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Advanced Dual Composition Control for High-purity Multi-component Distillation Column

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***Abstract*— The control of industrial dual high-purity methanol distillation columns is complicated since there are non-linearities involved. Due to economic factors, these distillation columns have strict product ethanol specification (less than 10 ppm), and require a high level of product recovery. Because of environmental factors the bottoms flow cannot contain more than 5 ppm of methanol for a prolonged period. Industrial methanol producers achieve this target by over refluxing the distillation column which creates a plant bottleneck.**

In this work, a control scheme was proposed to control a real life industrial dual high-purity methanol distillation column without exceeding specifications set by a commercial methanol producer with minimal reflux ratio. The control scheme keeps the product specification at the top by controlling the product flow, while an ethanol profile composition analyser located nearby the side draw is used to control the reboiler duty. The simulation results show that the proposed method can provide a reliable set-point track performance.

I. Introduction

Process modelling and simulation are well recognized in process engineering for critical process decision making, optimization and are used to predict certain process behaviors without putting the real process at risk [1], [2]. Though some general differences from real operations are expected in process modelling and simulation, a model can provide reliable process information [3]. In the process industry generally commercial process simulators (e.g. Aspen Plus, HYSYS and VMGSim) are used for modelling and simulation [4], [5].

Distillation is one of the most widely used industrial separation technique in process engineering. It is a mature and reliable technology in engineering practice but still difficult to control due to its highly non-linear characteristics, multiple inputs multiple outputs (MIMO) structure, presence of interactions between variables and the occurrence of severe operational disturbances. The modelling and simulation of distillation columns is indispensable for process dynamics and control analyses [6], [7], [8].

The control of distillation columns is a well-known area of process control, but mostly distillation columns with low to moderate impurities were studied and it is hard to find information about process dynamics and control of high purity distillation columns (e.g. dual high-purity methanol distillation column) [9], [10]. High purity distillation columns also show distinct characteristics (static and dynamic) making them more difficult and challenging to control. They are intrinsically mostly nonlinear in nature and often require nonlinear control [11], [12]. This paper focuses on high-purity distillation columns typical for a real industrial dual high-purity methanol distillation column with strict product ethanol ($\leq$ 10 ppm) and bottom product ($\leq$ 5 ppm methanol) specifications. A control scheme was proposed in this work to control the product composition at the top using the distillate flow, while an ethanol composition profile was used to control the reboiler duty.

This manuscript is organized as follows. After this general introduction, the high-purity distillation operating conditions and current control configurations are discussed in Section II. In Section III a dynamic model is developed. Dynamic behaviour analysis of the high-purtiy distillation based on the dynamic model is discussed in Section IV. A new control configuration is proposed afterward. Finally conclusions and limitations are addressed.

II. Process Description

Each distillation unit in the industry consists of a refining column, as shown in Figure 1.

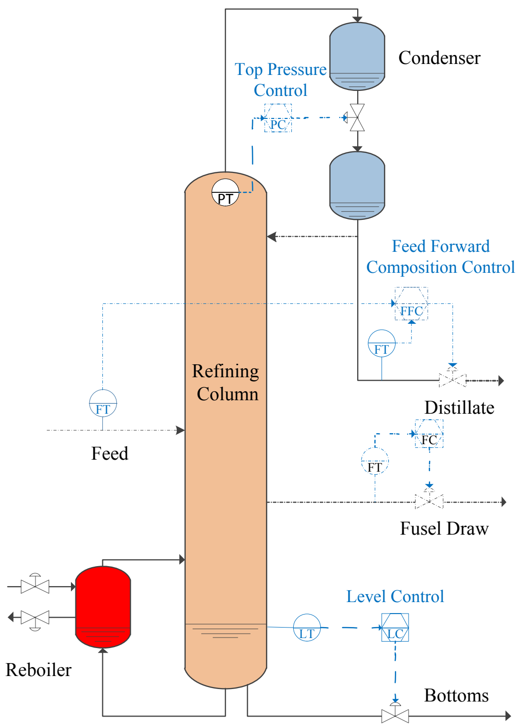

Fig. 1. Schematic of a distillation column with a topping tower and refining column

The crude methanol, which consists of methanol (80 %),

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ethanol (150 ppm w/w), butanol (95 ppm w/w), water (20%) and other light gases, is pumped into an 88 tray refining column. Methanol (product) is taken at the top of the refining column with 99.99% purity, while water is taken from the bottom. Ethanol is predominantly taken at the side draw, located near the middle of the column that is referred to in industry as the fusel draw. The product flow rate is mainly governed by the concentration of ethanol (ppm) in the product stream, where a strict level is enforced. Failing to meet the product ethanol specification would result in a substandard product with a lower commercial value.

