Temperature Inferential Dynamic Matrix Control of Reactive Distillation Systems

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Abstract: Two-temperature inferential control of the ideal and the methyl acetate double feed reactive distillation (RD) systems operated neat is evaluated using constrained dynamic matrix control (CDMC) and traditional decentralized control. For the ideal RD system, significant improvement in the stripping tray temperature control and the transient deviation in the bottoms purity is observed using CDMC. For the methyl acetate system, CDMC results in significant improvement in the control of the two tray temperatures as well as transient deviations in both the distillate and bottoms purity. Results also show that the magnitude of the maximum through-put change for which the control system fails is noticeably higher using CDMC.

Keywords: Reactive distillation control, dynamic matrix control, temperature inferential control

1. INTRODUCTION

Reactive distillation (RD) is now an established process intensification technology combining reaction and separation in a single column with potentially significant economic savings when the reaction kinetics and component relative volatilities are favorable (Siirola, 1995). When compared to conventional "reactor-separator" processes, the high non-linearity due to direct interaction between reaction and separation combined with fewer control degrees-of-freedom makes the design of an effective control system crucial to the successful implementation of RD technology.

In probably the first paper on RD control, Roat et al (1986) demonstrated that seemingly appropriate control structures succumb to a steady state transition for a moderately large through-put change suggesting the presence of high-non-linearity. Several later articles highlighted the presence of steady state multiplicity in various RD systems (see eg Mohl et al, 1999; Taylor and Krishna, 2000). The presence of steady state multiplicity can result in non-linear dynamic phenomena under open and closed loop operation. Sneesby et al (1997) considered the implications of steady state multiplicity on the operation and control of etherification columns. Kumar and Kaistha (2008a) demonstrated the occurrence of 'wrong' control action and closed loop steady state transition for the hypothetical quaternary ideal RD column studied by Al-Arfaj and Luyben (2000).

Given the high non-linearity in RD systems, the application of non-linear control techniques has been recommended in the literature. Among the prominent non-linear RD control works, Kumar and Daoutiditis (1999) implemented a non-linear inversion based control scheme for an ethylene glycol RD column. Model based gain scheduling has been applied to an ETBE RD column. Gruner et al (2003) report the non-linear control of an industrial RD column operated by Bayer. More recently, Kawathekar and Riggs (2007) have applied a non-linear model predictive control scheme to an ethyl acetate column.

Even as non-linear model based control is widely accepted in the academic community, industrial practice remains strongly biased towards the traditional decentralized PI control and where justifiable, linear model predictive control techniques such as DMC. This is probably due to the difficulty in developing a high fidelity non-linear process model and identifying the model parameters in an industrial setting.

A careful examination of the RD control literature reveals that the control of two-reactant double-feed RD columns operated neat (no excess of a reactant) such as the quaternary ideal RD system and the methyl acetate RD system, is particularly challenging due to the need for stoichiometric balancing of the two fresh feeds. Adjusting one of the fresh feeds to maintain an appropriate tray composition has been shown to be an effective means of maintaining this balance. The use of temperature measurements instead of composition, the former being much more rugged, reliable, cheap and with fast measurement dynamics, however causes the control system to succumb to non-linear dynamic phenomena such as 'wrong' control action in the methyl acetate RD system or a closed loop steady state transition in the quaternary ideal RD system (Kumar and Kaistha, 2008a). Application of linear MPC techniques, which have found industrial acceptance, may significantly improve the performance of a temperature inferential control system for such 'difficult to regulate' processes. This work addresses the same for the quaternary ideal and the methyl acetate RD systems.

2. BASE-CASE COLUMN DESIGN

Figure 1 shows a schematic of the double feed RD columns studied in this work. The reaction $A + B \leftrightarrow C + D$ occurs in the reactive zone. For the methyl acetate system, the components A, B, C and D correspond to methanol, acetic acid, methyl acetate and water respectively. For the ideal RD system, the component relative volatilities are in the order $\alpha_C > \alpha_A > \alpha_B > \alpha_D$ so that the reactants are intermediate boiling. The reaction kinetics and thermodynamic property models for the methyl acetate and the ideal RD system are taken from Singh et al (2005) and Al-Arfaj and Luyben (2000), respectively. The base-case design and operating conditions for the ideal RD system are taken from Kaymak and Luyben (2006). The internally heat integrated design of the methyl acetate RD system reported in Kumar and Kaistha (2008 b) is studied here. The salient design and operating conditions for the two systems are reported in Table 1.

