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Process Systems Engineering

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A novel soft sensor for measuring and controlling recovery in a high-purity, multi-component, side-draw distillation column

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distillation control, density

Abstract

The use of soft sensors for monitoring purposes is an established practice in the process industry. In this study, the focus has been on developing a soft sensor that can be used to monitor the product recovery rate of double-ended, high-purity distillation columns with a side-draw. To this end, this study specifically focuses on developing a cost-effective and accurate soft sensor for an industrial methanol distillation unit where a side-draw is used to meet the parts per million level impurity specifications. The novel soft sensor is based on the unique characteristics of the mass balance in this type of column, and uses the density measurement at the side-draw together with the flow rates of the side-draw and product draw to calculate the product recovery rate. The developed soft sensor was validated against real plant data as well as on a process simulation of an industrial methanol distillation column. The soft sensor demonstrated the ability to predict product recovery to an accuracy of 0.05% and showed good dynamic performance. The proposed soft sensor was next used as a process variable in the development of a supervisory scheme and a model predictive control scheme, which were able to operate the process at product recovery rates of 99.5% while honoring critical product and bottoms product specifications.

1.0 Introduction

The control of high-purity distillation columns has been an area of active interest for close to half a century ¹. From the on-set one key issue that has hindered the control of high-purity distillation processes has been the difficulty in accurately inferring key variables such as composition of a distillate stream ¹. Since these early times the key desirable attributes for inferential measurements have been the same: these are a high signal to noise ratio, fast response and low cost - among others ². The concept of soft sensors/ inferential measurements has been based on linking first principles based models and historical data to create algorithms that can link a measurable variable with the desirable one ². The use of soft sensors in distillation is a well-established practice, particularly those focused on composition inference that relies on temperature measurements³⁻⁵. Bettoni et al.⁵ used temperature measurements to estimate the composition of side-draw products. Their work showed that inferential control offered better performance than tray temperature control but failed to fully reject disturbances. Wang et al. ⁶ studied the control of a dividing wall column and compared control schemes with on-line analysers, and with temperature-inferred control. In recent years work has also been carried out on using adaptive fuzzy logic concepts in developing composition estimations in reactive distillation columns ⁷, the development of inferential controls for crude oil distillation units ⁸, and the development of a non-linear profile observer for high-purity distillation columns ⁹.

Similar to sensor development, the area of high-purity distillation control has been an area of active interest. In terms of control, high-purity distillation is a process with highly non-linear dynamics, that make it hard to control ¹⁰. Extensive work has been carried out on of high-purity distillation with applications such as cryogenic air separation ¹¹ as well as more theory oriented works ^{12,13}. Udugama et al ^{10,14-20} have also looked at this area of high-purity distillation columns

extensively in the recent years, especially an industrial methanol distillation column where a multi-component product stream needs to be distilled into a high-purity product in a side-draw distillation column.

Product recovery (β) is the ratio between the mass flow of the product to the mass flow of the product entering the column and as shown by Udugama et al.²¹ it is a key performance indicator of the economic performance of a distillation column. While gas chromatography sensors that monitor the concentration together with Coriolis flow meters that monitor the flow rates can be used to monitor these values, these sensors are expensive to purchase and operate, limiting their application to processes where a significant economic benefit can be realized by their introduction. Gas chromatography, for instance, requires trained technicians to provide accurate results, that make operation 70% of its overall cost²². Thus there is a need for the development of soft sensors that can perform the duty at the same level of accuracy and speed. In this work a novel density-based soft sensor for a high-purity multi-component methanol distillation column was developed and incorporated into a control structure.

This manuscript is divided into several sections. Firstly, in Section 2.0, some background on the industrial methanol distillation process is given. In Section 3.0 the development of the soft sensor is described in detail, while Section 4.0 details the development of both the decentralized and the MPC control schemes using the newly developed soft sensor. In Section 5.0 the developed controls are tested, with a traditional DV distillation control structure acting as a basis of comparison. Finally, conclusions are drawn in Section 6.0.

1
2
3 **2.0 Background**
4
5

6 In industrial methanol distillation a methanol/water mixture with trace amounts of ethanol
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8 (150 ppm) needs to be refined into AA grade methanol with less than 10 ppm ethanol. In
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10 addition, the bottom water stream is required to have a methanol concentration of <5-10 ppm to
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12 satisfy environmental standards. In order to achieve this double ended purity target, the side-
13
14 draw is used to remove the unwanted ethanol. For profitable operations the methanol recovery
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16 needs to be maximized and is typically operated at a recovery of 98%, while the re-boiler duty is
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18 kept to a minimum¹⁵. Figure 1 illustrates a typical methanol distillation column configuration.
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Figure 1. A schematic of a distillation column for which methanol is the top product and water is the bottom product, while ethanol is removed through the side-draw.

