Role of Multiplicity in Control System Design for a Methyl Acetate Reactive Distillation Column

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Abstract

The impact of steady-state multiplicities on the control of a methyl acetate reactive distillation (RD) column is studied. It is shown that input multiplicity, where multiple input values give the same output, can lead to “wrong” control action, leading to poor robustness. A new metric, rangeability, is defined to quantify the severity of input multiplicity in a steady-state input-output (IO) relation. Rangeability can be used in conjunction with conventional sensitivity analysis for the design of robust control structures for RD systems. The design methodology is illustrated for the temperature based control of an industrial scale methyl acetate column. Results for a synthesized control structure shows that controlling the most sensitive reactive tray temperature can lead to poor robustness due to low rangeability resulting in “wrong” control action for large disturbances. Controlling a reactive tray temperature with acceptable sensitivity but larger rangeability gives better robustness. It is also shown that controlling the difference in the temperature of two suitably chosen reactive trays gives better robustness of the control structure due to improved rangeability. The article brings out the importance of IO relations in understanding the complex dynamic behavior of RD systems.

Keywords: Reactive distillation control; input multiplicity; control system design

Introduction

Reactive distillation (RD) is a process intensification technique that combines reaction and separation in a single vessel and can replace conventional "reactor followed by separator" units at a fraction of capital and operating costs (Siirola, 1995). Although, RD is economical, the design of robust control systems for the same is quite challenging due to the non-linearity of the process resulting from the coupling of reaction and separation in a single column. Unlike ordinary distillation systems, the non-linearity can lead to the existence of steady-state multiplicities and non-monotonic temperature profiles. In view of these complexities, RD control has received much attention in the literature in recent years and remains an active research area. The large body of RD literature shows that many RD systems exhibit steady-state multiplicities (see for e.g. Taylor and Krishna, 2000; Kienle and Marquardt, 2003). The impact of these multiplicities on control performance and control system design has not been explicitly addressed in a systematic manner even as recent articles have alluded to avoiding the use of outputs showing input multiplicity in control loops (Hung et. al., 2006; Lin et. al., 2006).The impact of multiplicities on the control structure design is explicitly demonstrated in this work for an example industrial scale methyl acetate RD column.

Effect of multiplicity on RD Control

Steady-state multiplicities can be classified into input and output multiplicity as shown in Figure 1. Multiple inputs result in same output in case of input multiplicity while same input corresponds to different outputs in case of output multiplicity. In the case of an RD column, typically, input variables are reboiler duty, fresh feeds, reflux ratio and reflux rate while tray compositions, product purities and tray temperatures are regarded as output variables.

The implication of output multiplicity is on the start-up of a column. For example, there can be three distinct values of a tray temperature at the design values of fresh feeds and reflux ratio. Typically, these three distinct values would correspond to low, intermediate and high reaction conversion steady-states. Since the high conversion steady-state has a unique tray temperature, a simple temperature control loop with its set-point corresponding to this unique temperature, can be implemented to ensure that the column reaches the high conversion steady-state during start-up and then remains there in the face of disturbances. Thus, feedback control can be effectively utilized to prevent steady-state transitions and ensure proper column operation in case of output multiplicity.

On the other hand, the implications of input multiplicity on the RD column can be more severe. Consider input-output (IO) relation given in Figure 2 and assume that the output (y) is controlled using the input (u). Note that the controller is "direct" acting for the base-case shown (point 'o'). It can be seen that output is below the base case value between points 'o' and 'a' so that the controller would decrease the input to force the output back to its base-case value. However, the output is above the base-case value beyond point "a" and the "direct" acting controller would increase the input which corresponds to the "wrong" control action. The correct control action thus switches from "direct" near the vicinity of the base-case "o" to "reverse" for a large increase in the input (beyond "a"). Such a change in controller action is impractical so that for sufficiently large deviations, the column can drift continuously to either settle at a completely different steady-state (point 'c' in Figure 2) if the IO relation turns back again or until an operating constraint such as flooding or a saturated valve, is hit. The quantification of severity in the input multiplicity is thus more desirable.

