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Soft Sensor Development for Monitoring ASTM-D86 Index: Effect of Feed Flow Rate Change

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ABSTRACT

Changes in a crude oil flow rate to an atmospheric distillation unit can influence the quality of the products. This paper presents a modification method for a soft sensing model, including an update term, which makes it compatible with industrial variations. A modified soft sensing structure is adopted using the lookup table (LUT) method where steady-state soft sensing models are performed. The steady-state soft sensing models are proposed based on the local instrumental variable (LIV) technique for an industrial atmospheric distillation unit (ADU) at Shiraz refinery, Iran. The LIV-based soft sensors use tray temperature measurements to monitor the ASTM-D86 index of side products for a nominal flow rate (60,000bbl/day). The lookup tables have been developed based on the difference between the predicted values of the ASTM-D86 index and the corresponding simulation values to make update terms in different feed flow rates. The results present improvement in the predictions of LIV-based soft sensors, as well as acceptable control performance in feed flow rate variations. The comparison of soft sensing results with/without the lookup tables demonstrates that the proposed update term helps to predict product quality more precisely and is suitable for advanced monitoring scheme due to no complexity and low computational time.

Article Info

Keywords:
ASTM-D86 Index, Crude distillation column, Data-driven soft sensor, Local instrumental variable (LIV), Lookup table method

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I. INTRODUCTION

Crude distillation units (CDUs) are considered the principal process in oil refineries. The atmospheric distillation column (ADU) is the heart of a CDU and the most fundamental step in the refining process. The primary purpose of an ADU is to separate crude oil into its components (or distillation cuts, distillation fractions) including naphtha, kerosene, gas oil, etc. for further processing by other units. Crude oil is a complex blend of hundreds of hydrocarbons that makes it difficult to determine its product quality with distillation fractions. Typically, petroleum product quality is specified by ASTM standard methods. ASTM-D86 is the standard test method used to experimentally measure the batch distillation curve of a petroleum product at atmospheric pressure [1, 2].

The online monitoring of temperature, pressure, and flow rate is simply done by using available hardware sensors. However, online monitoring of product qualities is only possible by installing online sensors, which are very complex, hard-to-maintain, and expensive. One of the challenging issues in the quality monitoring or controlling of ADUs is the unavailability of suitable hardware sensors for online measuring of the ASTM index. The procedure of laboratory measurements for the ASTM analysis is also ponderous and time-consuming, so it is not practical to measure this quality more than once in a shift (e.g., 8 hours) or up to twice in 24 hours [3-5].

Since accurate and reliable measurements are required for control purposes, the lack of online measurement of product

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quality can be complemented by soft sensing methods. A soft sensor is a mathematical model that is used instead of a physical sensor when a physical sensor cannot be placed due to several reasons like non-availability of a sensor, economic constraints, placement constraints, etc. In the control theory field, these soft sensors are known as observers. If a system is observable, it is possible to fully reconstruct the system states that are used in the control structure from its output measurements using state observers. In the measurement and monitoring field, soft sensors are also known as observers if the relationships describe the process mechanistically [6, 7]. They have been successfully adopted in several applications to provide accurate and reliable estimates without requiring further expenditure on hardware sensors or laboratory measurements [8, 9].

There are two different approaches to design soft sensors: model-driven and data-driven. Model-driven soft sensors are based on prior knowledge of the system and use first-principle models to estimate the desired variables. Data-driven soft sensors use models that are based on available data of the system and extremely interesting in the process industries as they can quickly be developed without the need for insights into the complex mechanisms of industrial units. They describe the real process dynamics of complex processes more realistically [10-12]. Typical data-driven techniques to estimate the process variables include partial least squares (PLS) [13-15], principal component analysis (PCA) [16-18], artificial neural networks (ANN) [19-21], neuro-fuzzy system (NFS) [22-25], support vector regression (SVR) [26-28], and their modifications [29-32].

The state-dependent parameter (SDP) modeling approach is an identification and modeling technique that was introduced by Peter C. Young and co-workers [33] and first adopted for soft sensor development by Gharehbaghi and Sadeghi [34] and Bidar et al. [35]. The modeling approach is based on the data-based mechanistic (DBM) modeling philosophy. In the DBM philosophy, the non-stationary and nonlinear aspects of the system are reflected by varying parameter models, whether parameters are varying with time or state variables of the system. The identification procedure is based on a stochastic state-space formulation, which uses a recursive Kalman filter (KF), fixed interval smoothing (FIS), and iterative back-fitting algorithms [36].

Furthermore, the SDP modeling approach outperforms other traditional data-driven methods like PCR, PLS, ANN, SVR, and so on, due to its remarkable capability to describe the behavior of non-linear systems. As a result, SDP-based soft sensors have shown successful applications for the estimation of process variables. However, nonparametric methods like SDP suffer from the use of the back-fitting algorithm because the functionality of each SDP affects the estimation of the other SDPs, which produces other problems associated with the back-fitting algorithm.

To deal with this issue, Bidar et al. [37] proposed a novel SDP method by local instrumental variable (LIV). The LIV approach uses polynomial modeling combined with instrumental variable (IV) concepts to introduce the simultaneous estimation method of SDPs. The proposed method was applied to predict 95%ASTM-D86 of side products in a simulated ADU based on tray temperature measurements. LIV-based soft sensors were developed based on steady-state simulation data of an industrial ADU at a nominal feed flow rate of 60,000 bbl/day. The optimal performance was achieved with the help of LIV-based soft sensors in closed-loop control of the simulated process around the nominal flow rate.

However, in real crude distillation processes, the feed flow rate is variable due to operational and feed availability constraints. The persistence of such variations in the feed flow rate can raise serious challenges in the control of the process. Due to the highly nonlinear and ill-conditioned characteristics of ADU, LIV-based soft sensors have been trained with steady-state data at constant capacity while feed flow rate variations have a significant impact on the reliability of their estimates. The weakness of the proposed soft sensing model is to ignore the feed flow rate variation. Therefore, feed flow rate data like tray temperature measurements need to be properly incorporated into the soft sensing model. The slow and complex dynamic of ADU makes it difficult to gather dynamic data in different feed flow rates.