Table I Shows compositions and flow rates of all streams of the distillation column.

TABLE I
DISTILLATION COLUMN FLOW AND COMPOSITION INFORMATION

		Plant data	Units
Feed	Flow	142000	kg/hr
	Methanol	0.826	Mass Frac (%)
	Ethanol	150	ppm
	Water	0.179	Mass Frac (%)
	Butanol	95	ppm
Distillate	Flow	114500	kg/hr
	Methanol	99.99	Mass Frac (%)
	Ethanol	7	ppm
	Water	85	ppm
	Butanol	0	ppm
Bottom	Flow	24000	kg/hr
	Methanol	7	ppm
	Ethanol	7	ppm
	Water	99.94	Mass Frac(%)
	Butanol	0.05	Mass Frac (%)
Fusel	Flow	3100	kg/hr
	Methanol	85.54	Mass Frac (%)
	Ethanol	0.66	Mass Frac (%)
	Water	13.8	Mass Frac (%)
	Butanol	47	ppm

A. Current control Scheme

Due to the complex nature of high-purity distillation no complete control scheme is used to control the distillation columns, however the following controllers are present. Flow control of fusel, Ratio control between feed and product and level control of via the bottoms flow. The top pressure is controlled by the level of the condenser. The steam flow to the reboiler is controlled manually by operators, where the steam flow is adjusted on basis of the feed flow. In a typical non-high purity binary distillation operation the composition profile can be easily controlled by measuring the temperatures on one or several trays and keeping them at a certain level. In a binary or a pseudo-binary high-purity distillation operation a single online analyser can be applied.

In a methanol distillation column the feed to the column is a multi-component mixture and the required products are ultra-high-purity. In order to remove the medium boilers a side draw is indispensable. To operate such a column efficiently the ethanol composition profile needs to be managed rigorously. A Composition profile observer and controller provide the potential remedy.

III. MODELLING

Process modelling and simulation are well recognized in process engineering for critical decision making, optimization and control design. There are several comercial simulation software avaible nowadays such as HYSYS, Aspen Plus and VMGSim. In this paper, the high-purity distillation column was modelled using HYSYS with the property package Wilson-Virial/Poy. A shematic of a steady state model is shown in Figure 2. A purge stream Q-101 with zero flow had to be added for completeness.

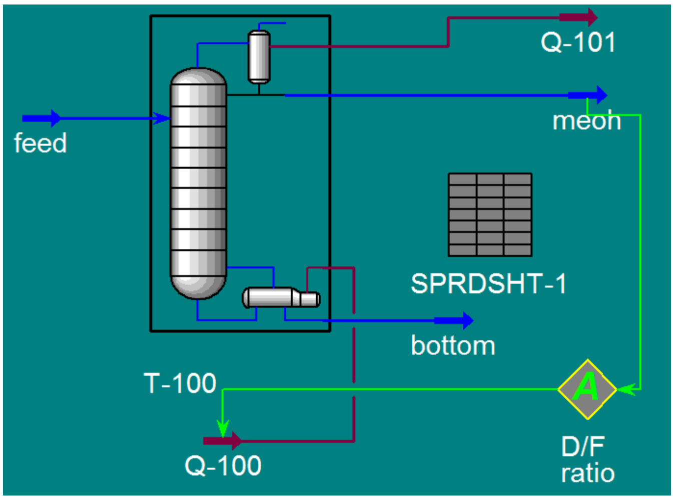

Fig. 2. Steady state model

The low ethanol concentration in the column complicated convergence. Attempting to converge the model directly to 10 ppm was unsuccessful, as the simulator was unable to find a feasible solution that satisfied all constraints in one go. Starting with a relaxed overhead ethanol specification of 50 ppm allowed the model to first converge to a relatively loose specification, allowing for the creation of a reference point. Subsequent convergence to lower ppm specifications uses this as a starting point. This method allowed to gradually tighten the ethanol specification down to 7 ppm. Once the model was converged to 7ppm, it was very robust in finding out new solutions. This steady state model was validated by industrial data.

