Soft sensor design for the optimisation of parallel debutaniser columns: An industrial case study

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Abstract: This work demonstrates a practical implementation of a soft sensor to estimate the C_5 hydrocarbon impurity in the butane product of a liquid petroleum gas (LPG) recovery system. Such a sensor can then subsequently be used to optimise the process. The process has two parallel debutaniser columns that feed a common LPG recovery system. The optimisation objective is to minimise the Reid vapour pressure (RVP) of the two debutaniser bottoms' products. This optimisation problem can be solved with a simple advanced control implementation. However, the ability of the controller to minimise the process variation and drive the process to the optimal point is directly influenced by the quality of the constraining process variable. In this case, the key controlled variable (CV) is the debutaniser overheads C_5 mass fraction. The designed soft sensor for this CV uses the general distillation shortcut (GDS) method, and is shown to represent the distillation column operation well. This work presents a derivation of the GDS method, and formulates a new approach for the feedback biasing of the two parallel debutaniser soft sensors.

Keywords: general distillation shortcut (GDS), industrial application of process control, inferential, liquid petroleum gas (LPG), soft sensor

1. INTRODUCTION

The use of catalytic polymerisation units for the production of high octane motor fuels is a widely implemented process in petroleum refining units (Leprince, 2001). The motor fuels produced from the catalytic polymerisation reactors need to be stabilised before being further processed. The stabilisation of the motor fuel is accomplished with a debutaniser, which separates out the liquid petroleum gas (LPG) components from the motor fuel. The motor fuel from the catalytic polymerisation unit is stripped in the downstream hydrotreater unit to meet a Reid vapour pressure (RVP) specification. The light components from the stripper in the hydrotreater are sent to the flare, while potential recovered LPG from the stabiliser is a valuable product in meeting market demand. This presents a control based optimisation opportunity, where the catalytic polymerisation motor fuel stabilisers could be utilised to minimise the motor fuel RVP.

The use of advanced process control for optimisation in the petrochemical industry is a mature field that generally results in significant benefits relative to the capital invested (Qin and Badgwell, 2003; Bauer and Craig, 2008). Such benefits can be realized for the feedback control of important but unmeasured variables by making use of soft sensors (Friedman, 1997). In this work, soft sensor design for the future use in a control strategy is presented.

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2. PROCESS DESCRIPTION

The LPG recovery section of the catalytic polymerisation unit that is investigated for potential optimisation using MPC is shown in Figure 1. The catalytic polymerisation production unit produces motor fuels, such as petrol and diesel, from a feed stream of C_3 and C_4 hydrocarbons. This is achieved by the fusion of the C_3 and C_4 olefin molecules into larger molecules through oligomerisation with the aid of a catalyst (Leprince, 2001). Butane and propane do not react in the catalytic polymerisation reactors and are carried on to the LPG recovery section.

The purpose of the V1 and V2 debutaniser columns is to separate the LPG from the polymerized effluent (petrol, diesel and heavy polymer). The $F_{V1,F}$ and $F_{V2,F}$ feed streams originate from two different catalytic polymerisation reactors and enter the column at approximately the middle tray. The debutaniser columns use high pressure saturated steam reboilers as an energy source. The $F_{V1,B}$ and $F_{V2,B}$ bottoms' stream of the debutanisers is predominately petrol and diesel, which is hydrotreated in the subsequent unit. The ($F_{V1,D}$ and $F_{V2,D}$) overheads distillate stream of the two debutanisers is fed into the D3 common surge drum. The combined streams feed into the V3 deethaniser, where the C_2 hydrocarbons and lighter impurities are stripped off.