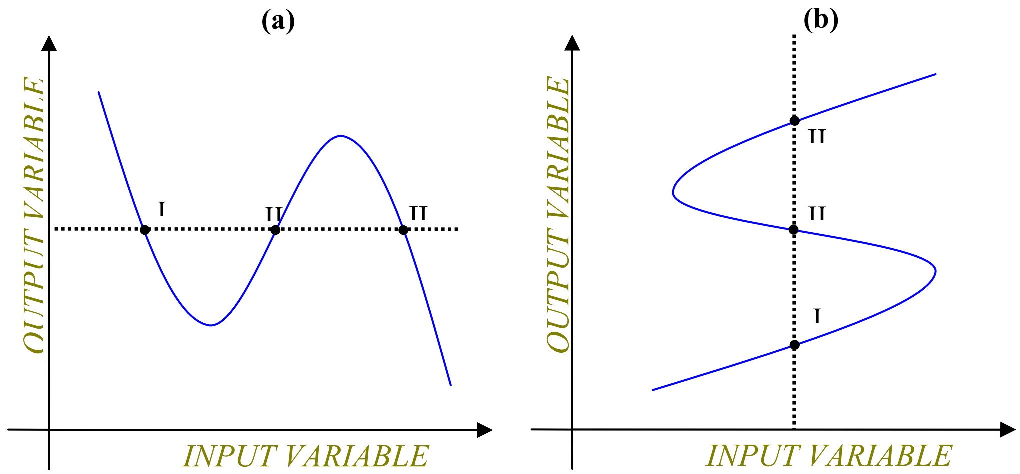

Fig. 1. Two types of steady-state multiplicities
(a) Input multiplicity
(b) Output multiplicity

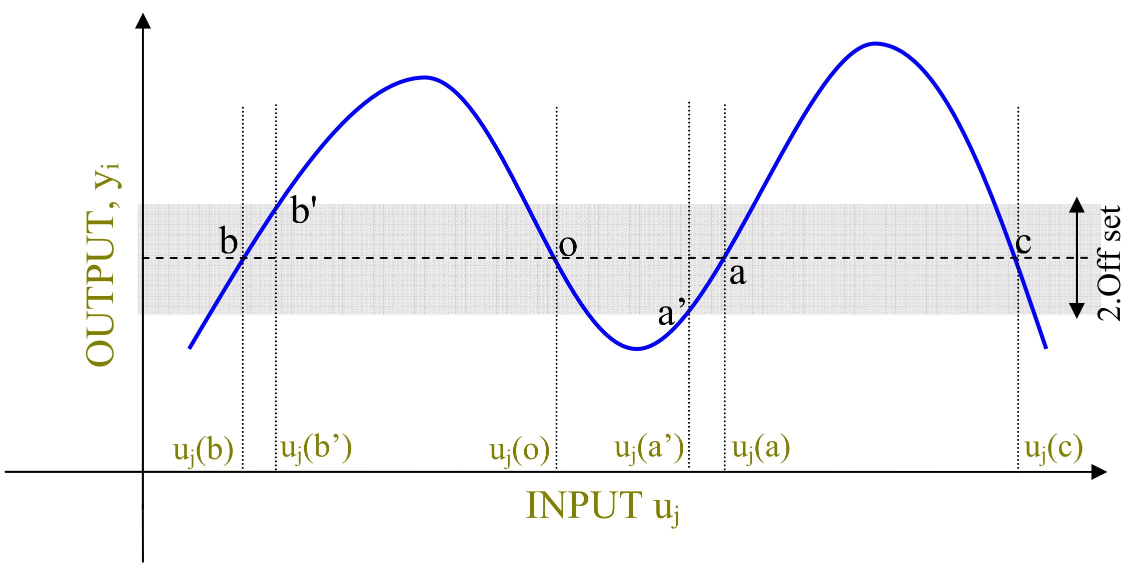

Fig. 2. A non-linear input-output relation with input multiplicity

3. Rangeability

In the above section, it has been argued that for a large enough disturbance in the input, input multiplicity can lead to "wrong" control action. If we consider Fig. 2, the output crossing its base-case value leads to non-uniqueness in the output with respect to the input. The limits on the input value are generally the points where output crosses its basecase value on the either side of its base case point. Now we can define rangeability of an output (y) with respect to the input (u). The rangeability of the input above its base-case value is defined as

$$R_{i,j}^{+} = u_j(a) - u_j(o) : u_j(a) \text{ is the first such crossing point above } u_j(o),$$

Similarly for decrement in input (u)

$$R_{i,j}^{-} = u_j(o) - u_j(b) : u_j(b) \text{ is the first crossing point below } u_j(o)$$