To carryout initial plant analysis it was necessary to build a dynamic model. This model was used to check for usefulness of temperature at all trays in predicting the composition at the product draw. The dynamic model was also used to understand the behaviour of the ethanol, methanol and water concentration within the column.

The dynamic model was built based on the steady state model. It was decided to eliminate the purge stream from the dynamic model as it was irrelevant to this task and since it reduces the complexness of the model. It was decided to have a flow specification for the feed flow into the column while having pressure specifications for all flow leaving the column, necessary changes were then made to the model including fitting valves and changing flow specifications to pressure specifications. Inlet pressure of the feed to the column was also lowered slightly as the hysys dynamic initialisation function found the specified pressure to be higher than stage pressure.

Minimal Control

Due to the relatively complex nature of distillation columns it was necessary to have some controller functioning, subsequent analysis revealed that the pressure at the top of the column needs to be maintained as well as the level in the reboiler needs to be maintained. To remedy these issues, the column pressure was controlled by the condenser duty while the column level was controlled by the bottoms flow (As shown in Figure 3).

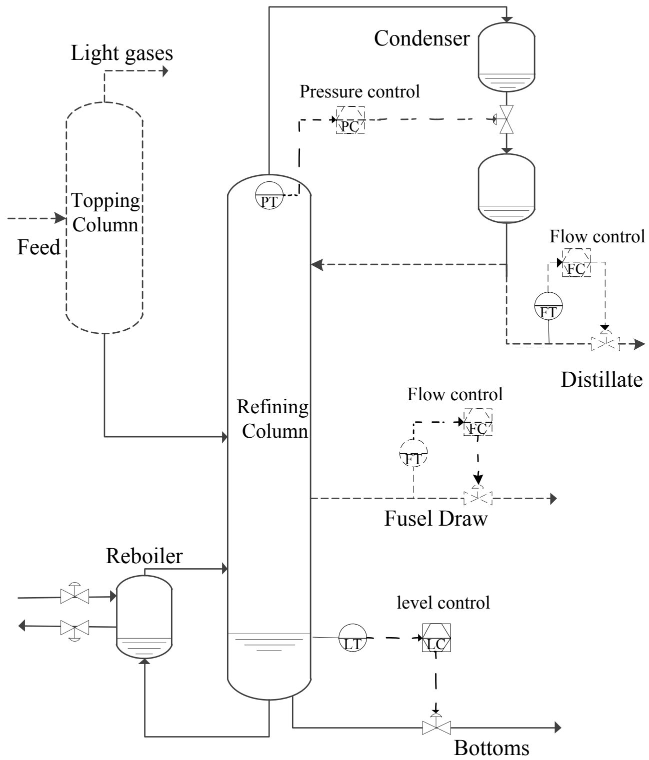

Fig. 3. Dynamic model with minimum control

Both controllers were then tuned using the HYSYS built in IMC tuning function. However subsequent runs carried out showed that both controllers were too aggressive and can amplify small fluctuations, then both controllers were detuned to achieve stability. A flow controller was subsequently introduced to the fusel draw to control the fusel flow at a desired set point.

IV. Results and Discussions

A. Temperature

Based on experience and literature it was expected that the temperature at the top part of the column would not be sensitive to changes in ethanol profile [1]. As a result temperature at the top of the column cannot be used to control the composition. However the analysis of the temperature profile (shown in Figure 4) shows that the temperature near the side draw can be used to predict the overhead ethanol specification (In general higher the product ethanol lower the temperature). Such a scheme in dynamic mode might be advantageous as it is able to pick up on disturbances in the bottom of the column, before they propagate to the top.