The feed to the V4 depropaniser is predominantly composed of saturated C_3 and C_4 hydrocarbons. V4 separates the propane and butane as two different product streams
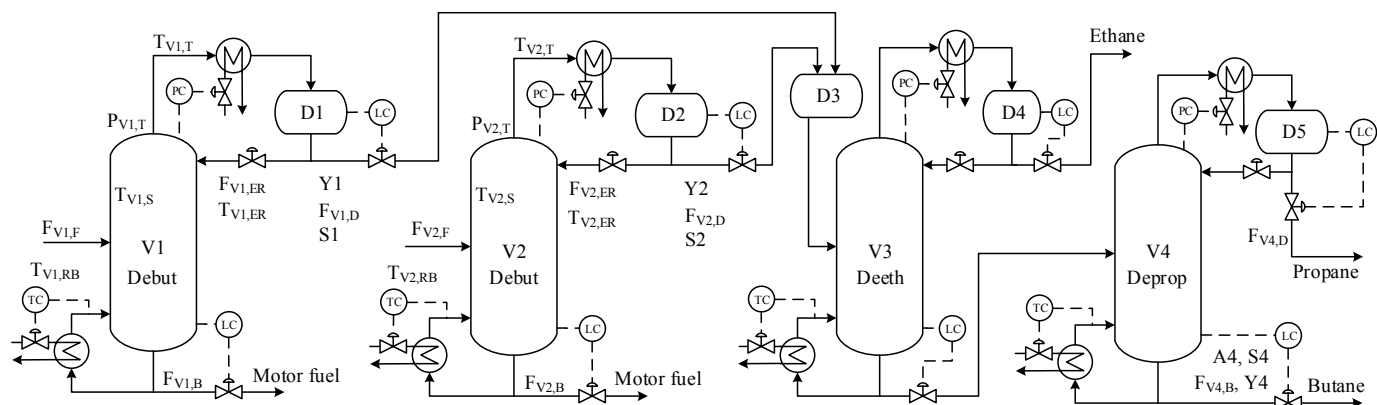
Fig. 1. Process overview showing the parallel debutanisers V1 and V2, the common deethaniser V3 and depropaniser V4. The lab sample points are S1, S2 and S4, and the analyser is A4. The soft sensors are Y1, Y2 and Y4.

that are sent to storage. The predominate use of the produced propane and butane products is for the blending of LPG to the correct specifications to be sold to the market. However, some of the butane can also be used as a blending component in the petrol pool if the RVP of the petrol blend is low. Market needs dictate the required product volumes, and blends are then adjusted to meet these needs. The butane product is therefore quite valuable due to some flexibility of its use. The propane can also be sent to the fuel gas system as a feedstock of high heating value (Muller et al., 2011).

3. OPTIMISATION OPPORTUNITY

Significant concentration of C_4 hydrocarbons is sometimes found in the gas to flare from the stripper column of the hydrotreating unit, which is downstream of the catalytic polymerisation unit. The hydrotreating unit further processes the motor fuels produced by the catalytic polymerisation unit. The cause of this valuable component flaring was found to be the requirement of the unit to meet the RVP specification of the hydrotreater petrol blending component product. Flaring results in valuable product loss, unnecessary energy consumption in upstream processing, and emission penalties (Wiid et al., 2019). However, significant C_4 hydrocarbon concentrations were also found in the feed of hydrotreater. Because of the constraint of the RVP specification, it is desirable to minimize the C_4 hydrocarbons in the hydrotreater motor fuels feed.

The main process lever that can be used to minimise the C_4 hydrocarbons in the hydrotreater feed is the operation of the V1 and V2 debutanisers. Therefore, the control philosophy is defined to maximise the separation of the two debutaniser columns and also to shift the cut to maximise the overheads distillate streams $F_{V1,D}$ and $F_{V2,D}$. However, when maximizing the separation and shifting the cut of the column to achieve this, the active constraint is a C_5 hydrocarbon mass concentration specification in the V4 butane product. Any C_5 hydrocarbons carried over with $F_{V1,D}$ and $F_{V2,D}$ cannot be removed by the following process equipment.

To achieve overhead composition control, a measure of the C_5 hydrocarbons in the distillate is required; however, there exists no analyser on these streams. A solution,

not requiring capital expenditure, is to create soft sensors Y1 and Y2 to infer the C_5 concentration using the existing instrumentation. However, there are maintenance implications that must be considered in the design of the engineering models that are used for inferential controlled variables.