If such crossing points do not exist, then $u_j(a)$ and $u_j(b)$ should be replaced by u_j^{max} and u_j^{min} respectively)

A modification for the above definition for rangeability can be given as follows. Instead of taking the value of the input where the output equals its base-case value, the value of the input where the output differs from the base-case by an offset is taken (corresponding points are marked as a' and b' in Fig. 2. This modification is appropriate in control point of view, because controller will see sufficient deviation in the set-point and the error in the output value will bring the output back to its basecase value in sufficient amount of time. Otherwise, at points where output exactly matches with the basecase value, controller will see no error and control action becomes negligible. It can be seen that incorporation of offset ensures that that output will be brought back to its basecase design value in a sufficient amount of time. From Fig. 2, the definition of rangeability is modified to

$$R_{i,j}^{+} = u_j(a') - u_j(o), \text{ for + change in u,}$$

and

$$R_{i,j}^{-} = u_j(o) - u_j(b') \text{ for – ve change in u.}$$

The steady-state IO relations are generated using homotopy continuation (Singh et al. 2005). It is shown that IO pairing with greater rangeability would provide more robustness to a control system and wrong control can be avoided. Identification of sensitive outputs with high rangeability is then a crucial step in the design of robust control structures for RD systems.

Case Study

A schematic of the methyl acetate column with all design parameters is shown in Fig. 3 (Al-Arfaj and Luyben, 2002). 95 mol% of pure methyl acetate is produced at the top of the column as distillate while the reaction conversion is 98%. Bottom stream from the column contains 96 mol % of water. Wilson model has been used for liquid activity coefficient calculation while vapor phase is treated as ideal. Marek's method is used to account for the vapor phase acetic acid dimerization on the VLE (Marek, 1955). The liquid and vapor phase enthalpies are calculated using the DIPPR method. An activity based reaction rate equation is used to model the reaction kinetics. Details of the column design, thermodynamic / kinetic models and parameters in this work can be found in Singh et al (2005). Steady state simulations are carried out using an in-house simulator developed using Naphtali-Sandholm method (Singh et. al., 2006) and the dynamic simulator uses the algorithm proposed in Jhon and Lee, (2003). Both steady state and dynamic simulators are developed in MATLAB package.

In this column, assuming the reflux drum and reboiler levels are controlled using the distillate and bottoms respectively, the available manipulated variables (inputs) for performing the regulatory tasks (maintaining stoichiometric balance and regulating the column internal flow) are the reboiler duty, the two fresh feeds and the reflux rate. The fixed reflux ratio policy is preferred over the fixed reflux rate policy as the former avoids output multiplicity (Singh et al. 2005).

The sensitivity of the tray temperatures to the three inputs, namely, reboiler duty, fresh acetic acid feed and fresh methanol feed, is plotted in Fig. 4. Temperature of Tray 18 and 34 are sensitive with respect to acetic acid while temperature of Tray 34 is sensitive with respect to methanol. All the reactive trays are insensitive with respect to methanol. By looking at the sensitivity diagram (Fig. 4), one control structure can be proposed in which fresh acetic acid used to control the reactive tray while methanol feed controls the bottom stripping tray temperature.