The objective of the present paper is to modify the LIV-based soft sensor model including an update term, which makes it compatible with industrial variations. An update term allows information about the feed flow rates to be included in the soft sensing model and improves their estimates. In other words, the flow rate-based corrector is proposed to develop a high-quality soft sensing model with good generalization abilities.

The lookup table (LUT) method is implemented to make update terms, which is based on ASTM-D86 differences (e.g. the difference between the outputs of LIV-based soft sensors and corresponding simulation values) obtained in different feed flow rates. The linear interpolation method is used to determine difference data for interpolated values. The difference data are augmented to the prediction values of soft sensors to maintain the 95%ASTM-D86 indexes at setpoint levels. As lookup table can produce a quick interpolation platform to link with soft sensing models, it can be easily combined with different soft sensing algorithms, including the effect of changes in influencing process variables.

The paper is organized as follows. Section II provides a brief overview of the SDP/LIV technique and then presents the modification by lookup table method. In this section, the issues of problem description (Section II.A), LIV-based soft sensor modeling (Section II.B), feed flow rate analysis (Section II.C), and lookup table method (Section II.D) are described in detail. Successful implementation results of the modified LIV-based soft sensors are provided and discussed in Section III. The paper is concluded in Section IV.

II. Modified LIV-based Soft Sensor Modeling Method

A. Problem description

Fig. 1 shows the flowsheet of the ADU considered in this paper including a crude tower, top condenser, two pumparounds, and three side strippers. The column has 43 trays and three main products including naphtha, kerosene, and gas oil, which are taken from three side strippers, and the atmospheric residue is sent to the vacuum distillation unit (VDU) for further processing. Further information about the case study is available in [38, 39].

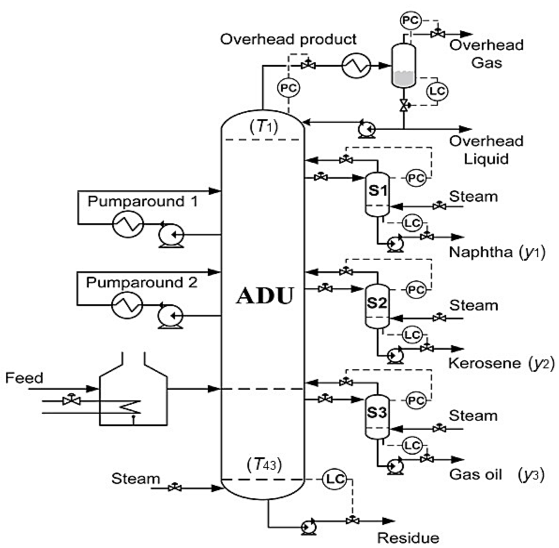

Fig. 1. The flowsheet of the atmospheric distillation column (ADU) [38].

The steady and dynamic simulations of the ADU were performed using the Aspen plus and Aspen dynamics, respectively. As is shown in [37], soft sensors were developed based on the LIV modeling approach to the continuous prediction of the 95%ASTM-D86 index of side products. Therefore, temperature measurements (e.g., T_1–T_{43}) inside the ADU and 95%ASTM-D86 index of naphtha (y_1), kerosene (y_2), and gas oil (y_3) were chosen as the input and output variables, respectively, and were initially used to identify soft sensing structures. Most informative temperatures were selected based on both correlation analysis and backward elimination method. The selected temperatures (three tray temperatures for each quality variable) and the corresponding output variables (y_1, y_2, and y_3) are given in Table I.

The LIV-based soft sensors were applied to the Aspen dynamic model of the ADU using MATLAB-Function blocks in Simulink while the proportional-integral plus (PIP) control structure was implemented. PIP is directly derived from Non-Minimum State Space (NMSS) form, which is essential for the True Digital Control (TDC) design. The PIP is considered as an extension to Proportional Integral (PI) and Proportional Integral Derivative (PID) control, but with additional feedback and input compensators introduced by the NMSS State Variable Feedback (SVF) control law. Since PIP control is a sequel to SVF control design, it can be utilized in any state space design method [38, 40].

TABLE I. SELECTED TEMPERATURES AND OUTPUT VARIABLES OF LIV-BASED SOFT SENSORS [37]

Product quality/ Output variable	Setpoint of output variable (°F)	Input variables
95%ASTM-D86 of naphtha (y_1)	385.7	T_4, T_{14}, T_{28}
95%ASTM-D86 of kerosene (y_2)	502.3	T_{20}, T_{21}, T_{43}
95%ASTM-D86 of gas oil (y_3)	623	T_{32}, T_{34}, T_{43}

Fig. 2 shows the location of the LIV-based soft sensors of the PIP controller and its application to the distillation column. The LIV-based soft sensors were developed at the nominal feed flow rate of 60,000 bbl/day. The detailed prediction results are presented in [37]. As the LIV-based soft sensors have been developed at a constant capacity, feed flow rate variations have a significant impact on the accuracy and reliability of the estimates. Therefore, the prediction performance of LIV-based soft sensors gets reduced. Accordingly, the feed flow rate analysis is discussed in Section II.C.