For the study in question, the feed of the column has been taken to be 142.5 t/hr and has a composition of methanol (82.6% wt), water (17.4% wt), ethanol (at a concentration of 150 ppm) and small amounts of butanol (< 100 ppm). The process aims for the recoveries and purities mentioned, which require side-draw flow rates of 3 t/hr, at an ethanol concentration of 0.66% wt. Detailed specifications for the process can be seen in Table 1, where the mass fractions in the process simulation have been validated against real plant data. Large deviations are seen only at the ppm level, where the percentage errors are in fact very small absolute errors.

Table 1. Mass balance specifications of the column separating methanol, water, ethanol and butanol based on industrial plant data.

		Plant data	Simulation	Units	Error (%)
Distillate	Flow Rate	115.5		t/hr	
	Methanol	99.99	99.99	Mass Frac (%)	0
	Ethanol	8	8	ppm	0
	Isobutanol	0	0	ppm	0
	Water	85	30	ppm	65
Fusel	Flow Rate	3.0		t/hr	
	Methanol	65	65	Mass Frac (%)	0
	Ethanol	0.66	0.68	Mass Frac (%)	3
	Isobutanol	47	59	ppm	26
	Water	34.4	34.3	Mass Frac (%)	0.3
Bottoms	Flow Rate	24.0		t/hr	
	Methanol	5	3	ppm	40
	Ethanol	0	0	ppm	0
	Isobutanol	500	550	ppm	10
	Water	99.94	99.94	Mass Frac(%)	0
Specifications	Re-boiler Duty	88.25		MW	-
	Methanol Recovery	98		%	-

2.1 Design and Thermodynamics

All simulations were carried out using VMGSim V.10 and AspenTech HYSYS V.8.8. The design inputs shown in Table 2 were used in setting up the steady state and subsequent dynamic simulations.

Table 2. Side Draw Distillation Column Design Parameters.

Design Parameter	Specification	Units
Condenser Pressure	134	kPa
Bottoms Pressure	209	kPa
Total Number of Trays	89	-
Location of Side-draw	13	Tray number (from bottom)
Column Diameter	6.1	m

In addition, the reboiler in the simulation was set to be a once through reboiler without baffles and the reboiler duty was directly specified. The *Wilson* model with a Virial equation of state together with a Poynting correction was used as the property package. This model determines the activity coefficients of each component in the mixture to calculate the fugacity of the liquid. The vapour fugacity is calculated using a Virial equation of state. The simulation solver then makes the required calculations using equilibrium and enthalpy models as well as using rigorous thermodynamics. It should be noted that the default thermodynamic parameters of the process simulators were used for these property packages and settings. These values were not further adjusted as relatively good agreement between the simulation and plant data was achieved¹⁴. The column was simulated with sieve trays, and based on tray manufacturer information the overall tray efficiency of the column was set to 80%, while the maximum flooding factor was set

to 120% . The flooding factor of 120% was in-line with F-factor calculations carried out by the authors in Udugama et al ¹⁸. In dynamics the simulation was stabilised at operating conditions by controlling the condenser and bottoms level (tower inventory) while also controlling the column overhead pressure. The dynamic behaviour of the column was in agreement with the industrial plant data that was available to the authors, but cannot be disclosed due to confidentiality restrictions.

During traditional operation the desired 98% recovery is not directly controlled, but inferred and back-calculated daily from process reports. However, it has been shown that an improvement of recovery to 99.5% can represent a yearly profit increase of USD 3.6 million²¹. As noted by Udugama *et al.*²¹ this is particularly attractive when the control installation costs are below USD 9 million. This could be achieved through the use of supervisory control layers, which are easy to understand and do not require complex software¹⁴. Cost, as mentioned, can be further reduced through the use of soft sensors which can accurately monitor and control recovery.

As it can be seen in Figure 1, a range of sensors and controllers are present on the column. Level and pressure sensors, along with the feed flow sensor are present for safety concerns, in order to ensure the distillation column is able to operate. The flowmeter in the distillation stream along with the composition sensor are required to specify the product properties necessary for the sales process; firstly, by monitoring and maintaining < 10 ppm ethanol for AA grade methanol standards and secondly to accurately quantify the amount of methanol produced by each unit¹⁵. In the distillate stream the flow sensor corresponds to a Coriolis flow meter that must be capable of accurately quantifying the mass flow. The composition control in the distillate stream corresponds to an on-line gas chromatography sensor. For the reasons mentioned, these devices are costly to install and operate, but they are also necessary.

