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Control of Reactive Distillation through the Multiple Steady State Conditions

Takehiro Yamaki, Keigo Matsuda*

Department of Organic Materials Engineering, Graduate School of Science and Engineering, Yamagata University, 4-3-16, Jonan, Yonezawa, Yamagata 992-8510, Japan
matsuda@yz.yamagata-u.ac.jp

In this paper, the controllability of reactive distillation (RD) on the multiple steady states (MSS) was analysed. We used the RD column for *tert*-amyl methyl ether (TAME) synthesis for a case study. The model was prepared five PI controllers which control liquid level, feed flow rate, pressure of column overhead and bottom product composition. Initial conditions of dynamic simulation were chose three cases each of upper, middle and lower branches on the MSS. Product composition was controlled for the ±10 % disturbances of feed flow rate and reflux ratio. However, pressure disturbance was failed to keep the set point. These phenomena are able to explain the bifurcation diagrams.

1. Introduction

Reactive distillation (RD) combined of the liquid phase chemical reaction and distillation separation has attracted much attention in the industrial and academic fields. Since RD column could simultaneously operate reaction and separation, this process has many advantages such as improvement of process performances and reduction of unit number than conventional multistep process. However, due to integration of different length and time scale operations, RD column lead to non-linear process characteristics (Taylor et al., 2000). In particular, many research groups study the multiple steady states (MSS). Nijhuis et al. (1993) reported that the MSS occur in a broad range of operating conditions. Mohl et al. (1999) have performed experiment with pilot-scale RD column, and the MSS has been found experimentally. Švandová et al. (2009) have studied the stability and operability on the MSS. From these investigations, the existence of the MSS has been evident into RD process, and many authors are suggesting that these analyses should help to avoid unsafe operation and design conditions. On the other hand, Ikoshi et al. (2010) have performed dynamic simulation on the MSS conditions, and step change of reboiler duty has been led to increase of product composition. Therefore, they have presented that the MSS conditions have a potential to increase the process performances, and it is required to investigate the controllability of RD column on the conditions.

Control of RD column for variable reaction systems is investigating. However, only few papers have addressed the control of RD column with the MSS. Kumar et al. (2008) studied the impact of MSS on the control of a simulated industrial scale RD column. Additionally, Kumar et al. (2009) reported that process dynamics of controlling RD column lead to non-linear behaviour by large throughput changes. These papers have been focused on the pairing of controller and the effect of throughput changes, the effect of the process dynamics with disturbances have not yet been studied.

This paper provides process dynamics and controllability of RD column on the MSS conditions. Bifurcation analysis was used to determine the region of the MSS. The dynamic simulation model with

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five PI controllers was developed, and we performed the process dynamics on the region of the MSS for three disturbances such as reflux ratio, feed flow rate and pressure.

2. Modelling of reactive distillation column

2.1 Steady state simulator

Figure 1 shows a schematic diagram of RD column for *tert*-amyl methyl ether (TAME) synthesis. The RD column consists of 33 trays, reboiler and condenser. The RD process has single feed stream on th 15th stage. The raw materials were fed 800 kmol/h. The bottom products is TAME and top is reactant and inert materials. Pressure of the top is set to 253 kPa. External reflux ratio is 5. The vapor-liquid equilibrium was calculated with Wilson-RK model. The mass transfer was assumed equilibrium stage approach. In the reactive section, the simplified reaction system includes 3 reactions was assumed:

$$2M1B + MeOH \leftrightarrow TAME \quad (1)$$
$$2M2B + MeOH \leftrightarrow TAME \quad (2)$$
$$2M1B \leftrightarrow 2M2B \quad (3)$$

The kinetics for the forward and reverse reaction is referred Al-Arfaj and Luyben (2004).

2.2 Dynamic simulator

Figure 2 shows a schematic diagram of RD column with five PI controllers. The model is exported from steady state simulator. The condenser and reboiler liquid level are adjusted using distillate flow rate and bottom flow rate, respectively. Pressure of the overhead is controlled condenser duty. In addition, the bottom TAME composition is controlled reboiler duty. Pressure, liquid level and flow rate controller condition was referred Luyben (2006). Only composition controller was tuned using Tyreus-Luyben tuning procedure with the ultimate gain and period from the relay feedback tests (Tyreus and Luyben, 1992).