The V4 bottom's butane product composition is monitored with regular lab samples (S4), which are taken every eight hours. Additionally, an analyser (A4) is installed on this product stream, which returns the composition analysis every 20 minutes. However, the A4 reading tends to be significantly less than the lab sample results. Due to this difference, the plant operators do not actually trust the analyser reading to control the process. In contrast, the S1 and S2 samples are only taken three times a week. This is not a sufficient sampling frequency for real time optimal control.

The financial benefits attained through the use of advanced process control are subject to the maintenance of the controller (Bauer and Craig, 2008), therefore it is important in the design of the controller to cater for maintainability. The installed analyser (A4) has considerable sustainable maintenance challenges which directly impacts any control scheme which aims to utilise the analysis reading. Not taking these maintenance challenges into account is a typical advanced control project mistake as described by Friedman (1992). To make use of this installed analyser, there are two main approaches that can be followed to resolve the issue:

(1) the maintenance plan needs to be improved to ensure measurement usability, or
(2) the analysis reading can be augmented using the real analyser readings together with the lab samples.

The first option is the ideal solution, because it is preferable to have a more trustworthy measurement. However, there is considerable effort that needs to be undertaken to achieve this option in a sustainable manner. Practically, the second option is faster to implement, and is the approach that is followed in this work. A simple scaling and biasing calculation is done, such that:

$$A4_{aug} = a_1 \cdot A4 + a_2 \qquad , \qquad (1)$$

where a_1 and a_2 are chosen such that the augmented analyser reading ($A4_{aug}$) best represents the S4 in amplitude and offset.

4. SOFT SENSOR DESIGN

The modelling of the soft sensors to be used as controlled variables for the composition control in the debutaniser real time optimisation control scheme is detailed below.

4.1 Composition inference method

To calculate the C_5 hydrocarbon mass fraction in the distillate stream of the debutaniser, the general distillation shortcut (GDS) approach is followed (Friedman, 1995, 1997; Friedman et al., 2002). This method has been widely used as an inference of the separation on a distillation column section through the use of readily available temperature and flow measurements to control product composition (Friedman and Reedy, 2001).

The method is derived from the formulation of the number of theoretical trays calculation by Colburn (1941). The number of theoretical trays calculation is for an equilibrium based model of a distillation column section. The number of theoretical trays (N) is given as:

$$N = \frac{\ln\left((1-P)M + P\right)}{\ln\left(1/P\right)} \qquad , \qquad (2)$$

where the substitutions for P and M are given in Table 1 for the enriching and stripping sections of a column. Additional parameters are the vapour to liquid ratio R and the equilibrium equation slope constant m. For the M parameter, $y_{F,i}$ and $y_{P,i}$ are the feed and product vapour compositions for the component i, while the $x_{F,i}$ and $x_{P,i}$ are the liquid feed and product composition for the component i.

Using the number of theoretical plates calculation, the inferential method by Friedman (1995) solves for the desired product composition in either the stripping or enriching section of the distillation column. It is assumed that the number of theoretical plates in a distillation column section remains constant, and that this number can be used as a tuning parameter in obtaining the best fit between the model and laboratory results. A further assumption is that the distillation equilibrium line slope m can be approximated using the distribution coefficient $K = y/x$ (Colburn, 1941). The resulting expression for component i is:

$$V_i = \left(\frac{(1/U_i)^{N+1} - 1}{(1/U_i) - 1}\right)(W_i - 1) + 1 \qquad , \qquad (3)$$

where the equation substitutions for V_i, U_i and W_i for an enriching and a stripping column section are given in Table 2.

The original work of Friedman (1995) only provided V_i for the stripping section of a distillation column. The expression for V_i for an enriching section was provided in Friedman (1997); however, it did not highlight the change in U_i. The enriching section equation with compensation

Table 1. Summary of the Colburn (1941) theoretical plate equations for an enriching and stripping section.