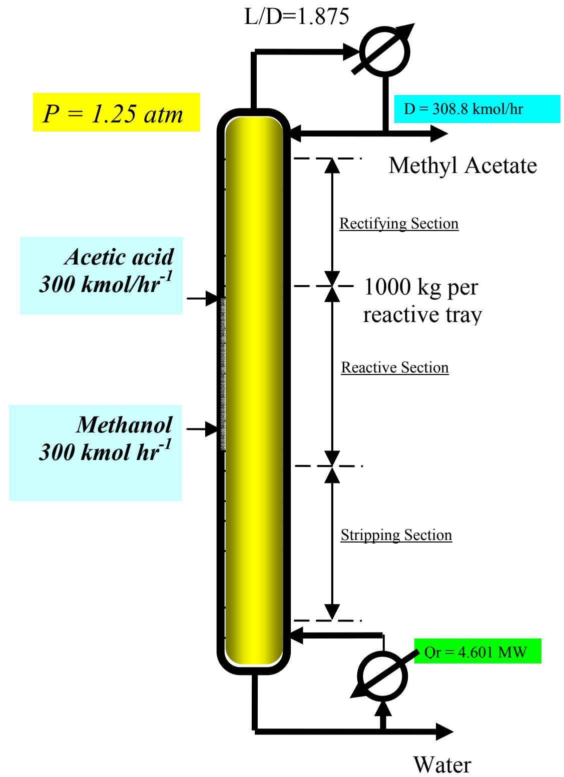

Fig. 3. Schematic of methyl acetate RD column

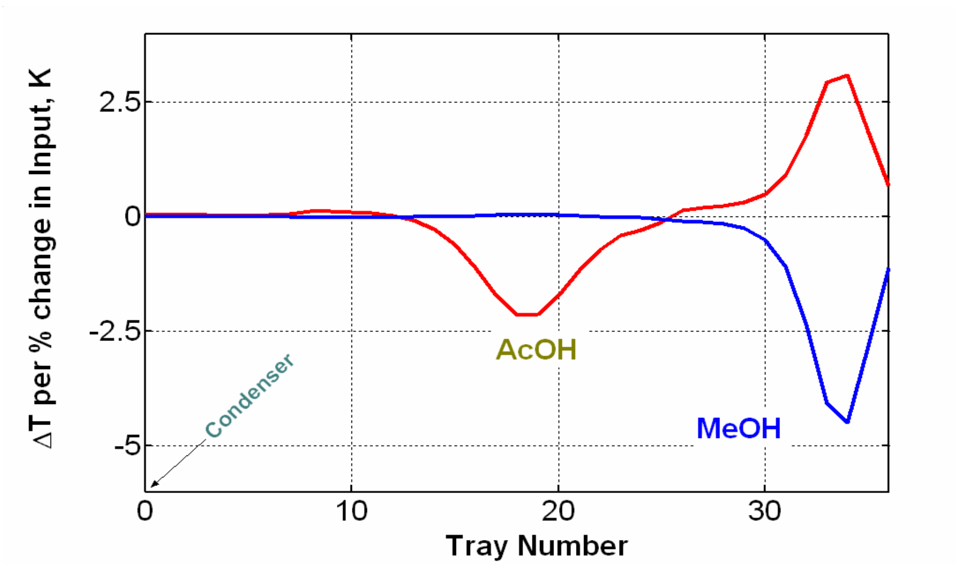

Fig. 4. Tray temperature sensitivities with respect to acetic acid (AcOH) and methanol (MeOH).

The steady-state variation in the sensitive tray temperatures with respect to changes in bothe feeds about their basecase individually is shown in Fig. 5. From this we can asses the non-linearity in the IO relation. The reactive Tray 18 temperature shows input multiplicity with respect to two fresh feeds where Tray 24 temperature does not show any multiplicity with respect to two fresh feeds. This input multiplicity occurs in the direction where the acetic acid becomes excess so that the control achieved for disturbances leading to excess acetic acid may be poor. Near the base-case, reactive Tray 18 temperature is flat with respect to the fresh methanol flow. Note that even as reactive Tray 18 is the most sensitive, it shows input multiplicity at the base-case for fresh acetic acid. Its rangeability with respect to acetic acid increase and methanol increase is respectively 8.8%, 0% respectively using 3K offset. Its use in a control loop may lead to porr robustness.

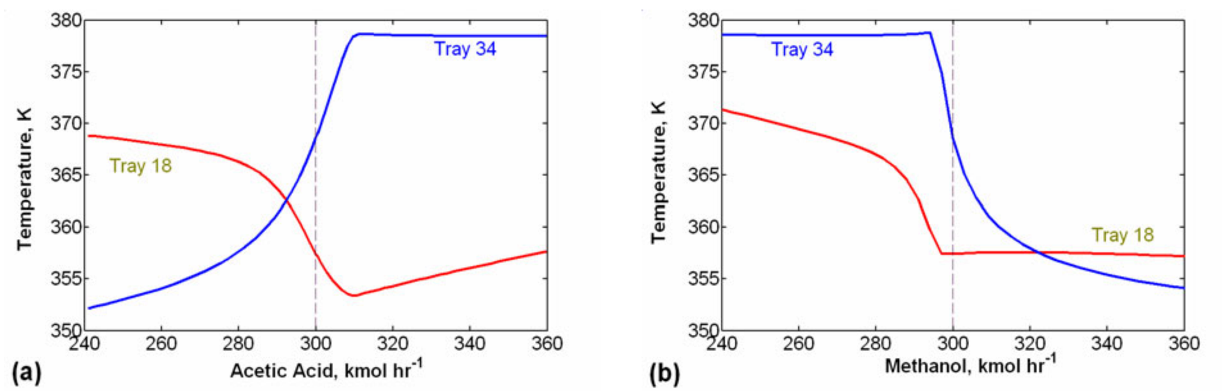

Fig. 4. Steady-state input-output relation of Tray 18 and Tray 34 temperatures.
(a) AcOH (b) MeOH