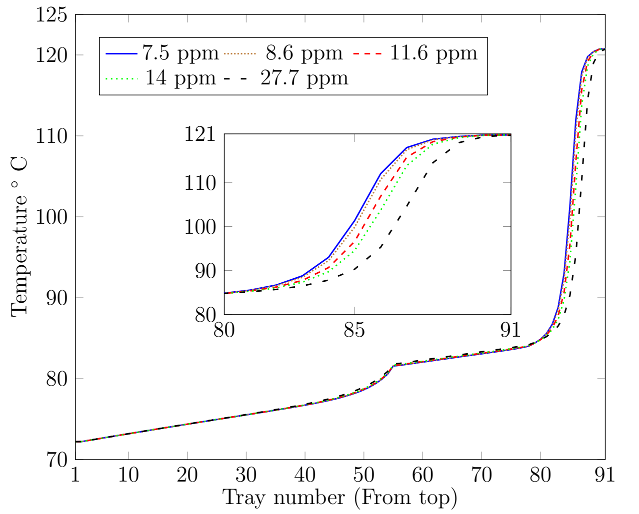

Fig. 4. Temperature profiles for different distillate ethanol concentrations

However subsequent analysis of this scheme showed the potential downfalls of such a scheme in practical applications since the feed composition to the distillation column can vary. If only looking at the temperature profile the controller may be fooled into thinking the ethanol concentration might be lower than the set point. In Figure 5, the influence of feed ethanol water and methanol concentrations on columns temperature profile is illustrated.

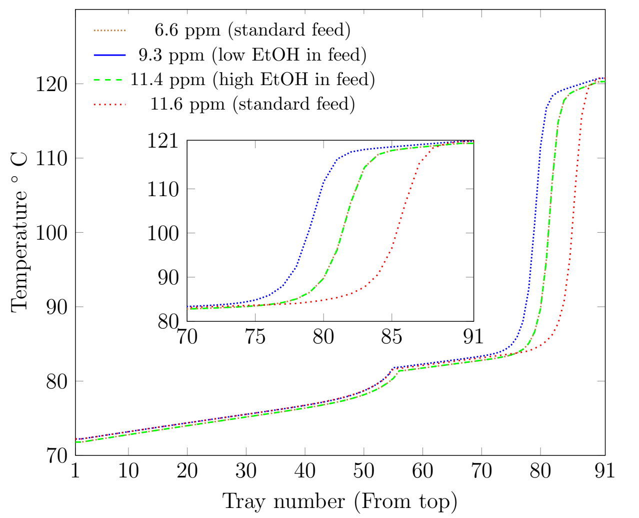

Fig. 5. Ethanol profiles for different feed conditions

The Reboiler duty has been kept at constant for runs made with different feed compositions and is the same at the 6.6 ppm product ethanol run with standard feed. The 11.6 product ethanol run with standard feed on the other hand has a lower reboiler duty. The Figure 5 shows that the temperature profile at the middle of the column can no longer be used to accurately predict product ethanol profile. In a high feed ethanol situation (250ppm ethanol in the feed) the product ethanol concentration would reach 11.6 ppm, but the temperature profile at the middle of the column would remain un-changed, thus being unable to detect the temperature change. Although the amount of ethanol entering through the feed has almost doubled in the high feed ethanol run, the percentage change to the feed mixture composition is minor. Since temperature at each tray is a function of the boiling point of the mixture at each tray a ppm change in the feed should not influence the temperature, however since more ethanol is arriving and no changes to reboiler duty (R/D ratio) are made the amount of ethanol in the produce increases.

In comparison a product ethanol concentration of 11.4 with standard feed is well detectable. In this instance feed conditions have not varied, however separation of all components are affected due to the lower reboiler duty. As a result the methanol-water separation would be effected and cause the temperature to shift. In the low methanol situation the methanol-water separation would be different. In this case the temperature will be higher near the middle of the column as more water is present and since water had a higher boiling point than methanol increasing the overall boiling point of a mixture. The amount of ethanol in the product has increased as the ethanol profile has shifted upwards due to the relatively higher temperatures at the middle of the column.

B. *Behaviour of ethanol, methanol and Water Profile*

Figure 6 also shows that the ethanol, methanol and water profiles are interlinked. As soon as one profile changes the other profiles will be dragged along. This is especially evident for the lower part of the column. Thus by controlling the ethanol profile near the fusel region by varying the reboiler duty it should be possible to control all three concentrations at the same time.