Traditionally, the external mass balance of the column is used to calculate the recovery

$$\beta_{external} = \frac{\dot{m}_{d, meoh}}{\dot{m}_{feed, meoh}} \quad (1)$$

In Eq. (1) the numerator ($\dot{m}_{d, meoh}$) is the mass flow of methanol in the distillate stream and the denominator ($\dot{m}_{feed, meoh}$) is the methanol mass flow rate in the feed. Implementing Eq. (1) in the process gives an instantaneous reading of the recovery. Unfortunately, it does not reflect the dynamics of the process, as any changes would immediately affect the reading, thus not representing the performance of the column. It also requires an additional composition sensor on the feed stream to achieve accuracies of +/- 0.1% for a meaningful recovery value. As mentioned, this type of sensor significantly affects the capital and running costs of the scheme, so other options must be considered.

3.0 Soft Sensor Development

In view of the steady state mass balance of the column illustrated in Figure 1, the product recovery can be re-refined as follows:

$$\beta_{mass\ balance} = \frac{\dot{m}_{d, meoh}}{\dot{m}_{d, meoh} + \dot{m}_{side, meoh} + \dot{m}_{bottoms, meoh}} \quad (2)$$

Where the denominator has been re-written as the methanol leaving the column in the distillate ($\dot{m}_{d, meoh}$), side-draw stream ($\dot{m}_{side, meoh}$), and bottoms stream ($\dot{m}_{bottoms, meoh}$). This is true because at steady state, the methanol entering the column as feed must be equal to the methanol leaving the column. Eq. (2) calculates the dynamic (or internal) state of the column and gives a good indication of the dynamic state of the recovery.

From this starting point simplifications can be made. To begin with, it can be reasonably assumed that the amount of methanol leaving through the bottom of the column is negligible, as the bottoms methanol concentration is typically < 5 ppm during normal operation at recoveries above 98%.

With this assumption the original equation, Eq. (1), can be re-written to find the ‘internal’ recovery of the column ($\beta_{internal}$) as follows:

$$\beta_{internal} = \frac{\dot{m}_{d, meoh}}{\dot{m}_{d, meoh} + \dot{m}_{side, meoh}} \quad (3)$$

Now analyzing the process mass balance further, the overall distillate flow rate can be assumed to be equal to the methanol distillate flow rate. This can be done because the methanol makes more than 99.95% of the distillate, thus:

$$\dot{m}_{d, meoh} = \dot{m}_d \quad (4)$$

This reduces Eq. (3) to:

$$\beta_{massflow} = \frac{\dot{m}_d}{\dot{m}_d + \dot{m}_{side, meoh}} \quad (5)$$

Since $\dot{m}_d$ is already monitored, the only remaining unknown is the side-draw methanol flow rate that can be expressed as follows:

$$\dot{m}_{side, meoh} = \dot{m}_{side} \times X_{meoh, side} \quad (6)$$

To monitor the side-draw flow rate, $\dot{m}_{side}$, a flow meter can be used while the side-draw methanol concentration, $X_{side, meoh}$, can be inferred based on a relationship between the density

and the composition. The correlation between the density of a water/methanol mixture and the methanol mass fraction is seen in Figure 2 and Eq. (7).

Figure 2. Relationship between composition and density at 298.15 K for water/methanol solutions.

$$X_{meoh, side} = 3.2262\rho_{side}^2 - 10.2500\rho_{side} + 7.0533 \quad (7)$$

A quadratic trend line was fitted to the data to obtain a simple relationship between the parameters. It should be noted that since density changes with temperature, this relationship is only valid at 298.15 K which is the temperature at this regression was taken ¹⁵

The side mass flow rate can then be coupled with the estimated methanol composition to calculate the methanol flow rate. The overall methanol recovery ($\beta_{density}$) becomes:

$$\beta_{density} = \frac{\dot{m}_d}{\dot{m}_d + \dot{m}_{side} X_{side, meoh}} \quad (8)$$

Eq. (8) is to be used by the soft sensor to determine the recovery during operation. This simple concept avoids installing additional gas chromatographs to the column. The proposed soft sensor would require a Coriolis flow meter on the side-draw stream to estimate its mass flow and

density, and would additionally use mass flow rate measurements from the already present Coriolis meter on the distillate to calculate recovery. Currently, density can be measured with Coriolis flow meters offering accuracies of $\pm 0.1 \text{ kg/m}^3$, which would enable accurate calculations of the recovery rate. Although, the technology requires regular maintenance, its location on the side-draw implies a relative smaller size than required on other streams, which directly reduces the costs of the meter. Using the Coriolis meter also avoids the need for even more costly and less robust composition analyzers. Its use would thus significantly reduce complexity while still estimating recovery within acceptable accuracies.