Pseudo output variables

Robust control requires sensitive IO pairing with large rangeability. Sometimes, IO pairings with moderate sensitivity and large rangeability may improve robustness of a control structure. The variation in the temperatures of some reactive trays with respect to fresh acetic acid is shown in Fig. 6. and also the rangeability of the sensitive reactive tray temperatures with respect to the acetic acid is tabulated in Table 1. In Fig. 6, notice that even as Tray 20 temperature is less sensitive than Tray 18 at the base-case operating condition as indicated by the local slopes, its rangeability is much better. Thus T_{20} appears to be a good compromise between sensitivity and rangeability as verified from Fig. 3 (sensitivity data) and Table 1 (rangeability data).

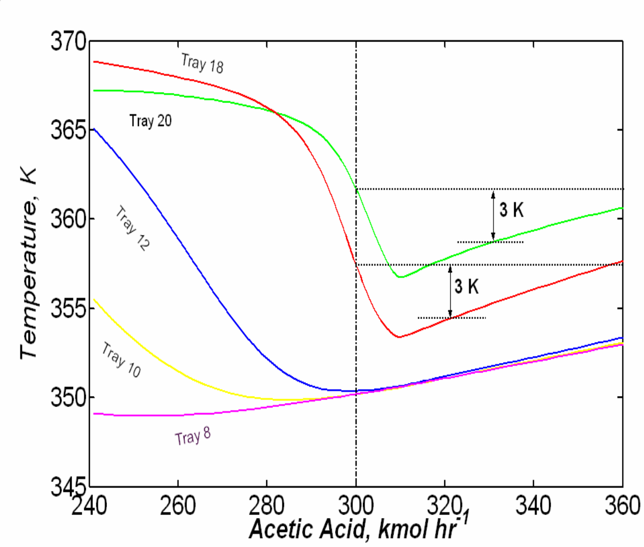

Fig. 6. Variation of reactive tray temperatures with respect to acetic acid.

Another alternative for improving rangeability is to control a pseudo-output, which is a suitable combination of reactive tray temperatures that mitigates input multiplicity to the extent that the pseudo-output does not cross its base-case value for the expected range of variation in the input. Then there exists a unique pseudo-output value corresponding to the base-case. In Fig. 6, notice that Tray 8 temperature is parallel to the sensitive reactive tray temperatures in the region of input multiplicity so that the difference between a sensitive tray temperature and Tray 8 temperature will lead to a pseudo-output with a flat response with respect to the input in the region of multiplicity.

Table 1. Rangeability of sensitive reactive tray temperatureswith respect to acetic acid and methanol

Tray Number	AcOH		MeOH	
	-	**+**	**-**	**+**
16	**> 20**	**0**	**> 20**	**0**
17	**"**	**0**	**"**	**"**
18	**"**	**8.8**	**"**	**"**
19	**"**	**10.9**	**"**	**"**
20	**"**	**11.1**	**"**	**"**
21	**19.2**	**7**	**"**	**"**

The difference in two reactive tray temperatures can thus give a pseudo-output with higher rangeability. Roat et al. (1987) have mentioned this possibility in their work. The choice of the two trays must be made carefully so that input multiplicity is mitigated for the expected range of variation in the inputs. This is evident in Fig. 7 which shows that T_{20}-T_8 does not cross its base-case value for a 20% increase and decrease in the fresh acetic acid whereas other combinations lead to a cross-over. For a 20% change in the inputs in either direction T_{20}-T_8 remains more than 4 K away from its base-case value. The rangeability with respect to acetic acid is thus >20% for both an increase and a decrease in the inputs. The large rangeability for T_{20}-T_8, also referred to as ΔT, implies its use as a controlled variable can lead to more robust control. As before, there remain one basic control structure, with three different outputs from the reactive section, namely, T_{18}, T_{20} and ΔT, being controlled. In the control structure nomenclature, these three different outputs are identified respectively, through superscripts 'a', 'b' and 'c'. A schematic of this basic control structure (CS1) is shown in Fig. 8.