$$A + B \leftrightarrow C + D$$

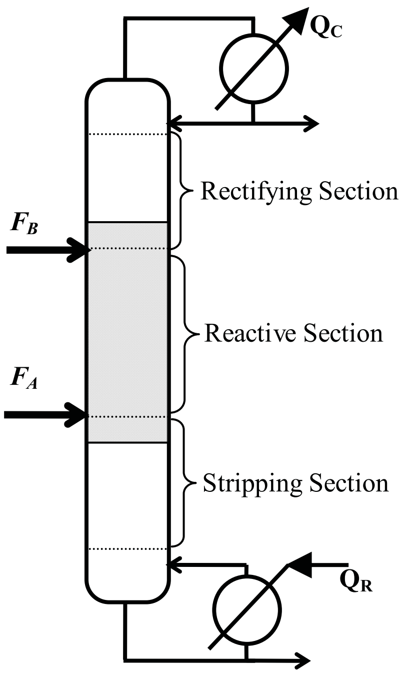

Figure 1. Schematic of a double feed reactive distillation column

Table 1: Design Parameters of Ideal RD system and Methyl Acetate system

	Ideal RD Column	Methyl Acetate RD column
Flow rate of feeds	$F_A = F_B =$ 12.6 mol/s	$F_{HAc}=F_{MeOH}$ =300 kmol/hr
$N_E/N_{RX}/N_S$ design	5/10/5	7/18/10
Feed tray locations	$n_{FA} = 9$; $n_{FB} = 12$	$n_{FMeOH} = 16$; $n_{FHAc} = 28$
Catalyst loading per reactive tray	0.7 kmol	300 kg
Pressure	8.5 bar	1.013 bar
Reflux ratio	2.6927	1.4877
Distillate rate	12.6 mol/s	308.63 kmol/h
Reboiler duty	0.8516 MW	3.66387 MW
Product purities	X_C,D = X_D,B = 0.95	X_{MeOAc},D=0.95 X_{H2O},B=0.96

3. TEMPERATURE INFERENTIAL CONTROL

3.1 Control Structures

Figure 2 & 3 plot the tray temperature sensitivities with respect to the two fresh feeds and the reboiler duty at constant reflux ratio for the ideal and methyl acetate columns. The sensitivity plots, suggest two candidate control structures, labeled as CS1 and CS2 for convenience. In CS1, F_A controls a sensitive stripping tray temperature while F_B controls a sensitive reactive tray temperature. The reboiler duty (Q_R) acts as the through- put manipulator. CS2 differs from CS1 in that the Q_R, instead of F_B is used to control a sensitive reactive tray temperature with F_B being the through-put manipulator. The two control structures are schematically depicted in Figure 4. Using bottom-up tray numbering, the temperature of Tray 2 (T_2), a stripping tray, and Tray 12 (T_{12}), a reactive tray, is controlled in the ideal RD column. In the methyl acetate column, the control tray temperature locations are Tray 2 (T_2) and Tray 13 (T_{13}). Note that in the ideal RD system, even as a rectifying tray temperature exhibits higher sensitivity than a reactive tray with respect to F_B (see Figure 2), it is not controlled due an inverse response with respect to F_B (Kaymak and Luyben, 2006) and severe input multiplicity resulting in a steady state transition for moderately large through-put changes (Kumar and Kaistha, 2008a).

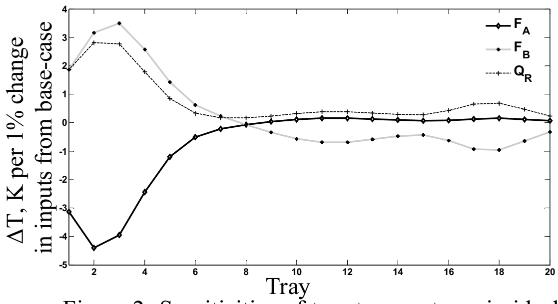

Figure 2: Sensitivities of tray temperatures in ideal RD system with respect to fresh feeds (F_A & F_B) and reboiler (Q_R) duty at fixed reflux ratio