B. LIV-based soft sensor modeling

The soft sensing model between temperature measurements (secondary variables) and each 95%ASTM-D86 index (primary variable) was identified based on SDP/LIV modeling in the following form [37]:

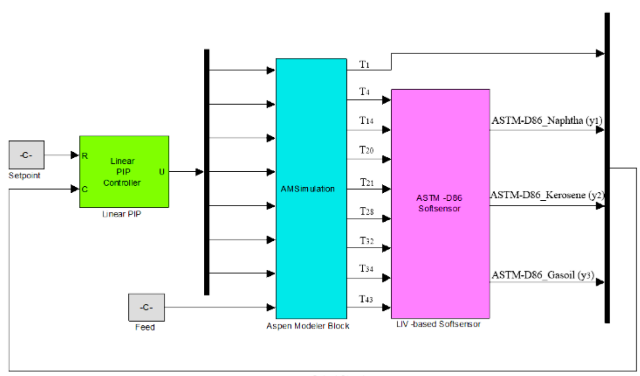

Fig. 2. The LIV-based soft sensors and PIP controller in MATLAB-Simulink [37]

$$\begin{cases} y_t = \sum_{i=1}^{n} a_{i,t} \cdot z_{i,t} + e_t \\ a_{i,t} = a_i\left(x_{1,i,t}, x_{2,i,t}, \ldots, x_{ns_i,i,t}\right) \end{cases}, \quad \forall t, \quad e_t = N\left(0, \sigma^2\right) \tag{1}$$

in which y_t is the model output, n is the number of SDPs/regressors, $z_{i,t}$ is the i^{th} regressor, and $a_i(.)$ is the SDP that is a function of the i^{th} correspondent states ($x_{j,i,t}$, $j = 1,2,\ldots,ns_i$). In the case where $a_{i,t}$ is not state-dependent, $ns_i = 0$. e_t is a zero-mean white Gaussian distributed unknown noise with variance σ^2 . In local polynomial modeling combined with the IV concepts, the functionality of each SDP from its corresponding states is defined by a local polynomial in the state variable space, where the parameters of these polynomials are locally estimated by the implementation of IV method. Therefore, $a_{i,t}$ can be defined as,

$$a_{i,t} = \mathbf{S}_{i,t}\mathbf{A}_{i,t} \quad i = 1,2,\ldots,n \tag{2}$$

where $\mathbf{A}_{i,t}$ is the vector of locally constant parameters of the polynomial demonstrating $a_{i,t}$ and $\mathbf{S}_{i,t}$ can be written as,

$$\mathbf{S}_{i,t} = \mathbf{S}_{0,i,t} \otimes \mathbf{S}_{1,i,t} \otimes \mathbf{S}_{2,i,t} \otimes \cdots \otimes \mathbf{S}_{ns_i,i,t} \quad , \quad i = 1,2,\ldots,n \tag{3}$$

and,

$$\begin{gathered} \mathbf{S}_{j,i,t} = \begin{bmatrix} 1 & x_{j,i,t} & x_{j,i,t}^2 & \cdots & x_{j,i,t}^{q_{j,i}} \end{bmatrix} \\ j = 0,1,2,\ldots,ns_i \end{gathered} \tag{4}$$

where $\otimes$ is the Kronecker tensor product symbol and $q_{j,i}$ is the order of polynomial describing $a_{i,t}$ with respect to $x_{j,i,t}$ such that $q_{0,i} = 0$. The number of parameters in $\mathbf{A}_{i,t}$ is obtained by $p_i = \prod_{j=0}^{ns_i}\left(1 + q_{j,i}\right)$. All members of $\mathbf{A}_{i,t}$ are state-dependent functions of $x_{j,i,t}$. Substituting Eq. (2) in Eq. (1) yields the model in vector form as,

$$y_t = \mathbf{z}_t\mathbf{A}_t + e_t \tag{5}$$

where $\mathbf{z}_t$ is the new vector of regressors and $\mathbf{A}_t$ is the vector of the parameters of local polynomials describing each state-dependent parameter. To identify the soft sensing model in the form of Eq. (1), the simulated datasets of input and output variables were established using the Monte Carlo method via linking the MATLAB-Simulink to Aspen dynamic model. The simulated data for building soft sensing models were obtained under the following conditions. The random signals of bounded and varying amplitude (within ±20ºF of the steady-state setpoints as given in Table I) with a nominal feed flow rate of 60,000 bbl/day were introduced as quality variations of side products during simulations. The simulation was performed as long as the steady-state operating condition was achieved (about 20 hr) to obtain the corresponding temperature profile (T_1–T_{43}). It assumes that there are no changes in pressure and tray efficiencies of the column.

A total of 1000 steady-state random data samples were collected and divided into the training dataset (500 samples) and testing dataset (500 samples). All representative temperatures were considered as states in one parameter and the corresponding regressor was chosen as one. In the online implementation of models, the temperatures were sensed and transferred to LIV-based soft sensors and the predicted outputs were taken and used in the PIP controller (see Fig. 2). The SDP method is a well-known modeling method, which was introduced into the field of soft sensing, so readers can refer to our previous papers [35, 37, 41] for more details on the SDP/LIV algorithm.

C. Feed flow rate analysis

Monitoring of control variable is shown that product quality can be affected by feed flow rate variations. Therefore, using only inferential temperature measurements cannot guarantee the desired value of setpoints because the tray temperatures do not correspond exactly to the product quality. Based on the process expert's knowledge, the acceptable operating range for the feed flow rate of the simulated ADU is from 50,000 to 65,000 bbl/day. To investigate the effect of feed flow rate, three simulation runs are conducted by changing the feed flow rate from 60,000 bbl/day to 50,000, 55,000, and 65,000 bbl/day. The input or feed flow rate signal of the ADU model is represented by a Ramp function. During each simulation run, the Ramp block slope and start time are set at ±3360 bbl/hr and 0.5 hr, respectively. The total simulation time is set at 20 hr as is required to reach a steady-state.

The PIP control structure and its parameters are the same as the nominal case (e.g., the feed flow rate of 60,000 bbl/day). The setpoints of the PIP controller are considered similar to the nominal values of 95%ASTM-D86, which are listed in Table I. After the system reached the steady-state condition, the results of product quality obtained by the Aspen IQ inferential quality software package and the LIV-based soft sensors are recorded. Aspen IQ is a built-in inferential sensor in the Aspen technology package, which makes online implementation and remote monitoring. The 95%ASTM-D86 values produced by Aspen IQ are considered as the “real” values. In each steady-state level, the difference between LIV-based soft sensor and Aspen IQ values or the difference data indicates system deviation from actual conditions.