	P	M
Enriching	mR	$\dfrac{y_{F,i} - m\,x_{P,i}}{y_{P,i} - m\,x_{P,i}}$
Stripping	$\dfrac{1}{(mR)}$	$\dfrac{x_{F,i} - x_{P,i}/m}{x_{P,i} - x_{P,i}/m}$

Table 2. Composition equation input summary.

	V_i	U_i	W_i
Enriching	$\dfrac{x_{Ni}}{y_{Ti}}$	$K_i R$	$\dfrac{1}{K_i}$
Stripping	$\dfrac{y_{Ni}}{x_{Bi}}$	$\dfrac{1}{(K_i R)}$	K_i

for U_i was given by Smets et al. (2007). In the derivation for the enriching section, it is assumed that total condensation occurs. Therefore, the composition of the overheads vapour is equivalent to the composition of the liquid in the distillate, giving $y_{T,i} = x_{T,i}$. This then allows the enriching section M from Table 1 to be defined as:

$$M = \frac{y_{N,i} - mx_{T,i}}{y_{T,i} - mx_{T,i}} = \frac{y_{N,i} - K_i y_{T,i}}{y_{T,i} - K_i y_{T,i}} \qquad , \qquad (4)$$

To solve for the molar composition of a component key in a binary distillation system, the steady state plate phase equilibrium equations can be used together with (3), and are given by:

$$\sum_i x_i = 1 \quad , \text{ and } \quad \sum_i y_i = 1 \quad . \qquad (5)$$

4.2 Debutaniser overheads C_5 mass fraction inferential

Important parameters for the inferential are the vapour to liquid ratio R and the diffusion coefficient K_i. A method for the determination of these two parameters from available instrumentation measurements, in different plant configurations, is detailed in Friedman (1997) and Smets et al. (2007). However, the method that is used for the determination of Y1 and Y2 differs from theirs, and is subsequently described.

The diffusion constant K_i is readily determined using Raoult's law and Dalton's law (Sorensen, 2014). The diffusion coefficient is equal to the fraction of the partial pressure of the component in relation to the total pressure:

$$K_i = \frac{p_i^{vap}}{P_N} \qquad , \qquad (6)$$

where p_i^{vap} is the partial pressure of the component and P_N is the total pressure at the tray where the partial pressure is calculated.

The partial pressure for a component is a function of the temperature (T) of the components. Multiple methods used for estimating the partial pressure are available (Sorensen, 2014). However, the Antoine equation is normally used for this inferential, because of the availability of coefficients for various compounds (Green and Perry, 2008). The equation is:

$$\log_{10}\left(p_i^{vap}\right) = A_i - \frac{B_i}{T + C_i} \qquad , \qquad (7)$$

where A_i, B_i and C_i are coefficients for the specific compound. The Antoine constants for pentane are taken from Osborn and Douslin (1974), and for butane from Das et al. (1973). The temperature input used, is from the measured tray $T_{V1,S}$ or $T_{V2,S}$.

The diffusion coefficients can be calculated using (6) together with the pressure at the measured tray (P_N). The pressure at the measured tray is approximated by taking the overheads pressure ($P_{V1,T}$ or $P_{V2,T}$), adding the average atmospheric pressure at the site (P_{atm}) and an estimated pressure drop per tray between the overheads and the sensitive tray. The pressure drop per tray is assumed to be 0.7 kPa. Therefore the pressure at the measured tray is

$$P_N = P_T + \Delta n \times 0.7 + P_{atm} \quad , \qquad (8)$$

where n is the number of trays between the top and the measured tray.