Finally it is important to pointout that on a mass basis almost 95% of the ethanol entering the column leaves through the side draw. Thus keeping the ethanol conenctraion in the side draw at a specified level by controlling the ethanol profile in the region around the side draw, will facilitate the control of the product ethanol concentration as well keeping the methanol specification at the bottoms draw.

V. Dynamics

The dynamic simulation was used to experiment with multiple control schemes. To control the product ethanol specification, the control schemes implemented included:

- Using the reboiler duty to control the product ethanol specification
- Using the product flow to control product ethanol specification
- Using ratio between feed and product flows to product ethanol specification

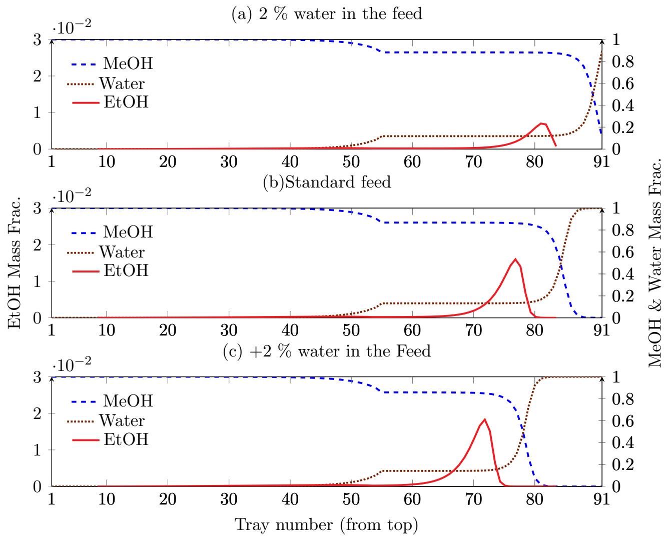

Fig. 6. Column composition profiles for different feed compositions

Despite these control schemes being able to give some degree of control, they were unable to keep the product ethanol at required specification all the time. The reboiler control scheme took too long to react and was letting out a large amount of methanol through the bottoms draw at times. Only controlling the product flow also creates issues with low rates of recovery and subsequently leads to methanol getting let out at the bottom. The feed to product ratio scheme did not take into account the dynamic interactions, as a result was unsuccessful. Subsequent analysis showed that a successful control scheme should manage the ethanol concentration profile throughout the column and control the ethanol profile near the side draw dynamically. This lead to the design of the control scheme proposed in this paper as shown in Figure 7.

In this control scheme the ethanol composition controller is using the product flow to keep the product ethanol specification. An ethanol composition profile observer is used to determine the reboiler duty where a pseudo process variable is created based on the composition observations of trays 73,75(the side draw location) & 77 (Trays numbered from top to bottom). This control scheme was developed based on the knowledge that the ethanol profile at the bottom of the column can be used to estimate the methanol profile. Thus by controlling the ethanol profile, one can influence the amount of methanol lost through the bottoms flow.

A. *Composition profile observer*

Based on this information it was decided to develop a control scheme where composition at trays 73, fusel draw & 77 are used to create a soft sensor control variable that can be used to control the reboiler duty. These trays were selected as the ethanol composition is relatively high around this region and since the fusel draw is located near this region. This control scheme dynamically controls the column ethanol profile movement and shape. The sensor was