3. Results

3.1 Bifurcation analysis

Bifurcation analysis in the steady state simulator was performed to establish appearance condition of the MSS in the developed model. Figure 3 shows the bottom TAME composition with the variation of

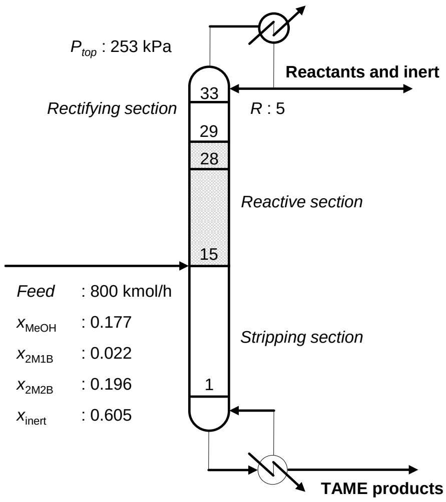

Figure 1: Schematic diagrams of RD column

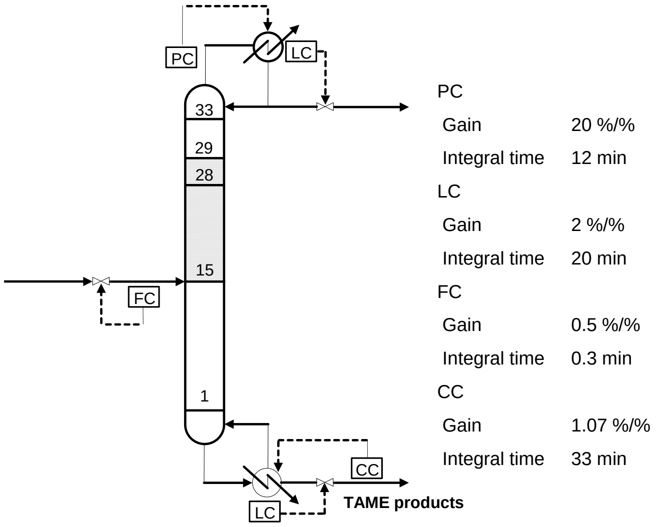

Figure 2: Schematic diagrams of control structure

the reboiler duty. It is found that the model developed RD column has the input multiple steady states which include three blanch such as upper, middle and lower. The MSS consist of reboiler duty between 25.50 MW to 26.57 MW, and bottom TAME composition has range from 0.39 to 1.0.

3.2 Process dynamics on the MSS conditions

To confirm the dynamics of RD column, the MSS conditions obtained bifurcation analyses were used. Figure 4 shows the reboiler duty with the variation of set point of composition controller. Note, reboiler duty is the value when the steady state was obtained after the set point change. Initial condition of set point was applied the value of 0.34 (i.e. reboiler duty 25 MW). Reboiler duty was changed along the value of set point, and the trajectory indicated the same result as the bifurcation analysis by steady state simulation. Thus, most of the conditions on the MSS except as set point above 0.999 were controlled for the disturbance of bottom TAME composition.

3.3 Controllability

The controllability for the three disturbances was considered in the MSS. Figures 5-7 show results of dynamic response of bottom TAME composition in the three disturbances: i.e. feed flow rate, reflux

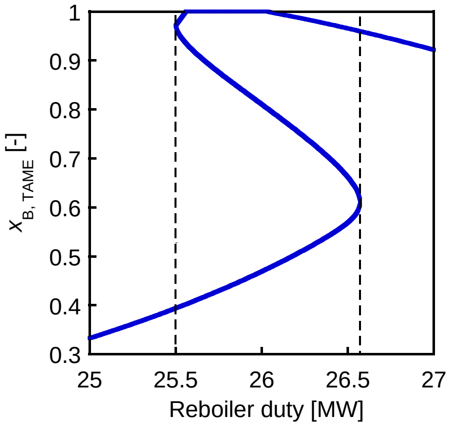

Figure 3: A bifurcation diagram for bottom TAME composition with the variation of reboiler duty