The calculation of the vapour to liquid ration (R) at the measured tray is approximated by dividing the calculated liquid equivalent vapour flow rate (F_V) by the calculated internal reflux (F_{IR}). The calculation of the internal reflux is given by:

$$F_{IR} = F_{ER} \times \left(1 + \frac{C_p}{\Delta H^{vap}}\left(T_T - T_{ER}\right)\right) \quad , \qquad (9)$$

where C_p is the specific heat capacity, and ΔH^{vap} is the enthalpy of vaporisation (Morgan, 1962). The measurement inputs are the external reflux flow rate ($F_{V1,ER}$ or $F_{V2,ER}$), overheads temperature ($T_{V1,T}$ or $T_{V2,T}$), and the external reflux temperature ($T_{V1,ER}$ or $T_{V2,ER}$).

The calculation of the liquid equivalent vapour flow rate (F_V) is approximated as the overheads vapour flow rate compensated for the subcooling effect of the reflux. Assuming that total condensation occurs, the overheads vapour flow rate equals the sum of the distillate ($F_{V1,D}$ or $F_{V2,D}$) and external reflux ($F_{V1,ER}$ or $F_{V1,ER}$) flow rates. The subcooling effect of the reflux on the vapour flow rate is calculated as the difference between the internal (F_{IR}) and external reflux flow rates. The liquid equivalent vapour flow rate is given by:

$$F_V = (F_{ER} + F_D) + (F_{IR} - F_{ER}) \quad . \qquad (10)$$

The GDS method for the enriching column section is used to infer Y1 and Y2. A binary distillation column is assumed which is deemed sufficient for this work. The heavy-key is chosen as the C_5 hydrocarbons, which is the desired inferred value. To solve for the heavy key molar concentration, $V_i = {x_{N,i}}/{y_{T,i}}$, $U_i = K_i R$, and $W_i = {1}/{K_i} - 1$ are introduced for both the heavy key $(i = H)$ and the light key $(i = L)$. These two equations, together with the plate equilibrium equations (5), can be solved for the heavy key. A constant bias (b) is included in the result to eliminate any offset in the inferred values. The heavy key molar concentration is:

$$y_{T,H} = \frac{1 - V_L}{V_H - V_L} + b \quad . \qquad (11)$$

The constants (A_H, B_H, C_H, A_L, B_L, C_L, C_p, ΔH^{vap}, N, and b) are estimated offline by fitting the inferential output (11) to lab sample data using numerical minimisation of a modified least squares parameter estimation cost function. The numerical minimisation algorithm that is used is the Nelder-Mead simplex method (Nelder and Mead, 1965).

The modified parameter estimation cost function uses the quadratic difference in standard deviation as an additional penalty in the cost function. This enables the parameter estimation to better fit some of the excursions in the sample data, and not fit the parameters to the average sample data. The parameter estimation is given by:

$$\min_{A_H, B_H, C_H, A_L, B_L, C_L, C_p, \Delta H^{vap}, N, k}(J) \quad , \text{ with}$$

$$J = \sum_k (x_k - \hat{x}_k)^2 + Q(\sigma - \hat{\sigma})^2 \quad , \qquad (12)$$

where x is the sample data and $\hat{x}$ is the inferred values, σ is the standard deviation of the sample data and $\hat{\sigma}$ is the standard deviation of the inferred values. The Q parameter is a tuning constant used to weight the standard deviation fitting.

The initial conditions for the Antoine constants, the specific heat and the enthalpy of vaporisation are taken from literature. The heavy key is assumed to be predominantly pentane, while the light key is assumed to be predominantly butane. The initial values for the enthalpy of vaporisation and the specific heat capacity are set to the butane values found in literature (Stephenson, 2012; Chen et al., 1975).

The resulting constants of the parameter estimation is shown in Table 3, and the inferential outputs of Y1 and Y2 are shown in Fig. 2 and Fig. 3 respectively. It must be noted that outliers and periods of process upsets were removed from the sample data prior to the fitting. The Pearson correlation for Y1 is 0.46, and for Y2 is 0.38. Although this is a correlation of moderate strength, the two soft sensors both captured many of the deviations. The fit is considered good, because the data source is irregularly taken lab samples and the sampling frequency is not high enough to capture process dynamics.

