these strategies, the control structure of reactive distillation column for dimethyl ether synthesis which can handle multiplicity problems will be obtained. This article will explain the algorithm on obtaining this control structure first. Next, the steady state base case will be explained. This followed by doing the sensitivity and rangeability analysis to choose which tray temperature is going to be chosen as controlled variable. This results two possible control structures, these two structures will be simulated dynamically to obtain control structure that has better control performances. This articles ends with the conclusions that can be drawn from the work.

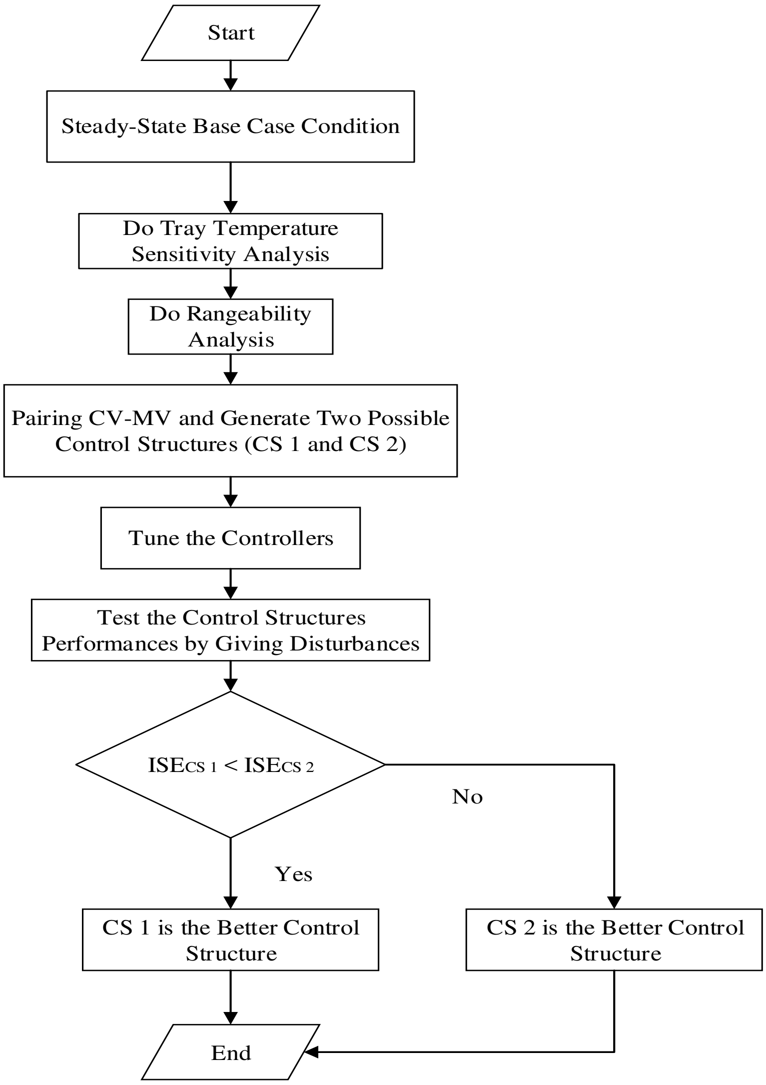

Figure-1. Algorithm of the work

METHODOLOGY

The design of an effective control structure requires some regulatory tasks followed by the selection of input-output pairings. Conventional heuristics says that the best input-output pairing is the most sensitive output to the input changes. In reactive distillation system, the rangeability of the most sensitive output will be low due to input multiplicity and thus impacting control robustness. In such situation, the choice of the output variable must be done by compromising between sensitivity and rangeability, not just by the sensitivity. The controlled variable must be the output with maximum rangeability and an acceptable sensitivity.The determination of control structure thus be done by firstly preparing the base case steady-state condition. This followed by doing the sensitivity analysis. Sensitivity analysis results some sensitive outputs, to the 10% input changes. For a reactive distillation column, the outputs (potential controlled variables) are the tray temperatures/compositions and the inputs (potential manipulated variables) are the fresh feed flowrates, reboiler duty and reflux ratio (or reflux rate). This sensitivity analysis is done by doing a steady-state input variation that results in output changes, and this results will be evaluated to obtain some sensitive output to be analyzed next in rangeability analysis. These sensitive outputs then are evaluated, and the outputs with better rangeability will be chosen as controlled variables and paired with corresponding inputs (manipulated variable). The pairings, will result some possible control structures (which is two possible control structure in this work). These structures will be tested by dynamic simulation to get both dynamic responses to some disturbances and from these response, the better control structures for this case can be determined by choosing which structure can handle the disturbance better.