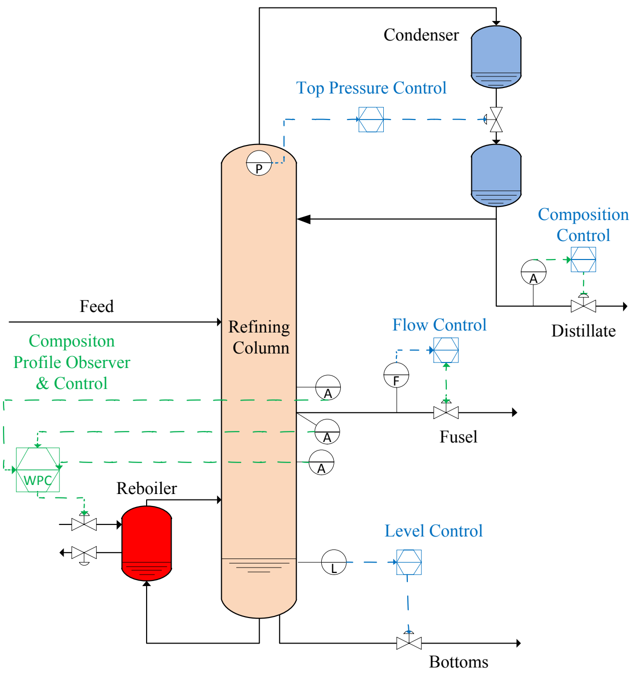

Fig. 7. Advanced composition control scheme

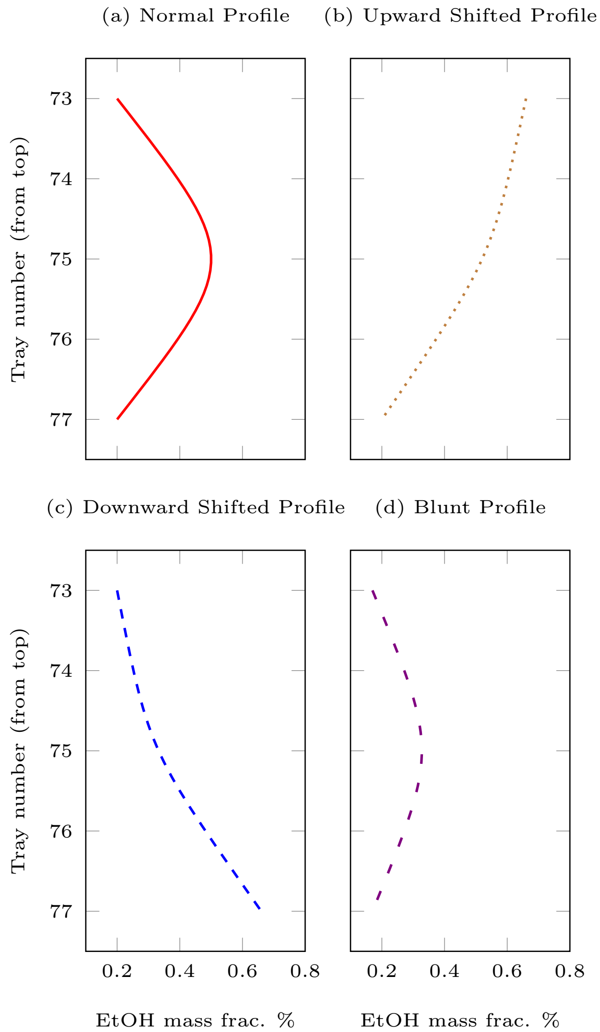

Fig. 8. Ethanol profile at the side draw with different conditions

developed based on the observations made in the temperature and composition observation section.

As shown in the Figure 8 (a) a single composition analyser at the fusel location would be sufficient to control the ethanol profile. The reboiler duty can be adjusted to keep the ethanol concentration to the fusel draw location at set point. However when a minor amount of excessive reboiler duty (+ 2%) is applied or an unforeseen disturbance occurs for a small period, the ethanol profile can shift to resemble the "upward shifted profile" in Figure 8 (b). In this circumstance if we only have a composition analyser at the fusel draw, a controller would interpret this signal as a lack of reboiler duty and increase the reboiler duty. This in turn makes the problem worse. The profile can also shift downward as illustrated in the "downward shifted profile" (shown in Figure 8 (b)) due to a lack of reboiler duty as well as unforeseen disturbances. In this case a controller with a single composition analyser would recognize reboiler duty needs to be increased, but this process will take time and would be sluggish to respond. Similarly the ethanol profile can become flattened as illustrated in Figure 8 (d) "blunt profile". In all these cases the ethanol concentration at the fusel draw has been lowered, as a result not enough ethanol will be extracted at the side draw and ethanol specification wont be met.

In this scheme the composition at trays 73, fusel draw & 77 are used to create a pseudo process variable to determine the reboiler duty. In normal operations the pseudo process variable is the composition of the ethanol at the side draw, the following logics are used to manipulate the pseudo process variable when disturbances occur. X represents the ethanol concentration in weight %.