4.3 Depropaniser bottom's product C_5 concentration

To compensate for unmeasured disturbances and non-linearities, it is desirable to bias the soft sensors using lab data. However, the S1 and S2 lab samples are taken at irregular time intervals, whereas the S4 lab samples
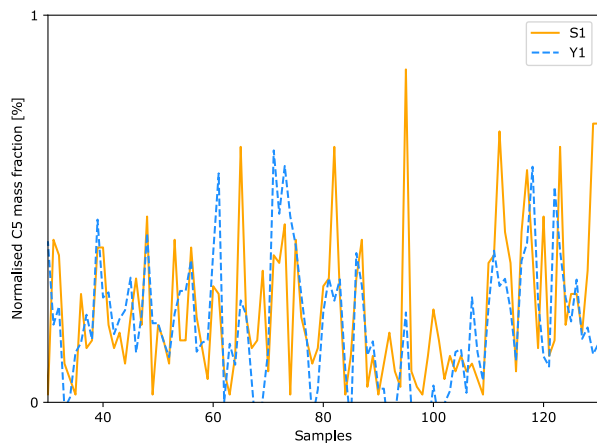
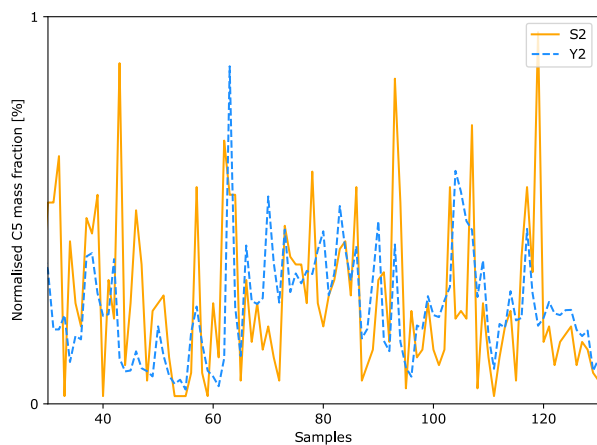Fig. 2. Y1 inferential fit against lab sample data.

Fig. 3. Y2 inferential fit against lab sample data.

Table 3. Constants used in the initial estimation and final calculation of Y1 and Y2. The units for C_p are J/(mol · K), and for ΔH^{vap} are kJ/mol.

	Initial	Y1	Y2
A_H	4	2.3	2
B_H	1070	1012	991
C_H	-40	219	360
A_L	4.45	4.6	16
B_L	1160	1174	1173
C_L	1.4	4.7	9.8
C_p	112	145	116
ΔH^{vap}	22.7	25.1	24.7
N	8	6	8

are taken three times daily consistently. This makes it desirable to able to use the data from the S4 lab samples. As an improvement, the $A4_{aug}$ analyser reading is used for more frequent and reliably timestamped compensation. This is due to lab samples often not being recorded at the exact time the sample is taken, causing potential erroneous biasing if used for error correction (Friedman, 2008).

To this end, the Y4 soft sensor for the bottom's product of V4 is created. This soft sensor uses an intermediate blending calculation of the $F_{V1,D}$ and $F_{V2,D}$ debutaniser
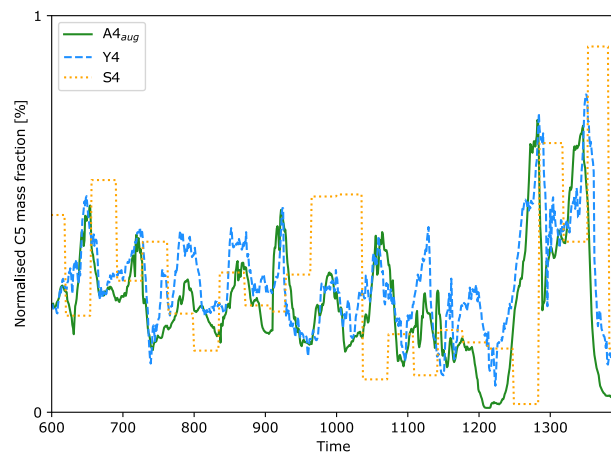