The data of different flow rates can be efficiently utilized to consider the feed flow disturbances, which can be used to make update terms. An update term allows information about the feed flow rate variations to be included in the soft sensor system to improve the resulting estimates. Accordingly, in the next step, the lookup table method is proposed to develop a flow rate-based corrector using an update term to compensate for varying crude oil flow rates.

D. Lookup table method

Many Simulink models rely upon discrete-valued functions for which the function values are defined as lookup tables. Such discrete-valued functions arise in applications for which no known closed-form algebraic definition exists. The one-dimensional lookup table (1-D) computes an approximated function that the function can be approximated by either a single continuous function or possibly a small number of disjoint continuous functions. Most lookup table blocks have the following interpolation methods available: flat (constant), linear, and cubic spline. Function values are defined as the lookup table between input value (breakpoint) and output value (table data), with an interpolation function used to evaluate intermediate values in the table data [42]. The 1-D lookup table model can be formulated as follows:

$$\Delta y = f(x) \tag{6}$$

In this case, there is one independent variable of feed flow rate (x) and one dependent variable of difference data (Δy), which makes the input-output pair. The first stage of a lookup table operation involves determining input values. The breakpoints of the lookup tables are considered at four levels of feed flow rate including 50,000, 55,000, 60,000, and 65,000 bbl/day, while the table data is different for each byproduct. The second stage involves generating table data that correspond to the supplied breakpoints. The table data can be prepared using the following steps:

1) The dynamic model runs at a flow rate of 60,000 bbl/day (nominal case), and $y_{predicted}$ and $y_{AspenIQ}$ are obtained through LIV-based soft sensors and Aspen IQ, respectively. $y_{predicted}$ and $y_{AspenIQ}$ are considered as 95%ASTM-D86 index of byproducts.
2) The dynamic model runs by varying the feed flow rate from 60,000 bbl/day to 50,000, 55,000, and 65,000 bbl/day, and after the steady-state is achieved, $y_{predicted}$ and $y_{AspenIQ}$ are recorded for each run.
3) Calculate the difference data (Δy) between $y_{predicted}$ and $y_{AspenIQ}$ of each run, which is determined by
$\Delta y =$ LIV-based soft sensor value $\left(y_{predicted}\right)$
- Aspen IQ value $\left(y_{AspenIQ}\right)$
for all product qualities.

The resulting data are tabulated and finally, the 1-D lookup table is formed with these data and when used in the dynamic model, it will give the update term for any feed flow rate level. Appropriate difference values for any given flow rate level are found by comparing the input flow rate to table data. If the inputs match the values of the flow rate level specified in breakpoint data sets, the block outputs the corresponding values. However, if the inputs fail to match values in the breakpoint data sets, the block performs interpolation between input-output pairs to determine an appropriate output value. In the block parameter dialog box, it can be specified how to compute the output in this situation. Then, the output value must be combined with the predicted values of the LIV-based soft sensor to achieve satisfied prediction performance.

III. Results and Discussion

To investigate the prediction performance of LIV-based soft sensors, a steady-state simulation of the nominal case (e.g., the feed flow rate of 60,000 bbl/day) was performed. The predicted results of the proposed soft sensors for the 95%ASTM-D86 index of three byproducts were compared with the Aspen IQ results through Fig. 3. y_1, y_2, and y_3 are the 95%ASTM-D86 index of naphtha, kerosene, and gas oil, respectively. It can be observed that the predicted quality of all byproducts is close enough to corresponding Aspen IQ values. It should be noticed that the difference between the LIV-based soft sensor and Aspen IQ results is slightly increased from the top product (naphtha) to the bottom product (gas oil) of the column. The difference data for 95%ASTM-D86 of naphtha, kerosene, and gas oil is 0.02% (0.07ºF), 0.04% (0.27ºF) and 0.06% (0.33ºF), respectively. However, in this case, the maximum difference in the 95%ASTM-D86 index is lower than 0.5ºF when the steady-state condition is reached. The reason for this increase in the difference between predicted results is that the complex conditions and internal interaction of the column affect the main variables in the top-down crude oil distillation column

[43]. The aforementioned reasons make the model response more accurate and simpler for naphtha rather than kerosene, and gas oil.

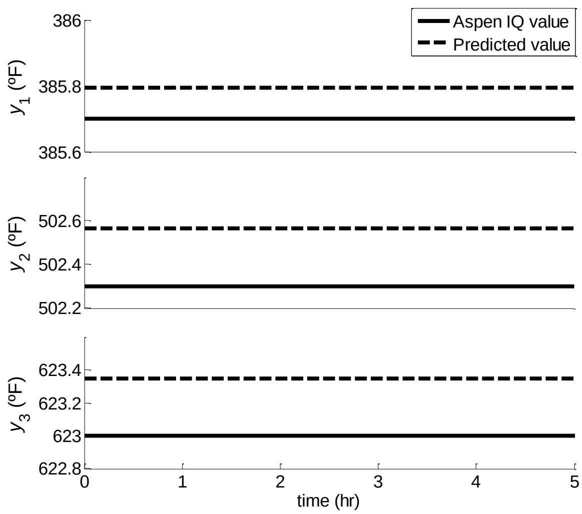

Fig. 3. The steady-state results of LIV-based soft sensors in the PIP control structure at a feed flow rate of 60,000 bbl/day

To investigate the prediction performance of the LIV-based soft sensors against feed flow rate variations, three simulation runs are conducted in the range of acceptable feed flow rate values. The change in feed flow rate from 60,000 bbl/day to 50,000 and 55,000 bbl/day and from 60,000 bbl/day to 65,000 bbl/day is continuously imposed through the Ramp function with the slope of -3360 bbl/hr and +3360 bbl/hr, respectively. While the simulation is run to reach a lower level of flow rates, e.g., a feed flow rate of 50,000 bbl/day, the steady-state parameters from the previous run with a higher flow rate level (e.g., a flow rate of 55,000 bbl/day) are used to initiate new simulation run. Table II shows the results of the LIV-based soft sensors and Aspen IQ, as well as the difference data (Δy) at each crude oil feed flow rate.