3.1 Soft Sensor Validation

An analysis of the sensitivity of the density to changes in product recovery shows that for every 1% change in product recovery a corresponding density change of $\sim 70 \text{ kg/m}^3$ is expected, which in turn corresponds to a 0.05% change in product recovery change resulting in a density change of $\sim 3.5 \text{ kg/m}^3$. Considering the accuracy of density measurement device such as Coriolis flow meters (as discussed in the above paragraph), it can be concluded that these density measurement devices are capable of capturing fine changes to density which in turn allows the soft sensor to make accurate predictions.

3.1.1 Influence of Ethanol

During normal process operations, concentration of ethanol in the side draw reaches 0.68% (weight) and has a density value which is closer to methanol than water²³. As a result of this, the density based recovery equation (Eq.8) would overestimate the amount of methanol present in the side draw. From a fundamental point of view this would result in the soft sensor to under predict the product recovery rate by 0.02% .

To further investigate this influence of ethanol, the validated process simulation was used to study the mismatch between the densities of pure methanol-water mixture and the actual side draw mixture of methanol-ethanol-water mixture (with trace butanol). Table 3 displays the results over the range of methanol concentrations that can be expected at the side draw (product recovery rates between 98% and 99.7%).

Table 3. Density mismatch between a pure methanol/water mixture and the actual side draw mixture

Methanol Concentration (Wt/Wt)	Density Mismatch (kg/m ³)
0.80	1.1
0.70	1.0
0.60	1.0
0.50	1.0
0.40	1.0
0.30	0.90
0.20	0.90

It can be seen that on average the density mismatch is $\sim 1 \text{ kg/m}^3$, which corresponds to $\sim 0.015\%$ mismatch in product recovery. Therefore, it can be concluded that the existence of ethanol (as well as butanol) in the side stream does not significantly affect the performance of the soft sensor. Moreover, the fact that ethanol concentrations are generally steady over a long period

(months) and that fact that the mismatch in density is consistent over the operating range allows for an off-set to be introduced to the soft-sensor to correct for the discrepancy.

From an operational point of view, it is important to note that components such as acidic compounds as well as ketones can sometime accumulate in the side draw region as discussed by Udugama et al. in ²⁰. In these instances it is important to ensure that the accumulation of these components is at relatively low levels ($> 0.25\%$ weight at the side draw) to ensure soft sensor accuracy.

3.1.2 Influence of Temperature

As discussed previously, the density vs methanol regression was obtained at 298.15 K. While in an industrial implementation the temperature of the mixture would be taken into account and then compensated for by the measurement devices ²⁴, it was decided to investigate the influence of temperature on the density measurement for robustness purposes. Table 4 shows the mismatch of density for a water/methanol mixture if the temperature of the mixture is 5 K higher than the standard conditions. The results shown are based on the validated process simulation. From analysing these results it can be seen that for a 5 K increase the soft sensor would under predict product recovery by 0.05%. Thus from a practical point of view, temperature compensation must be performed relatively accurately during the field implementation of this soft sensor.

Table 4. Density mismatch of the soft sensor for a 5 K increase in temperature

Methanol Concentration (Wt/Wt)	Density Mismatch kg/m ³
0.80	5.0
0.70	4.8
0.60	4.7
0.50	4.6
0.40	4.4
0.30	4.3
0.20	4.1

3.1.3 Dynamic Validation

To understand the dynamic behaviour of the soft sensor it was necessary to carryout step tests that compared the response of the external recovery, $\beta_{external}$ (Eq. 1), and the density recovery, $\beta_{density}$ (Eq. 8). To this end, reboiler duty step changes of 2.5 MW were performed on the process simulation while maintaining the product ethanol concentration at 7 ppm. $\beta_{internal}$ (Eq. 3), was also plotted for the purpose of comparison.

Figure 3. Step changes of re-boiler duty and its effect on recovery at SP=99.0%.

Figure 3 shows that the dynamics of all three recovery calculations are similar and all three calculations take a similar time to stabilise after step tests. However, it should be noted that in the step increase, the rise time of the external recovery calculation is somewhat slower than those of the density (soft sensor) and internal recovery calculations. It can also be observed that, the density based recovery rate (soft sensor) is in general recording a recovery value that is ~0.02% higher at all times. The reason for this slight mismatch was tracked back to the difference between the density vs methanol composition regression predicted by eq. 7 and by the process simulation. Further investigation into this matter revealed that the process stream where the density value was monitored in the process simulation was slightly overcooled, which resulted in this discrepancy. This mismatch was deemed to be minor hence, no further actions were taken.