Fig. 4. Sampled value, augmented analyser reading and calculated reading of the C_5 mass fraction in the V4 butane product plotted for 11.8 days with a 20 minute sampling interval.

distillate flow streams to give the approximated C_5 mass fraction entering the D3 drum:

$$Y3(t) = \frac{Y1(t) \cdot F_{V1,D}(t) + Y2(t) \cdot F_{V2,D}(t)}{F_{V1,D}(t) + F_{V2,D}(t)} \quad . \quad (13)$$

To compensate for the resulting mixing and delay due to the D3, V3 sump and V4 sump accumulators, the effect is approximated using a fixed dead time and fixed moving average window. Additionally, the concentrating effect due to the removal of propane in V4 is modelled using the butane product flow rate ($F_{V4,B}$) and the propane product flow rate $F_{V4,D}$. The mass fraction of C_2 hydrocarbons removed in V3 is low enough to allow its exclusion from the model. The resulting calculation for Y4 is given by:

$$Y4(t) = Y3_{av}(t - \theta) \cdot \frac{F_{V4,B} + F_{V4,D}}{F_{V4,B}} \quad , \quad (14)$$

where θ is the process dead time. The moving average window and the dead time were adjusted to minimise the phase difference between Y4 and $A4_{aug}$.

The Y4 soft sensor can then be compared to the $A4_{aug}$ reading to approximate the steady-state error in the Y1 and Y2 soft sensor calculations. The approximated error may then be used to correct Y1 and Y2 using the bias term b. The feedback approximate error is assumed to originate from Y1 and Y2 in ratio to the distillate flow rates $F_{V1,D}$ and $F_{V2,D}$ for V1 and V2 respectively. The b correction term for Y1 is given by:

$$\Delta b_{Y1} = a \cdot (Y4 - A4_{aug}) \cdot \frac{F_{V1,D}}{F_{V1,D} + F_{V2,D}} \quad , \quad (15)$$

where a is a tuning parameter dependent on the execution frequency and the desired rate of bias correction. The correction term for Y2 is similarly obtained.

The Y4 inferential output, together with the $A4_{aug}$ and S4 readings are shown in Fig. 4 for a period of 11 days. It must

be noted that no feedback biasing was done for this time period. The Pearson correlation between Y4 and $A4_{aug}$ for is 0.71. This is a strong correlation, and also indicates that the Y1 and Y2 soft sensors can reliably predict the debutaniser dynamic operation.

Care should be taken when implementing the bias update term for a soft sensor system that runs in closed loop, since there can be unexpected failures in the soft sensor system (Shardt and Huang, 2012; Shardt and Yang, 2016). During implementation the biases update values are first validated for standard operating regions and excessive rate of change.

5. CONCLUSION

The optimisation objective in this problem can be solved with an advanced process control scheme. However, the ability of this controller to minimise the process variation and drive it to the optimal point is directly influenced by the quality of the measurement. In this case, the key controlled variable is an overheads C_5 mass fraction soft sensor that is shown to represent the distillation column operation well. Additionally, it is shown how to use feedback biasing for the two debutanisers feeding a common LPG recovery section, where the measurement for the feedback has a significant process delay.

A C_5 hydrocarbon mass fraction soft sensor was developed and applied on an industrial case study consisting of parallel debutaniser columns. The soft sensor design is based on the GDS method, and compensates for dead time, mixed analysis streams, and long intervals between lab samples which are used for model error correction. The developed soft sensor is shown to predict the overheads C_5 mass fraction sufficiently well, and is recommended for use in advanced process control application.

Future work includes incorporating the soft sensor into an advanced control formulation and performing a post-implementation benefit audit. Further study includes comparing the GDS soft sensor approach with state-of-the-art black box soft sensor design, and comparing the GDS method to rigorous dynamical first principle models.

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