The difference data for each byproduct as depicted in Fig. 4 show significant variations when the feed flow rate change is imposed. It can be concluded that Δy values change with both feed flow rate and byproduct type. Fig. 4 shows that there is an almost linear relationship between the difference data and feed flow rate. However, the difference data is increased from the top-down column; in other flow rate levels, the gap between the difference data is also increased from naphtha to gas oil.

TABLE II. THE DIFFERENCE BETWEEN THE PREDICTED VALUES OF THE LIV-BASED SOFT SENSOR AND THE ASPEN IQ VALUES AT DIFFERENT FEED FLOW RATES

Feed flow rate (bbl/day)	Product	$y_{AspenIQ}$ (°F)	$y_{predicted}$ (°F)	Δy (°F)
50,000	Naphtha	385.6978	384.8201	-0.8777
	Kerosene	502.2982	508.7777	6.4795
	Gas oil	622.9988	631.3546	8.3558
55,000	Naphtha	385.6993	385.1145	-0.5848
	Kerosene	502.2996	505.6467	3.3471
	Gas oil	623.0001	627.8317	4.8316
60,000	Naphtha	385.6999	385.7936	0.0937
	Kerosene	502.3000	502.5650	0.265
	Gas oil	623.0000	623.3477	0.3477
65,000	Naphtha	385.7009	386.4092	0.7083
	Kerosene	502.3001	499.4574	-2.8427
	Gas oil	623.0000	614.8229	-8.1771

*Differences are calculated as $\Delta y = y_{predicted} - y_{AspenIQ}$

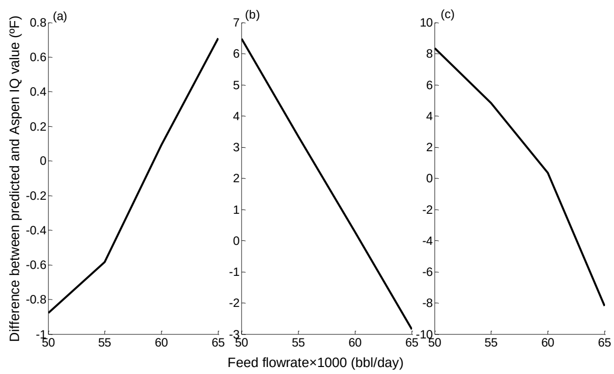

Fig. 4. The difference between the predicted and Aspen IQ values of (a) naphtha, (b) kerosene, and (c) gas oil against feed flow rate variations

In other words, Δy values for naphtha are lower than that for kerosene and gas oil at each flow rate level. The main reason behind this behavior is that the proposed soft sensor models have been developed based on steady-state data at a nominal flow rate of 60,000 bbl/day. Therefore, feed flow rate variations can directly affect the column performance and consequently reduce the prediction performance of the soft sensing system.

An accurate soft sensing system should be able to keep up with the desired product qualities while respecting the process under the variations in the flow rate of the crude oil feed. Accordingly, the lookup table method discussed previously in Section II.D is adopted to solve this issue. The Simulink model of the system is shown in Fig. 5, which includes the modified LIV-based soft sensor with LUT providing the input signal of the PIP control structure.

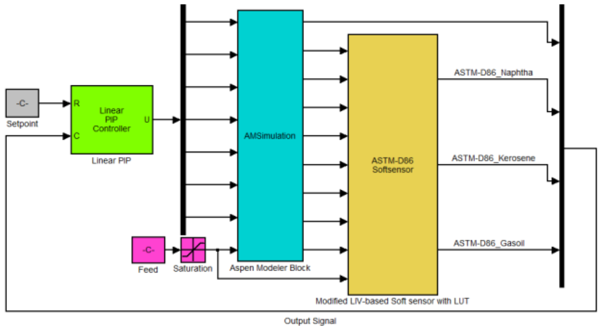

Fig. 5. Modified LIV-based soft sensor with LUT and PIP control structure in MATLAB-Simulink

Lookup table models are constructed individually for each byproduct, as shown in Fig. 6, which includes LUTs along with LIV-based soft sensors. For example, the input values of naphtha LUT are given by [50,000: 55,000: 60,000: 65,000], and the table data are difference values of [-0.8777: -0.5848: 0.0937: 0.7083] as given in Table II.

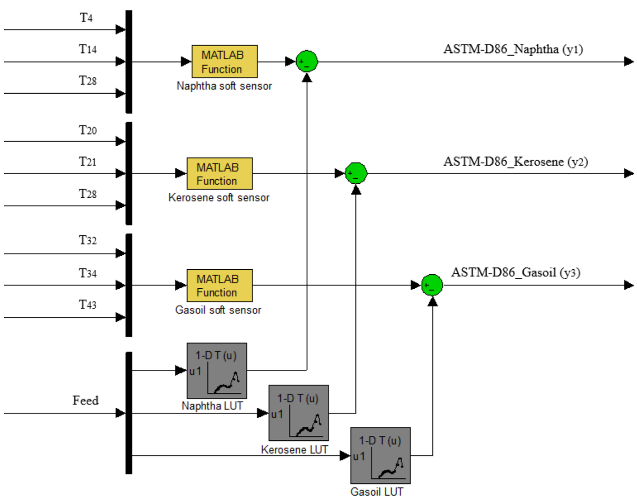

Fig. 6. Lookup table models in soft sensing structure

The kerosene and gas oil LUTs also contain a set of entries as shown in Table II. The linear interpolation method is used to determine the difference data for interpolated values. The modified structure shown in Fig. 6 includes three 1-D lookup tables for each byproduct where the outputs provide Δy values to the corresponding soft sensor for the prediction of product quality. The difference data are augmented to the prediction values of soft sensors to maintain the 95%ASTM-D86 index at the setpoint level. The ease of use in the proposed method can be justified by the fact that the lookup table is a standard library block in Simulink-MATLAB.