RESULT AND DISCUSSION

As the base case for this work, the schematic of the industrial scale dimethyl ether production reactive distillation column is shown in Figure-2. The column consists of 25 trays, with 7 rectifying trays, 13 reactive trays and 5 stripping trays. Pure methanol is being fed to 8th tray, reacting in the reactive trays resulting 99.99 mol % of dimethyl ether in the top product and 100 mol % of water in the bottom product.

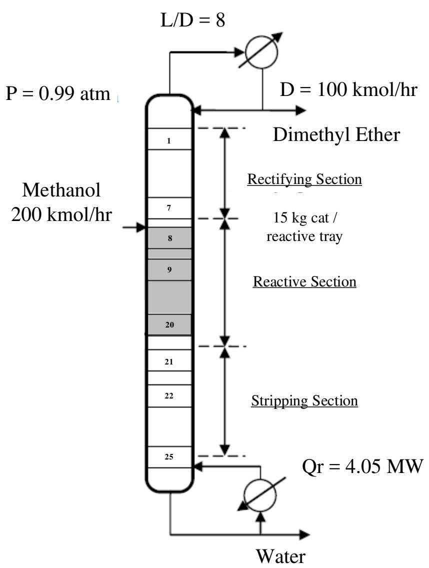

Figure-2. Schematic diagram for the base case steady-state condition

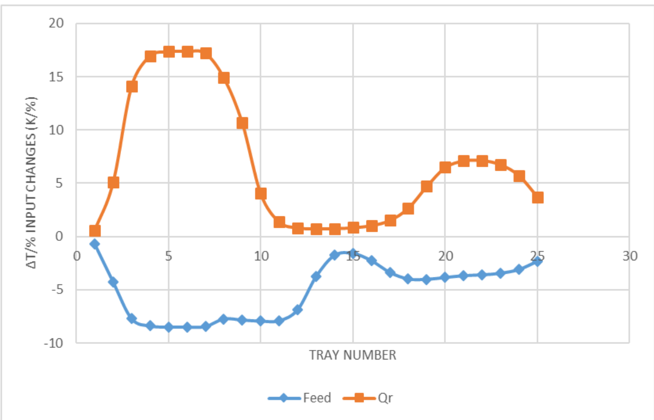

Figure-3. Sensitivity of tray temperatures to 10% change in inputs

The VLE model uses the Wilson equation. The reaction rate equation uses equation from Kiss & Suszwalak (2012). The experimental data was modeled as Eley-Rideal, but the equation was made as equivalent simple power law to simplify the simulation. The equations are as follows:

$$r_{DME} = kW_{cat}[MeOH]^m[H_2O]^n$$

and

$$k \;= A\exp\left(-\frac{E_a}{RT}\right)$$

Where A is a pre-exponential factor, 5.19×10^9 m^3 $kg\text{-}cat^{-1}s^{-1}$. Ea is activation energy, 133.8 kJ/mol. While m and n are reaction orders of methanol and water (m = 1.51 and n = -0.51). The specific steady-state and dynamic simulator for this work can be obtained from the authors.

1. *Sensitivity analysis*

The first step to design a control structure is to obtain sensitivity of the outputs with respect to the available inputs. The sensitivity of the tray temperatures to the two inputs, namely, feed flowrate and reboiler duty is plotted in Figure-3.

This sensitivity plot was done by steady-state input variation up to 10% input changes. There are two inputs, namely, feed rate and reboiler duty (Qr). The plot shows that for both inputs, the sensitivity profile is similar. Based on this sensitivity plot, six tray temperatures with highest sensitivity are obtained. These six trays are 3rd tray to 8th tray. These tray temperatures then taken to be tested in rangebility analysis. For reactive distillation control, the most sensitive tray temperature cannot be chosen as controlled variable just based on the sensitivity. Because reactive distillation is very nonlinear and thus showing input multiplicity behavior, thus the most sensitive input may have bad rangeability. This makes compromise between sensitivity and rangeability is needed for reactive distillation control structure design.