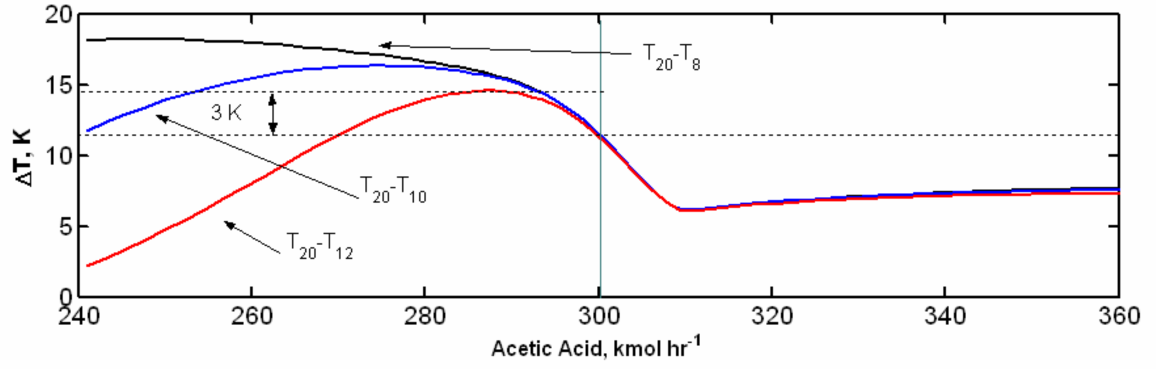

Fig. 7. Steady-state variation of difference between two reactive tray temperatures with Acetic acid

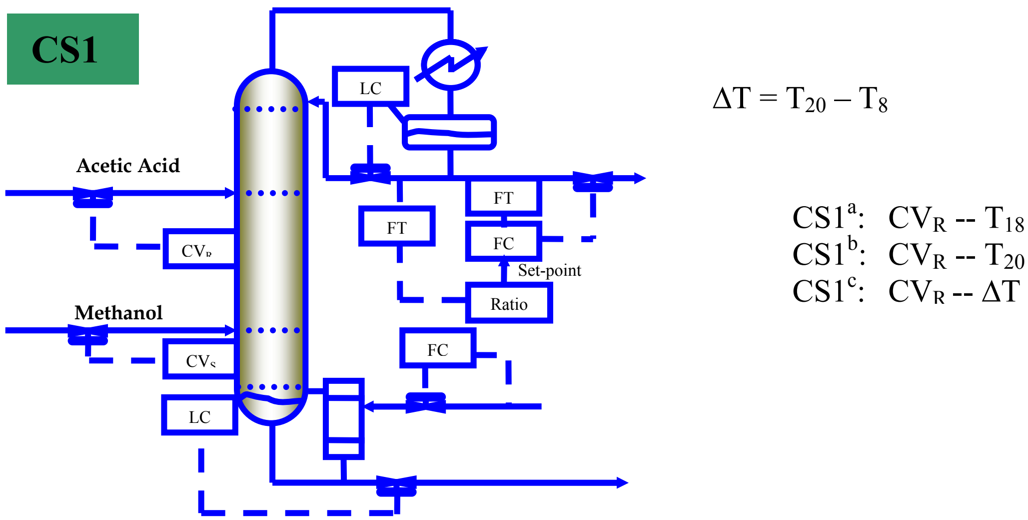

Fig. 8. Schematic of candidate control structures CS1 and CS2

7. Dynamic Results

The reset time for each loop in this control structure is obtained from the open loop step response to a small 1% change in the control input. As a conservative estimate, it is set to one-third of the time taken for the open-loop response to finally reach within 5% of its final steady-state value. Note that a first order response takes three time constants for 95% completion. The two controller gains must now be obtained. In CS1, the dynamic response of the reactive loop using acetic acid as the manipulation handle is slow so that its controller gain is set to the inverse of the process gain as a conservative estimate. The gain of the stripping loop is adjusted for a good closed loop response.