The modified Simulink model is run for the nominal case (e.g., a feed flow rate of 60,000 bbl/day) and the results are plotted in Fig. 7. The 95%ASTM-D86 of the various products satisfy the Aspen IQ values with no error. Therefore, LIV-based soft sensors provide good tracking as the error of their prediction is bounded for a bounded disturbance and the prediction converges to the actual quality value. The maximum prediction error for naphtha, kerosene, and gas oil soft sensors are 8.9336×10^{-5}, 2.6160×10^{-6}, and 1.3652×10^{-5}, respectively. The results of the modified soft sensor well match Aspen IQ values and hence the difference is practically zero after reaching the steady-state condition.

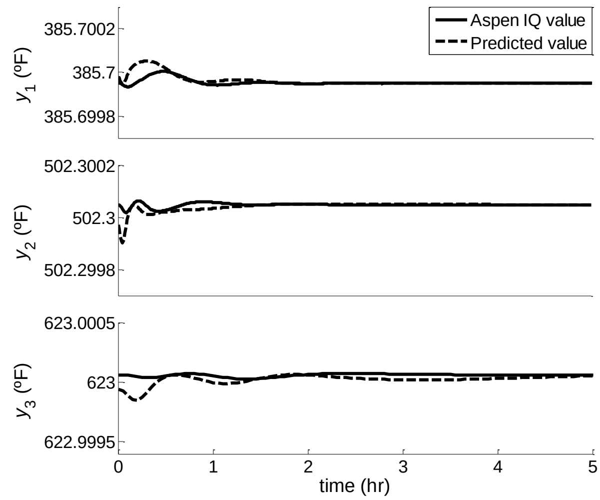

Fig. 7. The steady-state results of the modified LIV-based soft sensors in the PIP control structure at a feed flow rate of 60,000 bbl/day

The modified soft sensor is also tested to verify the prediction results through the simulation of two cases: (1) decreasing the feed flow rate from 60,000 bbl/day to 55,000 bbl/day, and (2) increasing the feed flow rate from 60,000 bbl/day to 65,000 bbl/day. The soft sensing models in both cases are the same. The Simulink models are run by applying a ramp signal of the feed flow rate to the system, whose prediction results are shown in Figs. 8 and 9.

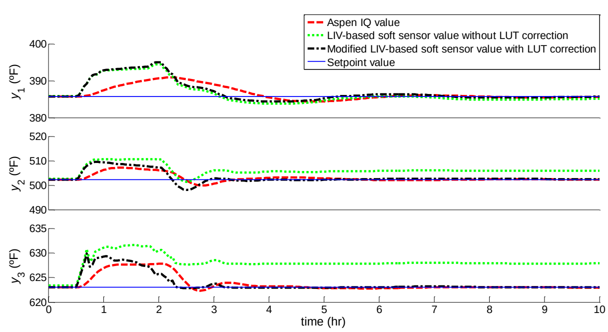

Fig. 8. The prediction results of the LIV-based soft sensor and Aspen IQ with/without LUT against a feed flow rate change from 60,000 bbl/day to 55000 bbl/day (case 1)

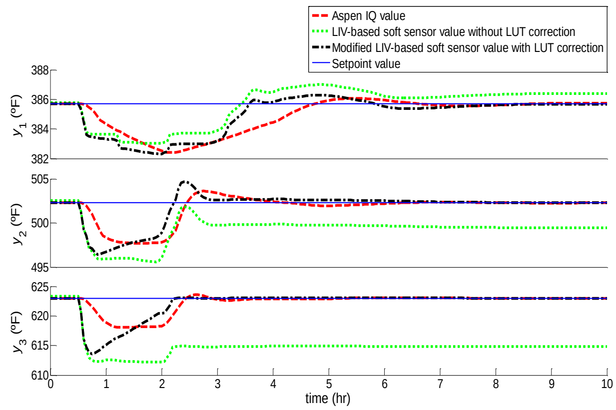

Fig. 9. The prediction results of the LIV-based soft sensor and Aspen IQ with/without LUT against a feed flow rate change from 60,000 bbl/day to 65000 bbl/day (case 2)

In Figs. 8 and 9, the results given by the modified soft sensor are compared to Aspen IQ values and also the results of LIV-based soft sensors without LUTs in each case. It can be seen that both increase and decrease trend were observed in the product qualities within 4 hours, indicating the system instability during the feed flow rate variations. In other words, flow rate level variations cause a transition period in sensing product qualities. However, the modified soft sensor provides good tracking in both cases. Figs. 8 and 9 indicate that the LIV-based soft sensors without LUTs do not provide a reliable estimate and fail to precisely match setpoint values even when the system reaches the steady-state condition. There is a significant difference between LIV-based soft sensors without LUT and Aspen IQ values, especially for kerosene and gas oil.

However, after applying the LUTs, the new difference values (Δy) are practically zero for naphtha, kerosene, and gas oil, which means that the predicted values are well-matched to Aspen IQ as well as setpoint values in both cases. Accordingly, the prediction results of modified LIV-based soft sensors are more reliable than LIV-based soft sensors. It is obvious that the modified model has the capability to operate efficiently within the feed flow rate range of 55,000-65,000 bbl/day.

The efficiency of the proposed method is its low computational complexity and processing time since the lookup tables are pre-calculated and stored in a MATLAB data file as a part of the simulation initialization phase or even stored in hardware in application platforms. The lookup table is an array that replaces runtime computation with a simpler array indexing operation. Moreover, the common method of reducing computational complexity in engineering applications is to use lookup tables [44]. The advantage of using the lookup table is that it is not time-consuming. As can be identified from Figs. 8 and 9, there is no delay in the prediction results of modified LIV-based soft sensors compared with Aspen IQ values.