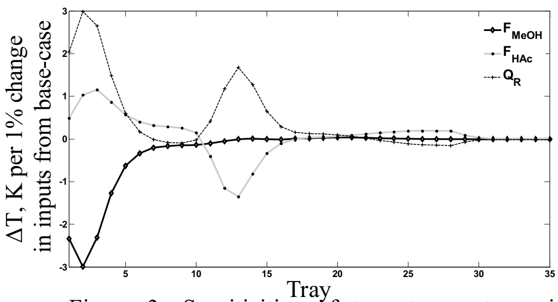

Figure 3: Sensitivities of tray temperatures in methyl acetate system with respect to Methanol feed (F_{MeOH}) and Reboiler Duty (Q_R) at fixed reflux

3.2 Dynamic Simulation and Temperature Controller Details

An in-house dynamic simulator is used to generate the open and closed loop dynamic simulation results for the two RD columns. With the two level controllers and perfect pressure control in place, a 2x2 temperature control system as in structures CS1 and CS2 is implemented. A 1 min lag is applied to the temperature measurements. The performance

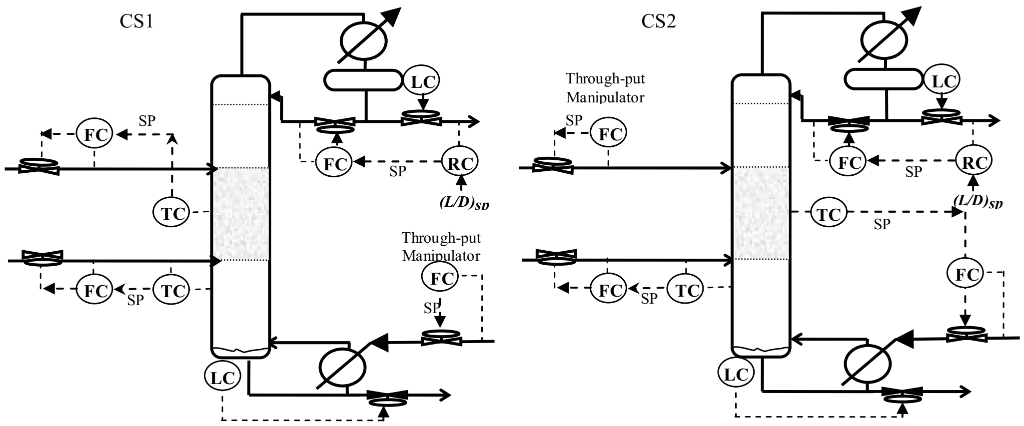

Figure 4. Schematic of used two point temperature inferential control structures

Table 2: CS1 & CS2 controller parameters for the ideal and methyl acetate RD column

Tuning parameters used in CDMC in the two systems						
System	MV	γ	CV	λ	P min	C min
Ideal RD Column with CS1	F_A	1	T_3	5	90	50
	F_B	40	T_{12}	10		
Ideal RD Column with CS2	F_A	1	T_3	5	90	50
	Q_R	4	T_{12}	10		
Methyl Acetate Column with CS1	F_{MeOH}	3	T_2	20	250	125
	F_{HAc}	4	T_{13}	25		
Methyl Acetate Column with CS2	F_{MeOH}	1	T_2	20	250	125
	Q_R	4	T_{13}	25		
Span of temperature measurements = 50K; All valves are 50% open at their design steady state. Slew rate constraints used in CDMC limits the rate of change of manipulated variable from zero to the base-case design value in no less than 2 minutes.						

of a 2x2 decentralized controller is to be compared with that of a 2x2 multivariable constrained dynamic matrix control (DMC) controller. For tuning the two decentralized PI temperature controllers, the relay feedback test is performed to obtain the ultimate gain and ultimate period of the temperature loops. The Tyreus-Luyben controller settings are then applied with appropriate de-tuning, if necessary. In the ideal RD column, both the temperature loops are tuned independently. In the methyl acetate column, sequential tuning is applied where the stripping loop is first tuned. For the DMC controller, appropriate valve saturation and slew rate constraints are applied. The slew rate constraint corresponds to the maximum rate of change of the DMC controller causing the output to saturate in two minutes. The sampling rate of the DMC controller is 0.5 minutes for the ideal RD column and 0.625 minutes for the methyl acetate RD column. The DMC step coefficient matrix is obtained using a +1% step change in the appropriate input. The tuning parameters used for CDMC are shown in Table 2.