2. *Rangeability analysis*

The steady-state variation of the sensitive tray temperatures obtained from sensitivity analysis as the two available inputs are varied about its base case is studied in rangeability analysis. The two available inputs in this case are feed flowrate and reboiler duty. This step's purpose is to assess the nonlinearity in the candidate input-output pairings. These input-output relations are plotted in Figure-4 for feed flowrate variation, and in Figure-5 for reboiler duty variation.

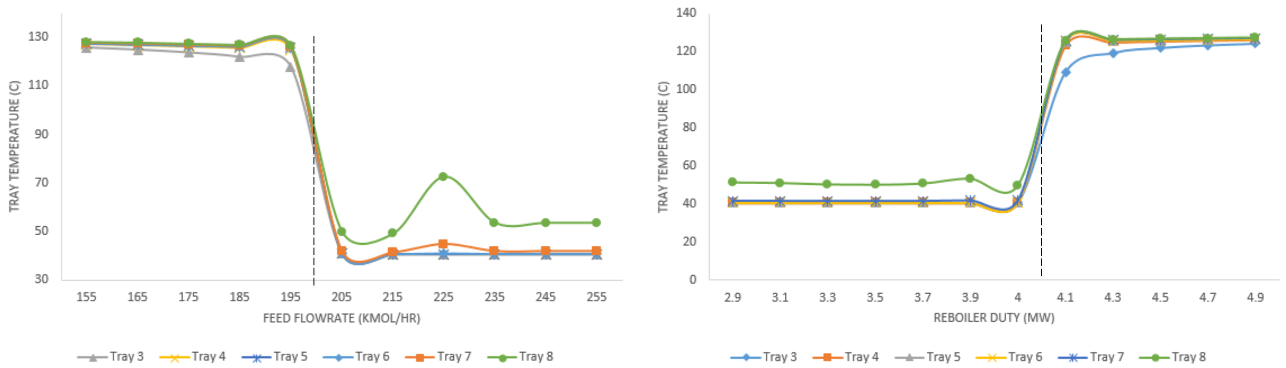

Figure-4. Steady-state input-output relation of six sensitive temperature trays to the feed flowrate and reboiler duty

The base case condition is illustrated by the dashed line, at feed flowrate 200 kmol/hr. For feed flowrate variation, the six sensitive tray temperatures do not show any input multiplicity for the base case temperature region. Tray 8 does exhibit some input multiplicity that observably from the peak and trough like transverse wave, but this multiplicity does not occur in the base case 8th tray temperature (89°C). Since the input multiplicity does not cross the base case temperature, the controller will have no "wrong" control action problem. This makes all six sensitive tray temperatures can be the output (controlled variable) and can be paired with the input (feed flowrate). Since all these temperature trays can be the controlled variable, the 5th tray temperature is chosen as the controlled variable and paired with feed flowrate as the manipulated variable because this tray temperature is the most sensitive among all these six trays.

As for the steady state variation of reboiler duty, as there is also no input multiplicity appeared around the base case temperature for all six trays. The base case is illustrated by the dashed line, in reboiler duty at 4.05 MW. This makes these six tray temperatures also can be chosen as the output for reboiler duty as the input. Thus the most sensitive tray temperature among these six will be chosen as the controlled variable, which is in this case also be the 5th tray temperature. Based on the sensitivity and rangeability analysis, two possible input-output pairings can be concluded as tabulated in Table-1.

Table-1. Two possible control structure based on sensitivity and rangeability analysis

Control Structure	CV (Controlled Variable)	MV (Manipulated Variable)
CS 1	5th Tray Temperature	Feed flowrate
CS 2	5th Tray Temperature	Reboiler duty