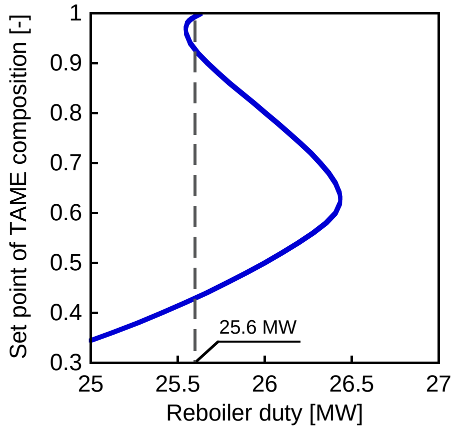

Figure 4: A trajectory of reboiler duty with the variation of set point of composition controller

ratio and pressure of overhead. Initial conditions, i.e. set point of composition controller, were applied 0.39, 0.93 and 0.99. Here, reboiler duty for these initial conditions is same value of 25.6 MW. The disturbances assumed ±10 % for the condition of steady state simulator as the base case. Additionally, each disturbance for all simulations was entered at 10 h from start calculation.

For the step change in the feed flow rate and the reflux ratio, each bottom TAME composition on the MSS conditions was controlled at set point of composition controller. The stabilisation of bottom TAME composition was taken a long time along the branch in the region of the MSS. For the +10 % step change in pressure of overhead, bottom TAME composition was regulated at the set point. However, the time required for the stabilisation on the set point 0.99 was longer than the case of disturbance of the feed flow rate and the reflux ratio. Additionally, the case of set point 0.93 and 0.99 was failed for the -10 % step change in the pressure of overhead.

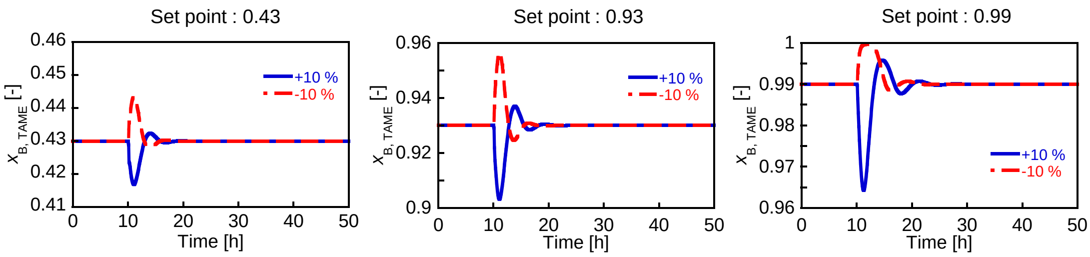

Figure 5: Dynamic responses of bottom TAME composition for ±10 % step change in the feed flow rate

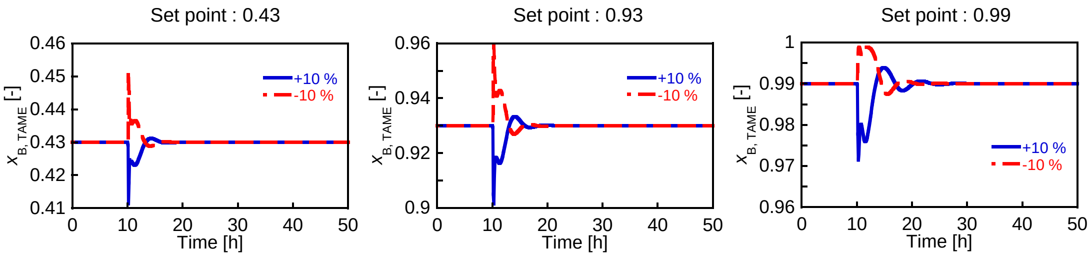

Figure 6: Dynamic responses of bottom TAME composition for ±10 % step change in the reflux ratio

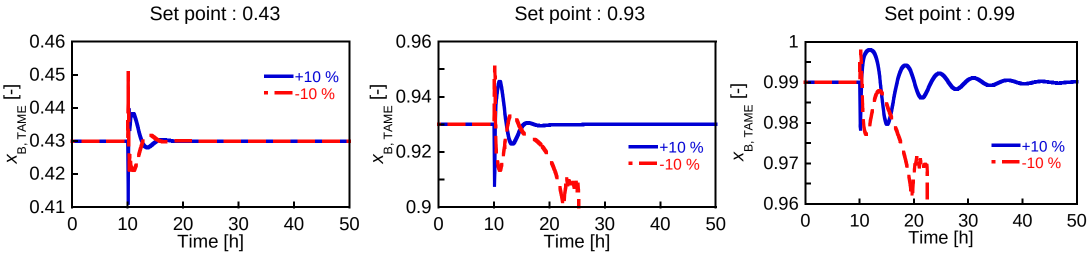

Figure 7: Dynamic responses of bottom TAME composition for ± 10% step change in the pressure of overhead