- $If X_{73} > X_{fusel}+0.1\%$ then $P_{seudo} = X_{fusel}+0.44\%$
- $If X_{77} > X_{fusel}+0.1\%$ then $P_{seudo} = X_{fusel}-0.44\%$
- $If X_{fusel} < 0.4\%$ then $P_{seudo} = 0.08\%$

These logic operations are designed to achieve the following objectives

- If the composition of ethanol at the top sampling point is greater than the fusel draw, the reboiler duty has pushed the profile upwards. Thus the reboiler duty needs to be lowered. This is triggered by an increase of the pseudo process variable over its set point by adding 0.44 %.
- If the composition of ethanol at the bottom sampling point is greater than the fusel draw, the profile is too low. Thus the reboiler duty needs to be increased quickly, which is done by decreasing the pseudo process variable by 0.44 %.
- The last logic is used to keep the ethanol profile sharp; this is required as a less defined ethanol bulge will result in not meeting the bottoms specification as well as recovery targets

If the ethanol profile is too sharp the controller will detect this as an increase in the pseudo process variable and would decrease the reboiler duty, hence a logic operation to carry out this action is not warranted. The values for the logic operations were arrived by a trial and error basis. These logic operations have the best mixture between aggressive control and robustness. To check the set point tracking ability of the overall composition control scheme, the product ethanol and fusel composition set points were changed while observing its effects on the ethanol composition at products and fusel.

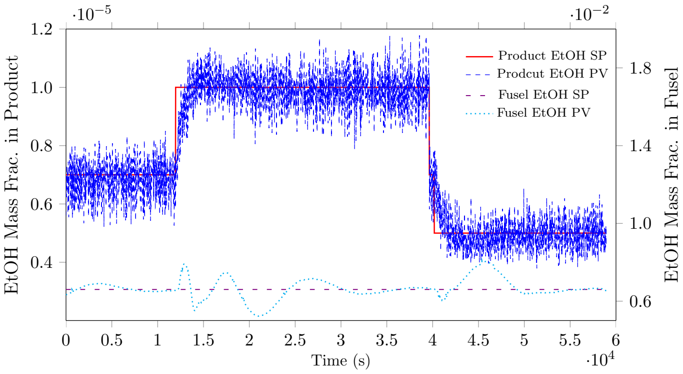

Fig. 9. Set point tracking characteristics of the proposed control scheme when the product ethanol specification is changes

In Figure 9 the set point at the product ethanol composition control was changed from 7 ppm to 10 ppm and down to 5 ppm. It is apparent that the product ethanol profile is capable of tracking this set point without exhibiting any bias. However it is also important to note that the product ethanol concentration is inherently noisy. This is mainly caused by the following factors: The product ethanol fraction is very low. As a result a minor fluctuation in a process variable can result in the product ethanol composition to fluctuate ± 0.5 ppm, even when no set point changes are carried out. The controller is tuned to be aggressive. Analysis carried out with no disturbance shows that the simulation has about ± 0.1 ppm noise which is acceptable. Figure 9 also clearly shows that the product composition controller has an influence on the fusel composition. The ethanol concentration at the fusel draw takes a long time to stabilize (about 8 hours) when a set point change is performed at the product control. This is not commercially significant as a variation in the side draws ethanol concentration has no economic ramifications. On the contrary, a slight variation in the product ethanol concentration has a significant commercial impact. It is important to note that set point changes of the product ethanol composition would be performed over days, not hours. However, if the value in the logic operations is changed to 0.15% the time taken for the ethanol composition at the side draw to settle down to a set point decreases significantly. Thus, if the operation warrants in future warrant both the compositions to be tightly controlled this action can be taken. The ethanol concentration in the side draw is always oscillating due to the control scheme trying to keep the ethanol profile at normal levels even when no set point changes are performed. As a result the ethanol concentration at the side draw location has only varied with-in acceptable limits where the composition controller at the product draw is able to maintain the product ethanol specification.

VI. Conclusions

A multi-component high-purity distillation column has been accurately modelled on steady state and dynamic state using a commercial process simulator. A dual composition control scheme with a side draw ethanol composition profile observer has been proposed and tested by set-point tracking. For the simulation results, the proposed method can provide reliable control performances.

In the future, the controller should be tested comprehensively against process disturbances and set point changes in the soft sensor. Also an automatic procedure should be developed to obtain soft sensor values according to different operational conditions should be developed.

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