IV. CONCLUSION

The modification of LIV-based soft sensor models for online monitoring of 95%ASTM-D86 index in the atmospheric distillation unit (ADU) has been addressed by incorporating the lookup table (LUT) method. The proposed LIV-based soft sensors were developed based on tray temperature measurement at a nominal feed flow rate of 60,000 bbl/day and applied to the Aspen dynamic model of the ADU using MATLAB-Simulink. In order to investigate the effect of feed flow rate changes, three simulation runs were carried out by varying the feed flow rate from 60,000 bbl/day to 50,000, 55,000, and 65,000 bbl/day. For each flow rate level, the prediction results of LIV-based soft sensors and Aspen inferential quality (IQ) were recorded when steady-state conditions were reached. The results show that difference values between LIV-based soft sensors and Aspen inferential quality (IQ) change either with the feed flow rate or with the byproduct type. Lookup tables were developed based on the feed flow rate and difference values and augmented with LIV-based soft sensor models in the PIP control structure. The results present improvement in the predictions of LIV-based soft sensors as well as acceptable control performance in feed flow rate variations. Therefore, the proposed update term using lookup tables is suitable for implementation in the advanced monitoring scheme due to simplicity and low computational time. It is important to emphasize that soft sensing models need not be retrained in feed flow rate variations using the lookup table method. Accordingly, this method can be easily combined with different soft sensing algorithms, including the effect of changes in influencing process variables.

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DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

A MATLAB-Simulink implementation file is available on request.

REFERENCES

[1] V. Kumar, A. Sharma, I. R. Chowdhury, S. Ganguly, and D. N. Saraf, "A crude distillation unit model suitable for online applications," *Fuel Processing Technology*, Vol. 73, No. 1, pp. 1-21, 2001.

[2] *ASTM D86: standard test method for distillation of petroleum products at atmospheric pressure*, 2010.

[3] T. Chatterjee and D. N. Saraf, "On-line estimation of product properties for crude distillation units," *Journal of Process Control*, vol. 14, No. 1, pp. 61–77, 2004.

[4] D. Wang, J. Liu, and R. Srinivasan, "Data-driven soft sensor approach for quality prediction in a refining process," *IEEE TRANSACTIONS ON INDUSTRIAL INFORMATICS*, vol. 6, No. 1, pp. 11-17, 2010.

[5] A. C. Serfidan, F. Uzman, and M. Turkay, "Optimal estimation of physical properties of the products of an atmospheric distillation column using support vector regression," *Computers and Chemical Engineering*, Vol. 134, p. 106711, 2020.

[6] C. M. Pappalardo and D. Guida, "System identification algorithm for computing the modal parameters of linear mechanical systems," *Machines* Vol. 6, No. 2, p. 12, 2018.

[7] B. Roset and H. Nijmeijer, "Observer-based model predictive control," *International Journal of Control*, Vol. 77, No. 17, pp. 1452-1462, 2006.

[8] P. Kadlec, B. Gabrys, and S. Strandt, "Data-driven soft sensors in the process industry," *Computers and Chemical Engineering*, Vol. 33, No. 4, pp. 795–814, 2009.

[9] H. Singh, A. K. Pani, and H. K. Mohanta, "Quality monitoring in petroleum refinery with regression neural network: Improving prediction accuracy with appropriate design of training set," *Measurement*, Vol. 134, pp. 698-709, 2019.

[10] H. A. Behrooz, "Robust set-point optimization of inferential control system of crude oil distillation units," *ISA Transactions*, Vol. In Press, Corrected Proof, 2019.

[11] F. Griesing-Scheiwe, Y. A. W. Shardt, G. Pérez-Zuñiga, and X. Yang, "Soft sensor design for variable time delay and variable sampling time," *Journal of Process Control*, Vol. 92, pp. 310-318, 2020.

[12] L. Fortuna, S. Graziani, A. Rizzo, and M. G. Xibilia, *Soft sensors for monitoring and control of industrial processes*. New York: Springer, 2007.

[13] H. J. Galicia, Q. P. He, and J. Wang, "A reduced order soft sensor approach and its application to a continuous digester," *Journal of Process Control*, Vol. 21, No. 4, pp. 489–500, 2011.

[14] J. Liu, "Developing a soft sensor based on sparse partial least squares with variable selection," *Journal of Process Control*, Vol. 24, No. 7, pp. 1046-1056, 2014.

[15] K. Zheng and K. Funatsu, "Partial constrained least squares (PCLS) and application in soft sensor," *Chemometrics and Intelligent Laboratory Systems*, Vol. 177, pp. 64-73, 2018.

[16] Z. Ge, "Mixture Bayesian Regularization of PCR Model and Soft Sensing Application," *IEEE Transactions on Industrial Electronics*, Vol. 62, No. 7, pp. 4336-4343, 2015.

[17] Z. Ge, C. Yang, and Z. Song, "Improved kernel PCA-based monitoring approach for nonlinear processes," *Chemical Engineering Science*, Vol. 64, No. 9, pp. 2245–2255, 2009.

[18] X. Shi and W. Xiong, "LWS based PCA subspace ensemble model for soft sensor development," *IFAC-PapersOnLine*, Vol. 51, No. 18, pp. 649-654, 2018.

[19] L. Fortuna, P. Giannone, S. Graziani, and M. G. Xibilia, "Virtual instruments based on stacked neural networks to improve product quality monitoring in a refinery," *IEEE Transactions on Instrumentation and Measurement*, Vol. 56, No. 1, pp. 95-101, 2007.

[20] J. C. B. Gonzaga, L. A. C. Meleiro, C. Kiang, and R. M. Filho, "ANN-based soft-sensor for real-time process monitoring and control of an industrial polymerization process," *Computers & Chemical Engineering*, Vol. 33, No. 1, pp. 43-49, 2009.

[21] K. Sun, S.-h. Huang, S.-S. Jang, and D. S.-H. Wong, "Development of soft sensor with neural network and nonlinear variable selection for crude distillation unit process," *Computer Aided Chemical Engineering*, Vol. 38, pp. 337-342, 2016.