4. RESULTS

A through-put change is considered as the primary disturbance to be rejected by the control system. The closed loop performance of the multivariable DMC and decentralized controller is now evaluated for the ideal and the methyl acetate RD columns.

Figure 5 plots the ideal RD column closed loop response to a ±20% through-put change using CS1 as the control structure. The response completion time is about 4 hours for both the controllers. Significantly tighter stripping tray temperature control (T_2) is achieved by the DMC controller while the reactive tray temperature control is comparable. This translates to tighter bottoms purity (x_D,B) control and no appreciable benefit in the distillate purity (x_C,B) control using the DMC controller.

Figure 6 plots the closed loop response to a ±20% through-put change in ideal RD column for CS2 using a decentralized and DMC 2x2 temperature controller. Significantly tighter T_2 and T_{12} temperature control is achieved by the DMC controller.

The closed loop response of the methyl acetate column to a ±20% through-put change is plotted shown in Figure 7. The CDMC temperature controller is far superior to the decentralized controller. The transient deviation in reactive T_{13} control is much smaller for the DMC controller. The tightness of the T_2 control is also better. The tighter temperature control translates to lower transient deviations in both the distillate (x_{MeOAC},D) and bottoms product purity (x_{H2O},B). Notice that with the DMC controller, the two fresh feeds move in tandem for a better stoichiometric feed balance during the transient with consequent improvement in the control performance. Figure 8 plots the closed loop response of CS2 to a ±20% through-put change for the methyl acetate RD column. For this structure also, the DMC achieves much tighter control of the stripping and reactive tray temperatures.

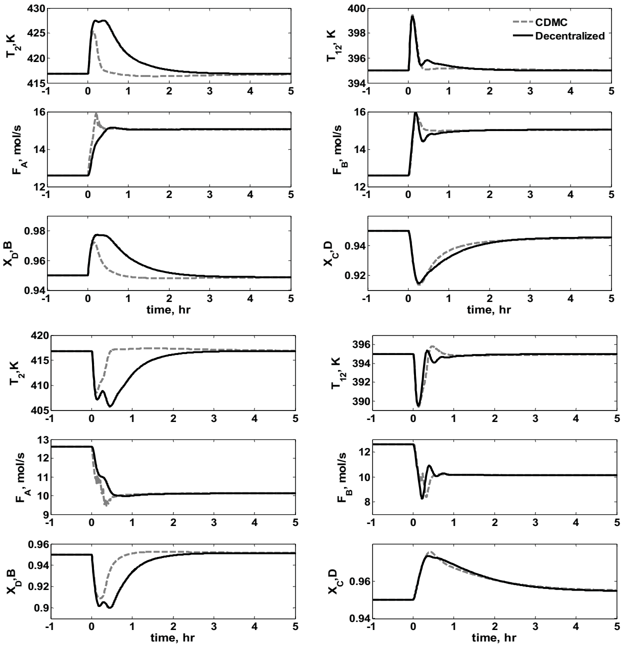

Figure 5. Closed Loop response in Ideal RD system with CS1structure for +20% (Fig A) and -20% (Fig B) change in throughput using CDMC & Traditional decentralized temperature controllers

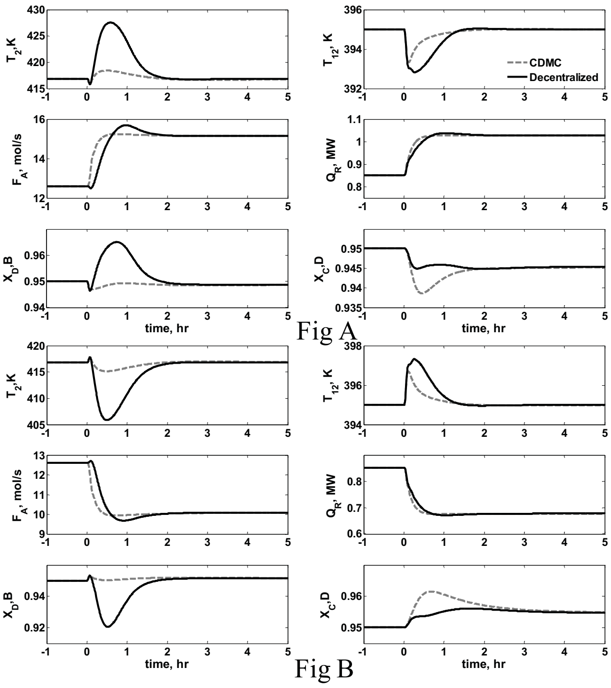

Figure 6. Closed Loop response in Ideal RD system with CS2 structure for +20% (Fig A) and -20% (Fig B) change in throughput using CDMC & Traditional decentralized temperature controllers