The dynamic response of the column to a 20% increase and a 20% decrease in the production rate handle set-point is obtained for the proposed control structure. The reboiler duty set-point acts as the production rate handle for the proposed control structure. Fig. 9 plots the manipulated and controlled variables for this CS1, namely the two fresh feeds and T_{18} and T_{34}, for a +20% and a -20% change in the reboiler duty. The figure clearly illustrates “wrong” control action by the acetic acid loop for a -20% change. Instead of decreasing, the controller increases the fresh acetic acid feed since T_{18} is more than its set-point and the “direct” acting controller thinks that to bring it back to set-point, more acetic acid must be added. From the plot, notice that the dynamic variation in the fresh feeds for a -20% change is such that methanol decreases quickly while the acetic acid decreases slowly. This leads to an excess of acetic acid being fed and the input multiplicity due to excess acetic acid, as seen in Figs. 8c and 8d leads to “wrong” control action. On the other hand, for a +20% step change in the reboiler duty, the methanol and acetic acid move together and excess acetic acid does not build so that the input multiplicity region is avoided. The maximum production rate decrease this $CS1^a$ can handle turns out to be -15%.

Similar to $CS1^a$, both $CS1^b$ and $CS1^c$ are able to handle a 20% increase in the reboiler duty. However, unlike $CS1^a$, both structures are able to handle a 20% decrease in the reboiler duty. The closed loop response of both feeds and deviation of controlled variables from their respective set-points for a -20% change in reboiler duty for $CS1^b$ and $CS1^c$ is shown in Fig. 10. Notice that “wrong” control action is avoided and the methanol and acetic acid follow each other much better than for $CS1^a$ (see Fig. 9) so that the multiplicity region is avoided. The improvement in control performance can be directly attributed to the higher rangeability that T_{20} and ΔT show. $CS1^b$ fails for a production rate decrease of 30% while $CS1^c$ is found to work even for a 40% production rate decrease (larger changes were not tested). This is in direct agreement with the fact that the fresh acetic acid shows greater rangeability with respect to ΔT than T_{20}. The significant impact of the choice of controlled variables on the robustness of a control structure is thus clearly illustrated. The key role of input multiplicity in understanding the dynamic results and the utilization of rangeability as a quantitative measure for the proper selection of controlled variables is also highlighted.

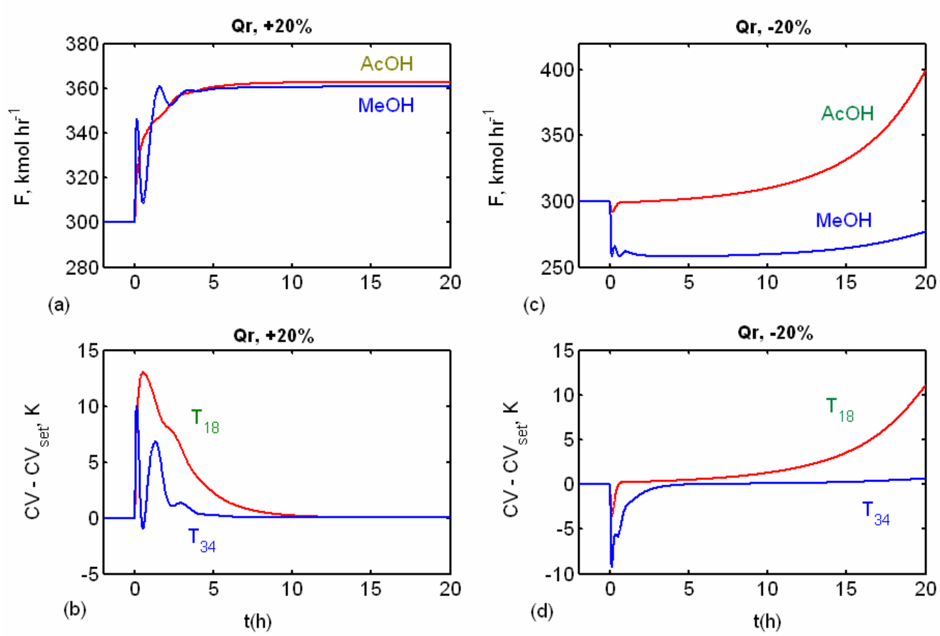

Fig. 9. Dynamic response of manipulated and control variables for ±20% change in reboiler duty for CS1[a] control structure.