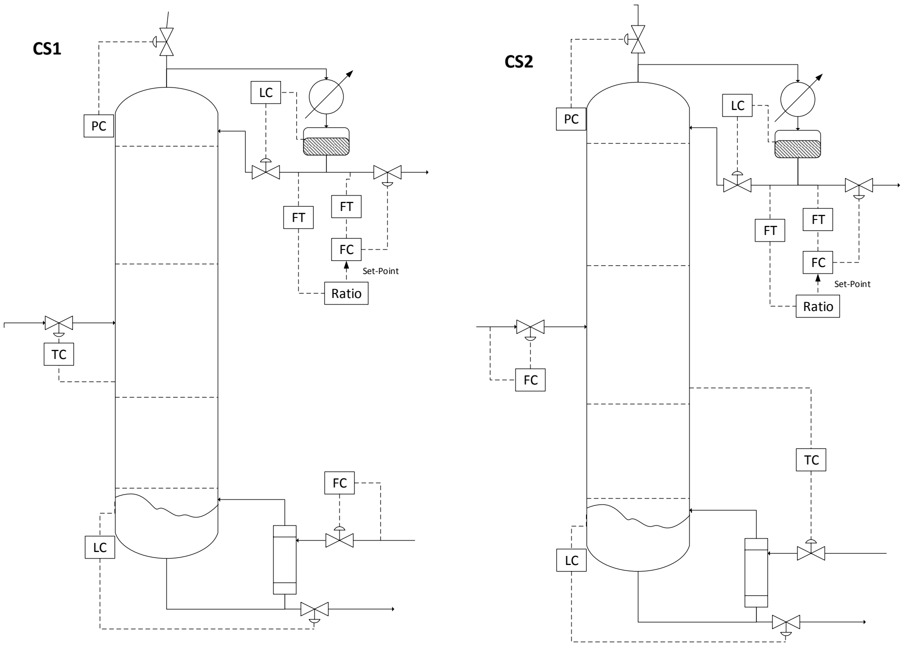

Figure-5. Schematic of candidate control structures CS 1 and CS 2

The schematic diagram for the two control structures is illustrated in Figure-5 above. For CS 1, the feed flowrate controlling the 5th tray temperature while reboiler duty controlling 5th tray temperature in CS 2. The other CV-MV pairings are the same for both control structure. Reflux ratio is controlled with ratio control, the purpose is to prevent the output multiplicity as stated by Kumar & Kaistha (2008) that constant reflux ratio policy will prevent output multiplicity. The bottom stage liquid level is controlled by manipulating bottom product rate, and distillate rate controlling the condenser liquid level. The vent stream is used to control the top stage column pressure to prevent the column overpressure.

3. *Controller Tuning*

The ATV (Auto Tuning Variation) method is used for controller tuning for both control structure. The tuning results PI controller parameters as tabulated in Table-2. With integral times units are in minutes.

Table-2. PI controller parameters

Controller	CS 1		CS 2	
	Kc	**Ti**	**Kc**	**Ti**
Column pressure controller	2	0	2	0
Temperature controller	0,03	109	0,5	20
Condenser liquid level controller	1,02	0	1,02	0
Bottom stage level controller	1,7	0,991	1,7	0,991
Feed flowrate controller	-	-	0,072	0,009
Reflux ratio controller	0,1	0,128	0,1	0,128

The ATV method is preferred over the conventional Ziegler-Nichols method in this work because the nature of Ziegler-Nichols method which is aggressive with a larger controller gain and shorter integral time. The ATV method is more suitable since the reactive distillation column involves fluid and thermal processes which are do not prefer high overshoot as the Ziegler-Nichols will bring to the process (Svrcek, Mahoney and Young, 2014).

4. *Dynamic results*

The dynamic performances of the two control structures discussed next. Each structure will be simulated dynamically and the dynamic response to some disturbance will be evaluated. The better control structure for this case will be the structure with more robust control performances.

4.1. *Control Structure* 1 (CS 1)

The dynamic performances in handling +5% disturbance (+5% step change in the production rate handle, which is for CS 1 is reboiler duty). The dynamic response graph showing that this disturbance does not give much trouble for CS1, as illustrated in Figure-6.

The response show that CS 1 has no problem in handling +5% disturbance, but not to -5% disturbance. Figure-7 below shows the dynamic response of CS 1 after the reboiler duty decreased 5%. The result for -5% step change in reboiler duty shows that CS 1 cannot handle -5% disturbance. The column appears to be upset after 5% reboiler duty decrease. The distillate rate becomes zero after 1 hour and the 5th tray temperature appears to have transition from the base case value (79 ^{o}C) into 35 ^{o}C. This is happened even after the fifth tray temperature, as the most sensitive output, being controlled. The result is contrary to the result of the work done by Kumar & Kaistha (2008), that feed rate controlling column temperature still can handle up to ±20% disturbance. This possibly because of the high reflux ratio used in this work (L/D = 8) will lead to tray hydraulic lags and thus the dynamic becomes slow. The effect of reboiler duty decrease to temperature decreasing is faster than the effect of feed rate increase to temperature increase. High reflux ratio also makes the liquid rate inside the column is far higher than the rate of the feed, so increasing the feed flowrate to increase the temperature is just like expel a drop of hot water into a bucket of cold water and of course the feed rate increase will not have affect the column temperature much.