To gain a better perspective on the performance of the controller algorithms and structures, the maximum through-put change that can be handled was studied. In both the ideal and the methyl acetate RD columns, a through-put decrease turns out to be the more severe disturbance with both CS1 and CS2 For the ideal RD column, CS1 using DMC fails for value for the decentralized controller is -45%. CS2 on the a

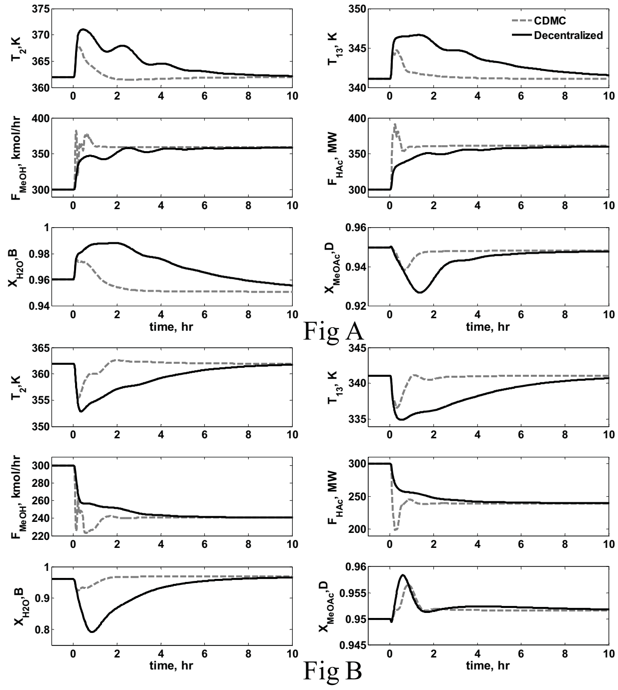

Figure 7. Closed Loop response in Methyl Acetate RD system with CS1 structure for +20% (Fig A) and -20% (Fig B) change in throughput using CDMC & Traditional decentralized temperature controllers

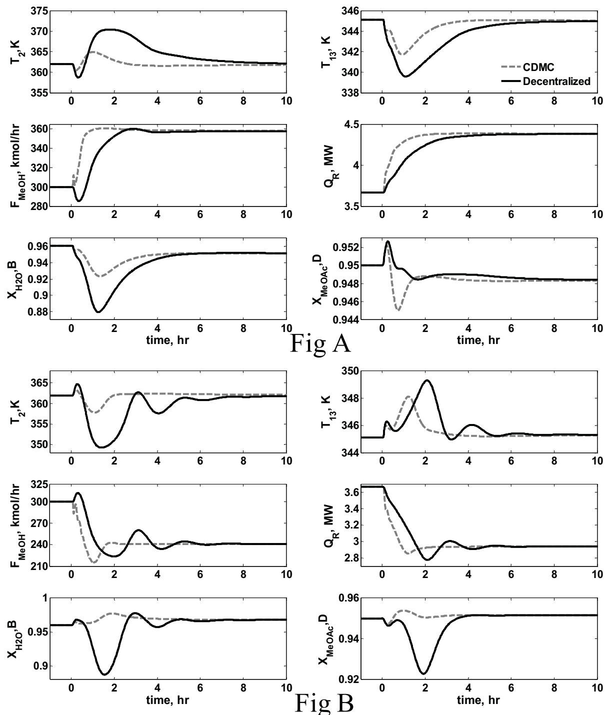

Figure 8. Closed Loop response in Methyl Acetate RD system with CS2 structure for +20% (Fig A) and -20% (Fig B) change in throughput using CDMC & Traditional decentralized temperature controllers

-70% step change in the through-put. The corresponding other hand fails for -65% and -55% through-put changes using respectively the DMC and decentralized control algorithms. For the methyl acetate system, CS2 with a DMC controller exhibits no improvement in the magnitude of the maximum through-put decrease handled. Column operation using CS1 with a DMC controller allows for a 60% through-put decrease to be handled where CS1 with decentralized control fails for a 45% through-put decrease.