[22] N. Bakhtadze, E. M. Maximov, and R. T. Valiakhmetov, "Fuzzy soft sensors for chemical and oil refining processes," *IFAC Proceedings Volumes*, Vol. 41, No. 2, pp. 46-50, 2008.

[23] E. AbdulJalee and K. Aparna, "Neuro-fuzzy Soft Sensor Estimator for Benzene Toluene Distillation Column," *Procedia Technology*, Vol. 25, pp. 92-99, 2016.

[24] T. Zhao, P. Li, and J. Cao, "Soft sensor modeling of chemical process based on self-organizing recurrent interval type-2 fuzzy neural network," *ISA Transactions*, Vol. 84, pp. 237-246, 2019.

[25] P. V. C. Souza, "Fuzzy neural networks and neuro-fuzzy networks: A review the main techniques and applications used in the literature," *Applied Soft Computing*, Vol. 92, p. 106275, 2020.

[26] P. Jain, I. Rahman, and B. D. Kulkarni, "Development of a soft sensor for a batch distillation column using support vector regression techniques," *Chemical Engineering Research and Design*, Vol. 85, No. 2, pp. 283–287, 2007.

[27] Y. Liu and J. Chen, "Integrated soft sensor using just-in-time support vector regression and probabilistic analysis for quality prediction of multi-grade processes," *Journal of Process Control*, Vol. 23, No. 6, pp. 793–804, 2013.

[28] S. Herceg, Ž. U. Andrijić, and N. Bolf, "Development of soft sensors for isomerization process based on support vector machine regression and dynamic polynomial models," *Chemical Engineering Research and Design*, Vol. 149, pp. 95-103, 2019.

[29] Q. Li, Q. Du, W. Ba, and C. Shao, "Multiple-input multiple-output soft sensors based on KPCA and MKLS-SVM for quality prediction in atmospheric distillation column," *International Journal of Innovative Computing, Information and Control*, Vol. 8, No. 12, pp. 8215-8230, 2012.

[30] Q. Jiang and X. Yan, "Weighted kernel principal component analysis based on probability density estimation and moving window and its application in nonlinear chemical process monitoring," *Chemometrics and Intelligent Laboratory Systems*, Vol. 127, pp. 121–131, 2013.

[31] X. Zhang, Q. Zhu, Z.-Y. Jiang, Y. He, and Y. Xu, "A novel ensemble model using PLSR integrated with multiple activation functions based ELM: Applications to soft sensor development," *Chemometrics and Intelligent Laboratory Systems*, Vol. 183, pp. 147-157, 2018.

[32] H. Liu, C. Yang, M. Huang, and C. Yoo, "Soft sensor modeling of industrial process data using kernel latent variables-based relevance vector machine," *Applied Soft Computing*, Vol. 90, p. 106149, 2020.

[33] P. C. Young, "The data-based mechanistic approach to the modelling, forecasting and control of environmental

systems," *Annual Reviews in Control*, Vol. 30, No. 2, pp. 169–182, 2006.

[34] H. Gharehbaghi and J. Sadeghi, "A novel approach for prediction of industrial catalyst deactivation using soft sensor modeling," *Catalysts*, Vol. 6, No. 7, pp. 93-109, 2016.

[35] B. Bidar, J. Sadeghi, F. Shahraki, and M. M. Khalilipour, "Data-driven soft sensor approach for online quality prediction using state dependent parameter models," *Chemometrics and Intelligent Laboratory Systems*, Vol. 162, pp. 130–141, 2017.

[36] P. C. Young, *Recursive estimation and time-series analysis*, Second ed. New York: Springer, 2011.

[37] B. Bidar, M. M. Khalilipour, F. Shahraki, and J. Sadeghi, "A data-driven soft-sensor for monitoring ASTM-D86 of CDU side products using local instrumental variable (LIV) technique," *Journal of the Taiwan Institute of Chemical Engineers*, Vol. 84, pp. 49-59, 2018.

[38] M. M. Khalilipour, J. Sadeghi, F. Shahraki, and K. Razzaghi, "Nonsquare multivariable non-minimal statespace-proportional integral plus (NMSS-PIP) controlfor atmospheric crude oil distillation column," *Chemical Engineering Research and Design*, Vol. 113, pp. 140-150, 2016.

[39] M. M. Khalilipour, F. Shahraki, J. Sadeghi, and k. Razzaghi, "Control Structure Design and Dynamic Modeling for Atmospheric Distillation Column: Effect of Increase Capacity," *International Journal of Industrial Electronics, Control and Optimization*, Vol. 1, No. 2, pp. 103-113, 2018.

[40] J. Sadeghi, "Modelling and control of non-linear systems using State-Dependent Parameter (SDP) models and Proportional-Integral-Plus (PIP) control method," Doctor of Philosophy, Centre for Research on Environmental System and Statistics, Lancaster University, United Kingdom, 2006.

[41] B. Bidar, F. Shahraki, J. Sadeghi, and M. M. Khalilipour, "Soft Sensor Modeling Based on Multi-State-Dependent Parameter Models and Application for Quality Monitoring in Industrial Sulfur Recovery Process," *IEEE Sensors Journal*, Vol. 18, No. 11, 2018.

[42] A. B. Hocking, M. A. Aiello, J. C. Knight, S. Shiraishi, M. Yamaura, and N. Arechiga, "Proving Properties of Simulink Models that Include Discrete Valued Functions," *SAE World Congress and Exhibition*, 2016.

[43] J. J. Macias, P. Angelov, and X. Zhou, "A method for predicting quality of the crude oil distillation," in *International Symposium on Evolving Fuzzy Systems*, Ambleside, UK, IEEE, pp. 214–220, 2006.

[44] W. Zhang, X. Chen, K. Cui, T. Xie, and N. Yuan, "DOA Estimation for Coprime Linear Array Based on MI-ESPRIT and Lookup Table," *Sensors*, Vol. 18, No. 9, pp. 1-11, 2018.

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