The temperature that fail to be increased will reduce the amount of vapor that can reach the condenser, and thus reduce the distillate rate. This can be seen in the Figure-7 above that the distillate rate becomes zero after 1 hour and the bottom rate becomes significantly increased. This concludes that CS 1 might not be the good choice as the control structure for this case.

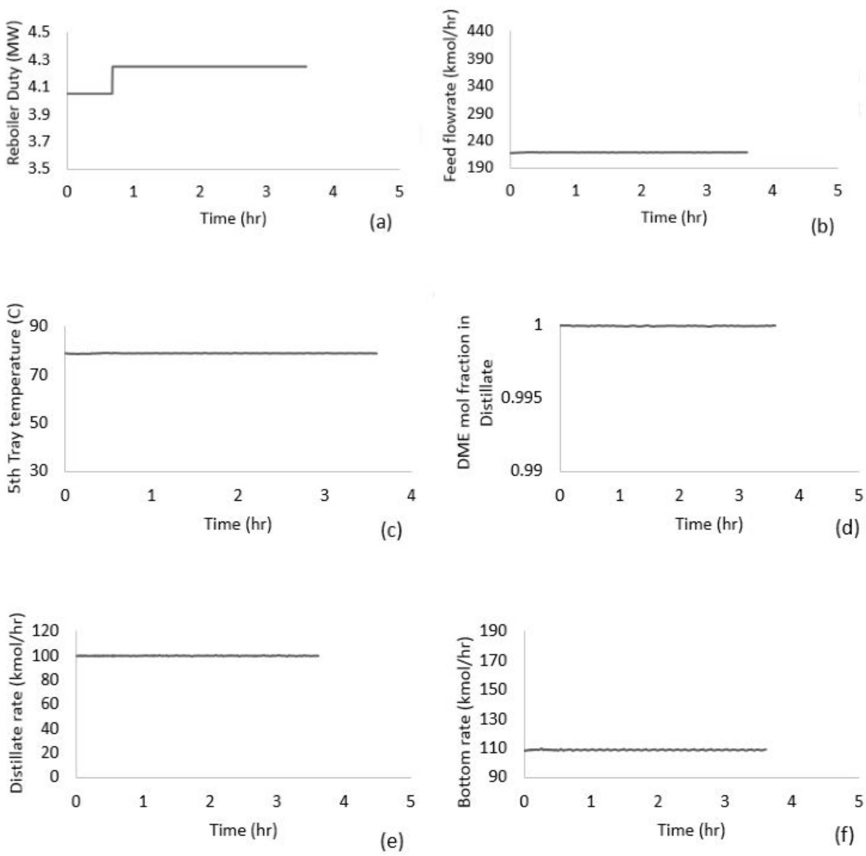

Figure-6. CS 1 response to +5% step change in reboiler duty with: a) Reboiler duty, b) Feed flowrate, c) 5th Tray temperature, d) DME mol fraction in distillate, e) Distillate rate and f) Bottom rate