4.0 Control Schemes

Two controller schemes, one decentralized and the other centralized, were designed in order to implement the soft sensor. The decentralized scheme is a structure based on supervisory control, so it can be implemented on a DCS and is the same as a simple DV control scheme. The

centralized MPC scheme, on the other hand, is more advanced and requires dedicated software, but can potentially be better and is used for comparison purposes.

To qualify these systems as successful, the following criteria has been defined:

- (i) Maximizing/controlling methanol recovery.
- (ii) Respecting the AA grade constraint on distillate ethanol content.
- (iii) Rejecting disturbances in feed.

4.1 Supervisory Scheme

The decentralized scheme used, was designed with the goal of providing an industrially compatible system that could meet the high-purity specifications while obtaining high recoveries and minimizing re-boiler duty. The system consists of a regulatory primary layer and a supervisory secondary layer consisting of a recovery constraint controller (RCC) and a dynamic re-boiler controller (DRC) and is based on the analysis and supervisory control structure developed by Udugama *et al.*¹⁵. This scheme will be referred to as Supervisory scheme.

The RCC takes the measurements of the current recovery ratio and ethanol content in the distillate stream. The controller changes the set point of the composition ($Y_{SP, QC}$) depending on the state of the column. In situations where the column β is higher than the desired set point, the $Y_{SP, QC}$ is tightened by the control structure to take advantage of the favorable recovery conditions and to bring the recovery back to set point. The aggressiveness of this reduction in set point is dictated by M_H which was set to a value of 2. Similarly, when β is lower than the desired set point, $Y_{SP, QC}$ is increased which in turn increases the recovery rate back to set point. The aggressiveness of this increase in set point is dictated by M_L which was set to a value of 6.

The value of M_H and M_L have been set based on work carried out in Udugama *et al.*¹⁵ where the M_H value was three times smaller than M_L . This means the controller responds much more aggressively to a low recovery rate situation than a high recovery rate situation. This is because a low recovery rate situation is economically undesirable, while a high recovery rate situation only needs to be managed to ensure that in the long term the mass balance of the column is kept in check. The maximum rate of change was set to 0.1%/min to avoid abrupt variations in the set point. The set point is calculated as a function of recovery as follows:

$$Y_{SP, QC} = Y_{SP} - M_H 10^{-6 \frac{\beta - \beta_{SP}}{[\%]}} \quad \text{if } \beta_{SP} \leq \beta \quad (9)$$

$$Y_{SP, QC} = Y_{SP} - M_L 10^{-6 \frac{\beta - \beta_{SP}}{[\%]}} \quad \text{if } \beta_{SP} \geq \beta \quad (10)$$

Eq. (9) represents a high recovery scenario, while Eq. (10) represents a low recovery case. In both cases the recovery measurements are based on $\beta_{density}$. The flow rate of the side-draw stream was set to 3113 kg/hr in order to avoid ethanol accumulation in the column. The side-draw flow rate value is based on industrial plant settings and is in turn set by practical limitations due to the requirement to recycle this side draw stream back to the reformer section (specifically the saturator) of a methanol production facility²¹. In this instance it was decided to hold this flow value constant due to the fact that varying this may affect the density based measurements.

The recovery set point, $\beta_{density}$ and feed mass flow rate are then sent to the DRC. This controller is comprised of a feed forward controller and a feedback trim controller. The feedforward controller adjusts the re-boiler duty depending on the feed flow rate, as shown in Eq. (11), while the trim controller receives information from the RCC regarding the recovery and makes small adjustments to the re-boiler. The schematic of the system is shown in Figure 4.

$$\frac{\dot{Q}_{Reb}}{[kW]} = 0.6707 \frac{\dot{m}_{Feed}}{[kg/hr]} - 4200 \quad (11)$$

Figure 4. Supervisory control scheme, where SS stands for soft sensor.

4.2 MPC Scheme

A model predictive controller (MPC) scheme using a 2x2 multi-input, multi-output (MIMO) controller was designed, where each input affects both outputs. The inputs selected were the methanol $\beta_{density}$ and the ethanol content of the distillate stream, $X_{d, eth}$. The outputs were the set point of the $X_{d, eth}$ controller and the re-boiler duty.