4. Discussion

The dynamic response results for ±10 % step change in pressure of overhead show that effect of the pressure for the reaction and separation performance is more important than the variable of feed flow rate and reflux ratio. Only the case of pressure disturbance was led to failure for control of bottom TAME composition. Thus, we have analysed the effect of pressure and reflux ratio for the process performance using bifurcation diagrams. Figure 8 shows the bottom TAME composition with the variation of the reboiler duty and the pressure or the reflux ratio. For the increase of the reflux ratio, the region of the MSS shifts in the direction toward the large reboiler duty. The range of bottom TAME composition within the MSS was same results about 0.4 to 1.0. On the other hand, the region of the MSS varies widely depending on the pressure of overhead. Compared with the base case results, it is clearly found that the range of bottom TAME composition within the MSS decrease about 0.32 to 0.82 in the operation of the pressure 227.7 kPa. Reduction of pressure is led to decreasing temperature, and decreasing temperature in reactive section produces low reactive performance for TAME synthesis. Therefore, the case of pressure 227.7 kPa obtained maximum bottom TAME composition of 0.82. Since the operation of low pressure (227.7 kPa) was not reached TAME composition over 0.82, the case of set point 0.93 and 0.99 was failed for the -10 % change in the pressure.

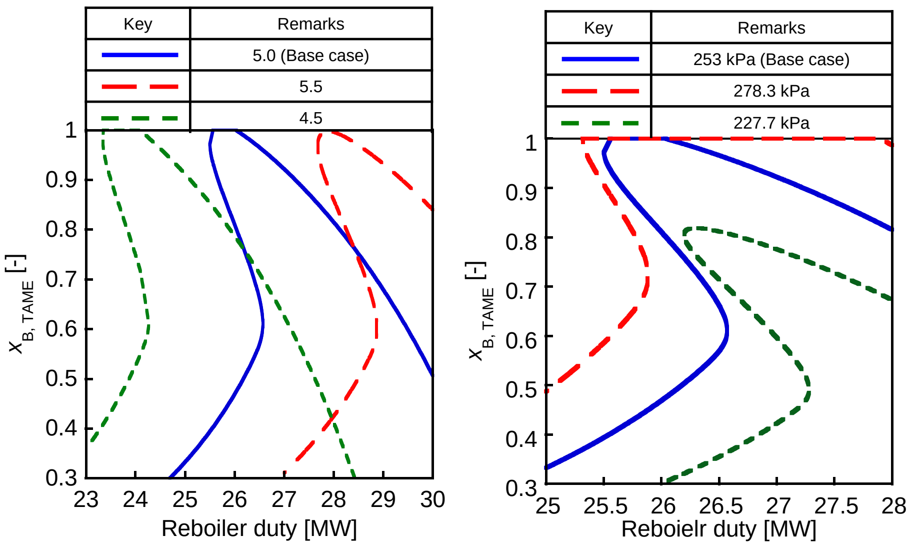

Figure 8: Bifurcation diagram with effect of operation condition: (a) reflux ratio, (b) pressure

5. Conclusion

In this work, the *tert*-amyl methyl ether (TAME) synthesis case study was used to consider the process dynamics and controllability on the MSS conditions. Five PI controllers were prepared for control of condenser and reboiler liquid level, feed flow rate, pressure of column overhead and bottom TAME composition. For the change of composition controller set point, reboiler duty indicated the MSS such as bifurcation results of steady state simulation. Three initial conditions as upper, middle and lower brunch of bifurcation diagram was used to highlight the controllability for the disturbances of feed flow rate, reflux ratio and pressure of column overhead. Bottom TAME composition on the MSS was controlled for the disturbance of feed flow rate and reflux ratio, but the pressure disturbance was led to failure control for set points at upper and middle brunch. The controllable range was estimated using bifurcation diagrams.

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