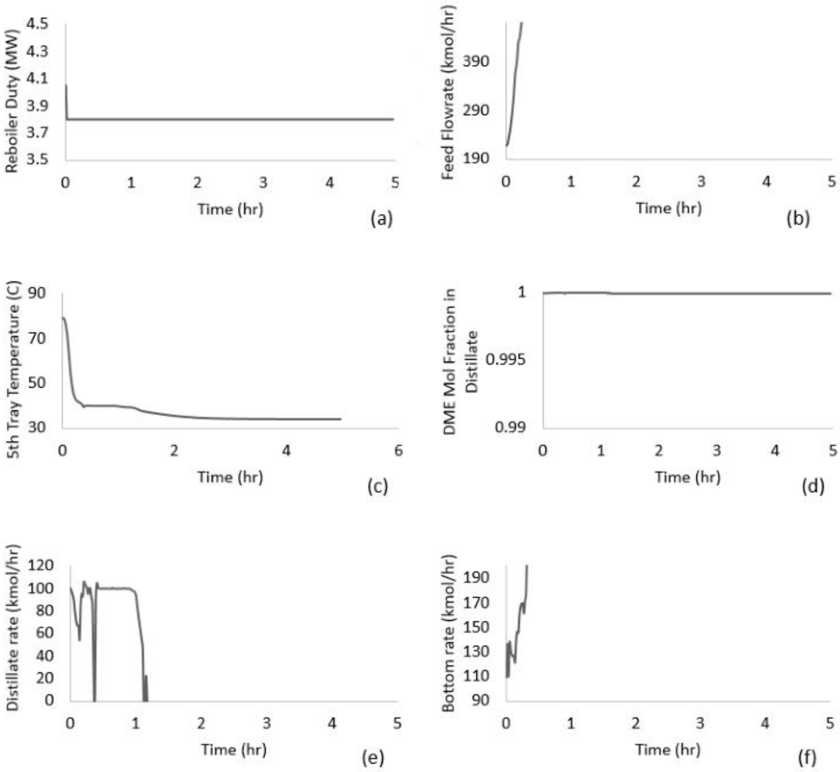

Figure-7. CS 1 response to -5% step change in reboiler duty with: a) Reboiler duty, b) Feed flowrate, c) 5th Tray temperature, d) DME mol fraction in distillate, e) Distillate rate and f) Bottom rate

4.2. *Control Structure* 2 (CS 2)

Unlike CS 1, in the CS 2, column temperature is controlled by reboiler duty. This control structure appears to be able to handle disturbances better than CS 1. The result shows that CS 2 can handle up to ±25% disturbance, which is step change in the feed flowrate. The dynamic response of CS 2 after +25% disturbance is showed in Figure-8 below.

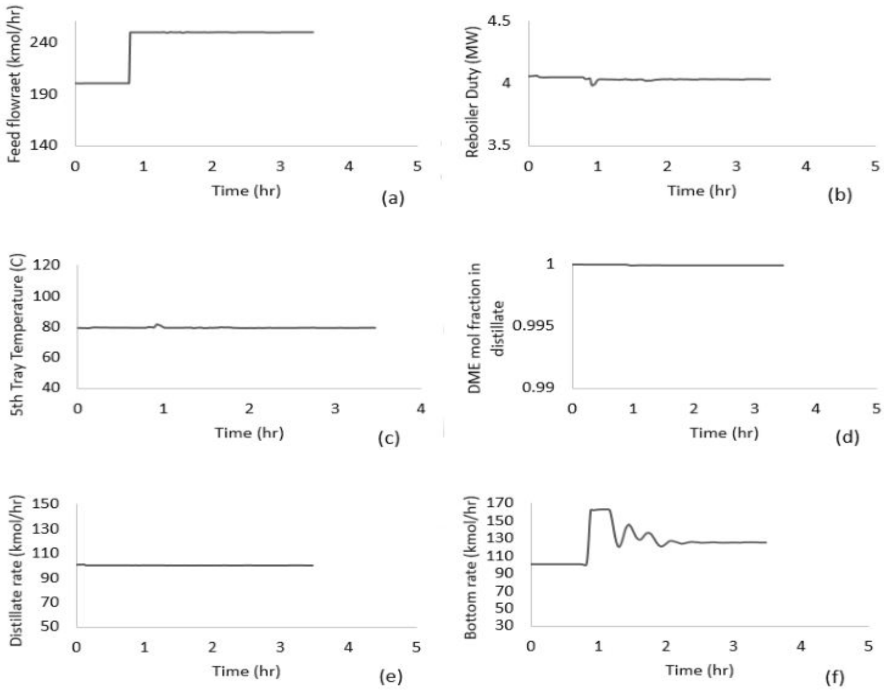

Figure-8. CS 2 response to +25% step change in feed flowrate with: a) Feed flowrate, b) Reboiler duty, c) 5th Tray temperature, d) DME mol fraction in distillate, e) Distillate rate and f) Bottom rate

CS 2 can handle +25% disturbance well. The dynamic of 5th tray temperature appears to not have much overshoot (below 10°C). This because the fast and sensitive of 5th tray temperature change to the reboiler duty change. This also possibly caused by the same reason why CS 1 failed, that is high reflux ratio. As stated before, high reflux ratio makes the feed increase not have much effect on column temperature. Thus the temperature overshoot is not too high to be handled by CS 2. Aggressive response showed for the bottom rate. The bottom rate appears to have aggressive behavior because of relatively high steady state gain and low integral time for the bottom stage liquid level controller.