The model was built through open loop tests. The effect of re-boiler duty and distillate flow rate step changes were observed on the $X_{d, eth}$ and $\beta_{density}$. The complex process dynamics observed

through the tests, lead to the normalization of the data in order to create transfer functions that were then inserted into the MPC module as the process model. A general unconstrained MPC module available on Aspen HYSYS was used for the process simulations, but other MPC modules would also be suitable, such as unconstrained or constrained MPC controllers from Aspen PLUS (DMC or DMCplus) or MATLAB. For a constrained optimization the key variable with a hard constraint would be the ethanol composition which must be kept below 10 ppm wt. However, preliminary simulations (as confirmed in the results in Section 5.0) illustrate that at the current set point of 8 ppm wt., this threshold is not crossed for expected process disturbances. These results indicate that adding constraints would have little benefit, while it may lower the energy savings of the MPC, through more aggressive disturbance handling. Since the authors cannot see an added benefit in introducing a constrained MPC module, which would be more time consuming to set up and maintain in an industrial setting, the general unconstrained MPC module was used. However, it is important to note, that in case there is a need to handle constraints actively, a constrained MPC must be set up as this will lead to more superior overall performance in comparison to an unconstrained MPC module. The MPC module was tuned by setting a range of parameters and variables. After a series of simulations, the sampling interval (k) was given a value of 10 min. In a similar manner suitable values for the prediction horizon (P), and the control horizon (M) were found. The prediction horizon represents the number of sampling intervals into the future, while the control horizon is the number of control moves into the future that the MPC considers when predictions are made¹⁵. These parameters were set to 50 and 2 respectively. Values for the process variable and manipulated variable weighing matrices (Γ_u and Γ_y respectively) were also required. These were found through flow rate step changes and observations on their effect on $\beta_{density}$ and $X_{d, eth}$. The observations lead to values of 0.5 for Γ_u

and 1 for Γ_y . These parameters determine the controller's ability to reject disturbances and the size of its actions. In this particular case these parameters were tuned to have a balance between not exceeding product ethanol concentration and the amount of additional reboiler duty that was used to achieve this outcome. The relatively small Γ_u chosen, results in larger actions and better disturbance rejection, but lower stability. Figure 5 shows the resulting scheme for the MPC.

Figure 5: MPC Control Scheme.

5.0 Disturbance testing

A validated process model developed by Udugama *et al.*¹⁵ was used to implement the two control structures described in Section 4.0. In addition, a traditional DV control structure was developed where the distillate flow was used to control the product ethanol specification at 7

ppm while the re-boiler duty was used to control the bottoms methanol concentration at 3 ppm. The product and bottoms set-point for the DV control structure were chosen to allow a sufficient operating window for the DV controller to meet product and bottoms specifications of the column, while it is also important to note that the DV controller does not control product recovery hence the recovery values seen are a result of the controller set points. Moreover, the DV controller in practice will also require a gas chromatograph to monitor the bottoms methanol composition.

5.1 Feed Step Tests

Flow rate step changes of 5700 kg/hr (4%) were made. A change of this size is an extreme scenario, where the column suddenly takes in a large amount of liquid. The results show that the disturbance is rejected successfully by both the Supervisory and MPC schemes. As it can be seen in Figure 6, the DV and MPC schemes have large $\beta_{external}$ overshoots, while the Supervisory scheme does not change significantly. In the case of the MPC, the overshoot can be attributed to the small Γ_u value. The responses seen by the re-boiler duty and $X_{d, eth}$ through the MPC and Supervisory schemes are quite different. For instance, there is a required increase in re-boiler duty to overcome the increase in flow rate. In the case of the MPC this increase in duty is gradual, while the Supervisory scheme sees a more sudden change which is then reduced slightly by the feedback trim controller. The result is a steady state with lower energy requirements for the MPC, compared to the Supervisory scheme. When looking at $X_{d, eth}$ the Supervisory scheme set-up sees the decrease in recovery, and thus increases the set point of the distillate. As the

recovery stabilizes, so does the ethanol mass fraction, although at a lower set point than before the disturbance. The MPC on the other hand, oscillates with no major overshoots.

Figure 6. Flow rate step change effect on external recovery to the left, to the right its effect on ethanol mass fraction and re-boiler duty are shown.

Table 5 shows the scaled integral squared error (ISE) for the different schemes at a set point of 99.5% using the Supervisory scheme as the basis. These values indicate that the DV and MPC schemes are able to control the $X_{d, eth}$ tightly and close to the desired set point, compared to the Supervisory scheme. On the other hand, the Supervisory scheme does a better job of controlling $\beta_{external}$. This occurs, because as explained, the Supervisory scheme allows for the $X_{d, eth}$ to increase in order to maintain the recovery at the set point.