5 DISCUSSION

The Integral Abslolute Error (IAE) of product purity is plotted in Figure 9 & 10 as the magnitude of the through-put change is increased. Regardless of the control structure and the RD system, the 2x2 DMC control provides tighter product purity controller for large through-put changes.

We have considered a through-put change to be the primary disturbance for the double feed ideal RD systems operated neat. In some situations, variation in the fresh feed composition may also constitute a principal disturbance into the column. To test for the closed loop control performance of the temperature inferential control systems under consideration, we consider a 5 mol% step change in the purity of either feed as a disturbance. For the ideal RD system, component B in F_A and component A in F_B are the feed impurities. For the methyl acetate RD system, water is taken as the impurity in the fresh feeds. Table 3 reports the IAE of the two controlled tray temperatures and the distillate and bottoms purity for the two RD systems using CS1 and CS2. In both the RD systems, the reactive tray temperature control is poorer while the stripping loop temperature is better than decentralized controller. The inferior reactive temperature control is possibly due to the change in the step response coefficients for the altered feed conditions. Inspite of the poorer reactive temperature control, the data in the Table 3 suggests that the deviations in the distillate and bottoms purity for the DMC and decentralized controller are comparable. The DMC controller can thus withstand a feed composition disturbance.

Table 3: Comparison of Controllers for Regulatory Performance with impure fresh feed as disturbance with Integral Absolute Error (IEA's) key control variables

	Disturbance	Control Variable	CS1		CS2	
			CDMC	Decentralized	CDMC	Decentralized
Ideal RD Column	Pure F_A & Impure F_B with Z_B=0.95, Z_A=0.05	T_{12}	72.85	29.285	43.70	46.504
		T_2	334.83	433.47	266.01	695.89
		Top Purity	0.46	0.63	0.703	0.76
		Bottom Purity	0.59	0.88	0.56	1.27
	Pure F_B & Impure F_A with Z_A=0.95, Z_B=0.05	T_{12}	96.28	45.78	35.50	48.65
		T_2	296.61	202.32	143.31	347.67
		Top Purity	1.33	1.09	0.88	0.581
		Bottom Purity	0.612	0.58	0.47	0.35
Methyl Acetate RD Column	Pure F_{H2O} & Impure F_{HAc} with 5 % water	T_{13}	67.26	58.26	68.86	28.94
		T_2	126.38	460.02	120.77	425.32
		Top Purity	0.047	0.046	0.06	0.036
		Bottom Purity	0.429	1.40	0.41	1.20
	Pure F_{HAc} & Impure F_{H2O} with 5 % water	T_{13}	41.19	167.94	52.65	82.71
		T_2	125.61	535.69	137.49	371.41
		Top Purity	0.49	0.51	0.516	0.51
		Bottom Purity	0.45	2.68	0.350	1.62

The asymmetry in the closed loop results (see e.g. Figure 5) suggests the presence of non-linear effects. To investigate this, Figure 11 & 12 plots the variation in the two tray temperatures with respect to the fresh feeds and the reboiler duty at constant reflux ratio. In the ideal RD system, input multiplicity in the stripping tray temperature (T_2) for excess F_B and lower F_A is evident. The reactive tray temperature (T_{12}) exhibits input multiplicity as F_A and F_B are decreased. For the methyl acetate RD system, even as a crossover with respect to base-case steady state does not occur for the range of variation in the column inputs shown, the reactive tray temperature exhibits gain sign reversal with respect to the fresh acetic acid feed. Also, notice the severe directionality in the steady state reactive tray temperature response with respect to the fresh methanol feed with a very small decrease in temperature as the feed rate is increased and very large increase as it is decreased. This extreme directionality, at least partially, explains the asymmetry. The input-output (IO) relations (Figure 11 & 12) can also be used to understand the control system failure mode to large through-put changes. For example, for CS1 with a decentralized controller, for a -50% through-put change, the F_B valve ends up shutting down in slightly under an hour with F_A maintaining T_2 at its set-point. The control system failure mode likely corresponds to 'wrong' control action due to input multiplicity.