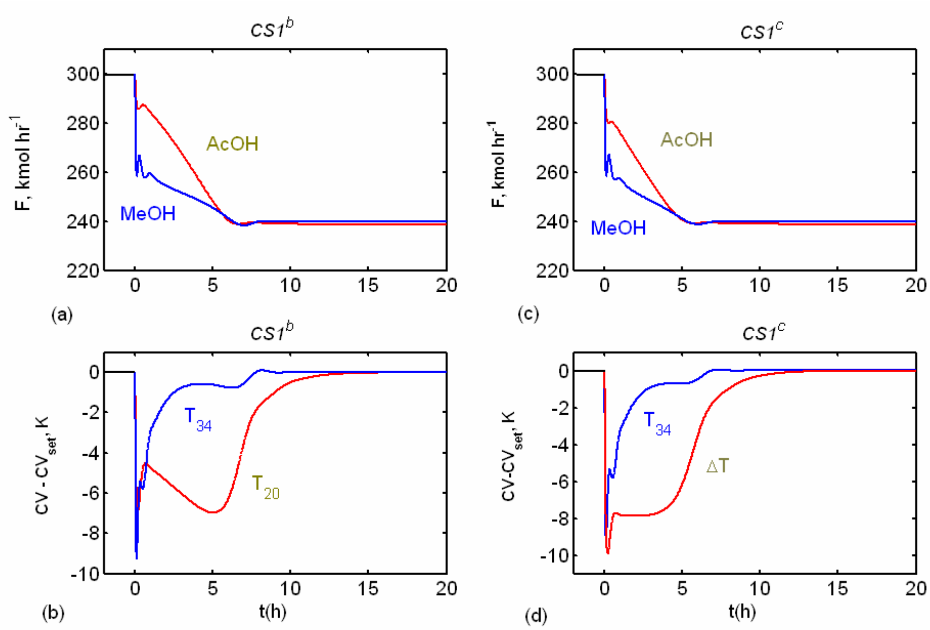

Fig. 10. Manipulated and controlled variable dynamic response for -20% change in reboiler duty for CS1[b] and CS1[c].

Discussion

The dynamic simulations show that the “wrong” control action occurs whenever a large amount of unreacted acetic acid “breaks-through” from the reactive section into the stripping section. This can happen when the acetic acid is fed in large excess relative to methanol or if the reboiler duty is lowered sufficiently. The IO relations in Fig. 6 also suggest as much where the reactive tray temperatures show input multiplicity when the acetic acid feed is increased or when the reboiler duty is decreased. The key to robust column control then lies in ensuring that such a “break-through” is prevented via proper choice of the controlled and the manipulated variables

The idea of preventing acetic “break-through” into the stripping section also suggests that the liberal use of ratio controllers can significantly improve the robustness of a control structure since changing the three inputs in ratio would prevent an excess of acetic acid from building and consequent “break-through” into the stripping section. For example, CS1 can be modified so that the two fresh feeds are kept in ratio with the reboiler duty and the temperature controllers adjust the ratio set-point. Through rigorous dynamic simulations, it was found that such a control structure easily handles a 30% production rate change in both directions regardless of the controlled variable used (T_{18}, T_{20} or ΔT). On the other hand, a control structure implementing a ratio controller between the two feeds with the reactive loop adjusting this ratio set-point remains susceptible to “wrong” control action for a large step decrease in the reboiler duty. The reason is the input multiplicity corresponding to a reduction in the reboiler duty (Fig. 5b). A sudden large decrease in the reboiler duty allows acetic acid to “break-through” into the reactive section. Clearly, the insights gained from steady-state IO relations are invaluable in understanding the complexities of RD control.

Conclusions

The methyl acetate case study shows that input multiplicity can lead to “wrong” control action for large disturbances moving the column towards the multiplicity region. The effectiveness of column regulation thus depends on both the direction and magnitude of the disturbance. A new metric, rangeability, has been proposed to quantify the severity of input multiplicity. Rangeability can be used in conjunction with conventional tools such as sensitivity analysis and Niederlinski Index for the design of effective control structures. Dynamic results for the control structure proposed show that contrary to conventional wisdom, controlling the most sensitive output results in poor robustness due to the low rangeability of this output. On the other hand outputs with acceptable sensitivity and greater rangeability provide more robust control. Also, a suitable combination of outputs can result in greater rangeability so that controlling this pseudo-output enhances the robustness of the control system. Rangeability is thus a useful tool for the proper selection of controlled variables for RD column control.

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