Table 5. ISE of the main variables for a feed disturbance expressed as the integral squared error compared to the Supervisory scheme.

Variable	Control Scheme	ISE (%)
$\beta_{external}$	Supervisory	100.00
	MPC	2760.78
	DV	1992.31
$X_{d, eth}$	Supervisory	100.00
	MPC	8.24
	DV	6.94

5.2 Routine Cyclic Disturbances

Cyclic disturbances were applied to help compare the schemes under conditions that resemble those of the ‘real world’. Once more, only feed flow rate variations were performed. Sinusoidal disturbances with an amplitude of 5700 kg/hr (4%) were applied at two different time periods, t_{short} = 50 min and t_{long} = 2000 min. Figures 7 and 8 show the effects of the flow rate changes on $\beta_{external}$, $X_{d, eth}$ and re-boiler duty for the three schemes.

Figure 7. Cyclic changes of flow rate and its effect on external recovery for the three schemes.

The long period is shown on the left and the short period on the right.

Figure 8. Cyclic changes of flow rate and its effect on ethanol concentration at the top and reboiler duty for the three schemes. The long period is shown on the left and the short period on the right.

The results also show that the $\pm 0.1\%$ accuracy requirements are met by both schemes. Larger $\beta_{density}$ measurement results were obtained throughout the different systems, though by a difference lower than 0.1% . This further demonstrates that the accuracy of the soft sensor is suitable for the monitoring and control of recovery. However, since the $\beta_{density}$ measurement is

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3 constantly higher than $\beta_{external}$, the set point could be adjusted by less than 0.1% to obtain the
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5 desirable external recovery. This could be particularly useful for the MPC which sees lower
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7 recoveries than the Supervisory control system.
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11 Examining the long period fluctuations, it can be seen that the response times for the recovery
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13 (6 - 9 hr) are similar for all three schemes. Similar response times are also seen for the re-boiler
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15 duty (0 - 1.5 hr). Additionally, there are only minor differences in energy requirements (0.2 -
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17 0.8 MW difference). The Supervisory scheme obtains 0.1 - 0.15% higher mean values for
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19 $\beta_{external}$. As explained earlier this occurs due to the controller's 'lee way' on $X_{d, eth}$, to quickly
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21 return to the specified recovery. MPC shows overall lower mean recoveries, but has tighter
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23 control on $X_{d, eth}$ (0.7 ppm lower means). For the short period fluctuations, the $\beta_{external}$
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25 amplitudes of the DV and MPC schemes are significantly larger than those seen in the
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27 Supervisory control scheme. The response times are also different, with MPC showing a slower
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29 adjustment of the re-boiler duty (0.3 hr slower than the Supervisory control). This occurs because
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31 for the MPC to react, both $\beta_{density}$ and $X_{d, eth}$ must have been affected, which for feed flow rate
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33 disturbances can take some time, as previously noted by Udugama *et al.*¹⁴. Tables 5 and 6 further
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35 illustrate these points by providing the quantitative comparisons.
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5.3 Controller Performance

Table 6 shows that for a long period disturbance, the three schemes have similar amplitudes for $\beta_{external}$ and re-boiler duty, while $X_{d, eth}$ is more tightly regulated by the MPC and DV than the Supervisory scheme. For the short period disturbance, the amplitude of the re-boiler duty and $X_{d, eth}$ are smaller for MPC and DV, while the $\beta_{external}$ amplitude is significantly smaller for the Supervisory control scheme.

The disturbance rejection ability of each scheme has also been quantified as the ratio between the disturbance of the process variable coming out and the disturbance going into the process (4% feed flow):

$$Disturbance\ Rejection = \frac{Disturbance\ amplitude\ \% \ out}{Disturbance\ amplitude\ \% \ in} \quad (12)$$

These values were then expressed as a percentage of the Supervisory scheme, as presented in Table 4. The calculation allows for a more obvious view of which scheme decreases the disturbance the most, with low values indicating a greater reduction. These results once more reinforce that the Supervisory scheme has a tighter control of the recovery, while the MPC does a better job at reducing disturbances for $X_{d, eth}$ with smaller changes to the re-boiler duty. This is seen more significantly in the short period disturbances, since the MPC lags on acting upon changes in the recovery value.

Table 6. Amplitude of key variables at a recovery set point of 99.5%. Those values which were considered more attractive have been highlighted. The disturbance rejection has been presented using the Supervisory scheme as the basis of comparison.