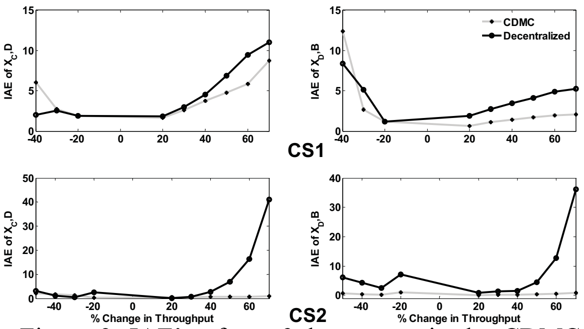

Figure 9: IAE's of top & bottom purity by CDMC and decentralized control using CS1 & CS2 in Ideal RD column for large throughtput changes

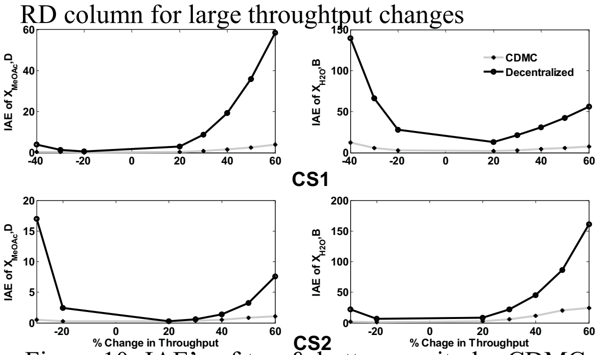

Figure 10: IAE's of top & bottom purity by CDMC and decentralized control by CS1 & CS2 in Methyl Acetate RD column for large throughtput changes

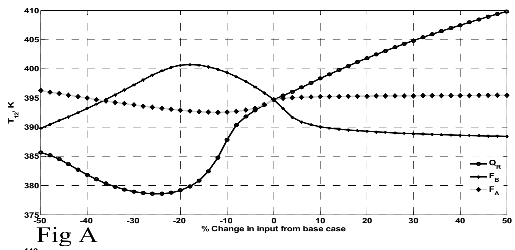

Fig A

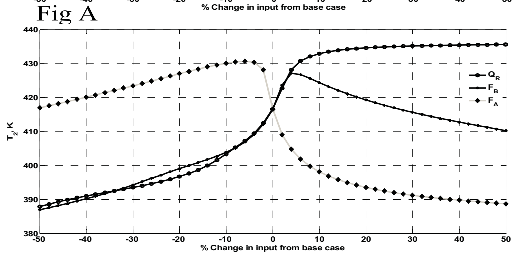

Fig B

Figure 11: I/O relation in Ideal RD system

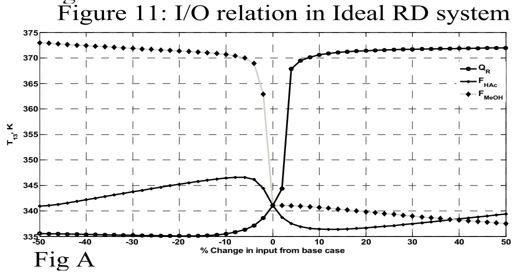

Fig A

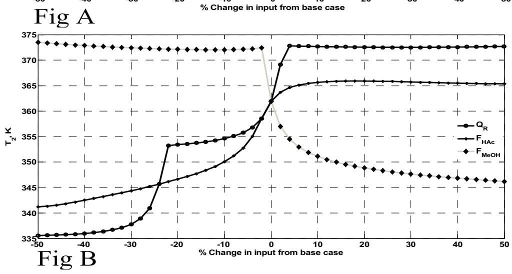

Fig B

Figure 12: I/O relation in Methyl acetate column

It is comforting to note that in spite of the highly non-linear IO relations, a linear control system (decentralized or DMC) effectively rejects such a severe disturbance without succumbing to non-linear dynamic phenomena.

6. CONCLUSIONS

In conclusion, this work demonstrates that the application of constrained dynamic matrix control for two-point temperature inferential control of double feed RD columns operated neat improves the control system performance in terms of the maximum through-put handled and/or the tightness of product purity control achieved. Specifically, in the ideal RD column, significantly tighter bottoms purity control is achieved In the methyl acetate column, tighter control of both the distillate and bottoms purity is achieved using the DMC controller for both the structures. The maximum through-put decrease handled is noticeably higher in CS1 while no such benefit was observed for CS2. These results suggest an overall incentive for the application of linear model predictive control algorithms over conventional decentralized of the highly non-linear RD systems.

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