This good dynamic performance also showed if CS 2 is given -25% disturbance. CS 2 dynamic response for -25% disturbance is showed in Figure-9 below. This result shows that CS 2 is better control structure for this case than CS 1. CS 2 successfully handle up to ±25% disturbance, while CS 1 have failed to handle -5% disturbances.

This result also asses the effect of column base case design to the control structure design. Because as stated before, the base case has high reflux ratio that cause high liquid rate inside the column. This leads to CS 1 failure that uses feed rate (which is far less than the liquid rate inside the column) to control the column temperature that seems far more influenced by the liquid rate inside column. Contrary to the CS 1 result, CS 2 do not have much problem in handling the disturbances because of the same reason. This concludes that CS 2 is the proper control structure choice for this case.

CONCLUSION

This article has demonstrated the method of determining control structure of reactive distillation column for Dimethyl Ether (DME) synthesis. The method uses sensitivity and rangeability analysis as demonstrated by Kumar & Kaistha (2008). These two analysis are done because the steady-state multiplicity problem in reactive distillation needs the compromise between output sensitivity and rangeability. From the sensitivity and rangeability analysis, 5th tray temperature was chosen as the controlled variable for two possible inputs (feed flowrate and reboiler duty). These two possible input-output pairings result in two control structures, namely CS 1 and CS 2. Proper choice of the structure of course the structure with better control performances, which is CS 2, that can handle up to ±25% disturbance. This because the base case design that has high reflux ratio is not controllable if CS 1 is used, this showed as CS 1 failed to handle -5% disturbance.

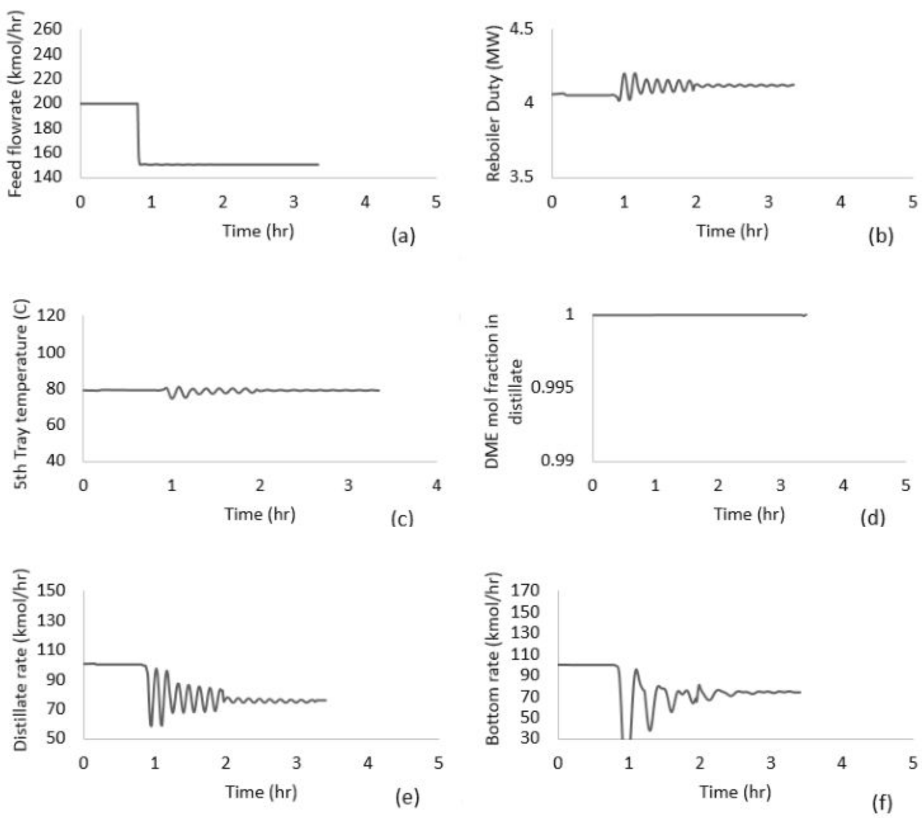

Figure-9. CS 2 response to -25% step change in feed flowrate with: a) Feed flowrate, b) Reboiler duty, c) 5th Tray temperature, d) DME mol fraction in distillate, e) Distillate rate and f) Bottom rate

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