Process Variable	Control Scheme	Long Period	Disturbance Rejection Long Period (%)	Short Period	Disturbance Rejection Short Period (%)
$\beta_{external}$ Amplitude (%)	Supervisory	0.33	100.00%	0.48	100.00%
	MPC	0.31	94.08%	5.80	1209.79%
	DV	0.33	101.42%	5.50	1161.24%
Re-boiler Duty Amplitude (MW)	Supervisory	3.50	100.00%	4.05	100.00%
	MPC	3.50	100.22%	1.55	38.60%
	DV	3.50	102.09%	1.20	30.29%
$X_{d, eth}$ Amplitude (ppm)	Supervisory	0.75	100.00%	1.03	100.00%
	MPC	0.21	30.35%	0.50	53.99%
	DV	0.20	32.46%	0.34	40.22%

Both the Supervisory and MPC schemes maintain the ethanol content below the 10 ppm requirement for both long and short period disturbances. However, Table 7 shows that the MPC struggles to reach the recovery set point, and obtain recoveries over 0.1% smaller than the Supervisory scheme. This reduction in recovery, in turn results in lower energy requirements for the MPC, which are nonetheless similar to those of the Supervisory scheme in relation to the energy consumption of the DV controller. Considering the complexities of MPC systems and the small differences in mean re-boiler duties, the Supervisory scheme seems to be the more attractive scheme. The Supervisory scheme achieves the $X_{d, eth}$ requirements, while obtaining higher recoveries and a tighter control over this variable. Having said this, the tighter control of MPC over the ethanol content allows for a greater buffer zone in the quality of the product. It may also be possible to improve the overall performance of the MPC with further tuning. Since both schemes succeed at regulating the parameters of interest with the use of the proposed soft sensor, the choice of scheme will ultimately rely on economic and operational decisions. It is also important to note that in both long and short period disturbances the production rate of the supervisory control scheme is slightly higher than the MPC and is somewhat higher than the DV controller

Table 7. Average values of key variables at a recovery set point of 99.5%. Those values which were considered more attractive have been highlighted.

Process Variable	Control Scheme	Long Period	Short Period
Feed Flow Rate Average (kg/hr)	Supervisory	142550	142559
	MPC	142509	142482
	DV	142567	142504
$\beta_{external}$ Average (%)	Supervisory	99.42	99.48
	MPC	99.27	99.36
	DV	98.03	98.16
Re-boiler Duty Average (MW)	Supervisory	89.87	89.95
	MPC	89.67	89.18
	DV	88.03	87.99
$X_{d, eth}$ Average (ppm)	Supervisory	8.52	8.53
	MPC	7.86	7.67
	DV	7.00	7.00
Product flow Rate Average (kg/hr)	Supervisory	117063.4	117141.4
	MPC	116853.1	116936.9

	DV	115440.5	115542.5
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Overall the results show good accuracy and control of the recovery, in particular the Supervisory scheme. As previously discussed, this control allows for high recoveries to be achieved and in turn higher profits for the plant. The use of density to track composition and recovery thus shows great potential for the improvement of current distillation processes at a lower cost than can be achieved through traditional methods.

A similar overall controller performance can be observed when comparing the product recovery, ethanol composition and reboiler duty variations recorded in Udugama et al ¹⁴ (where similar MPC and supervisory control structures were developed but with the use of direct (external) recovery calculations) to those recorded in this study. The product recovery rate and reboiler duty that is achieved using the density-based controllers can be regarded to be similar to that of using direct recovery calculations. However, it is also important to note that some of the dynamic responses of the ethanol and recovery are somewhat different. Specifically, in density-based control, the recovery amplitude during short feed flow disturbances is larger than the external recovery-based controls. This is likely due to the different underlying process dynamics and the subsequent controller tuning which is more aggressive. As a consequence the product ethanol concentration (which is directly linked to product recovery) is also different. It is also important to note that the supervisory control in this work has a static flow rate and is not changed. Secondly both MPC and the Supervisory controller are using the density based recovery measurement and have been tuned accordingly to give the best response.

6.0 Conclusions

This study looks at the development and use of a density-based soft sensor to monitor and control recovery in a multi-component distillation column. To this end the study compared the traditional recovery reading against the new recovery measurement proposed, with the findings showing that the necessary accuracy of 0.05% is achieved with the operations envelope. Three different control schemes were designed on a validated industrial process simulator; (i) a decentralized scheme, (ii) an MPC scheme, and (iii) a simple decentralized DV scheme with no recovery tracking. An analysis of the three schemes shows the use of the soft sensor allows for better control of recovery while obtaining AA grade methanol. The use of this soft sensor represents a cheaper alternative to traditional recovery calculations. Its implementation in complex control systems offers a source of cost reduction for these schemes.

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