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A data-driven soft-sensor for monitoring ASTM-D86 of CDU side products using local instrumental variable (LIV) technique

Bahareh Bidar, Mir Mohammad Khalilipour, Farhad Shahraki, Jafar Sadeghi*

Center for Process Integration and Control (CPIC), Department of Chemical Engineering, University of Sistan and Baluchestan, Zahedan 98164, Iran

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ABSTRACT

Atmospheric crude distillation unit is the main unit operation in petroleum refining industries. The main difficulties in quality control of column are the availability of quality measurements. The design of product quality estimator will help improve quality monitoring and control performance in oil refinery industry by accurately predicting the side products properties, simultaneously. The objective of this paper is to design and implement state dependent parameter (SDP) based soft sensors using local instrumental variables (LIV) technique for an industrial atmospheric crude distillation unit. On the basis of tray temperature measurements of the column, soft sensor models for estimation of 95%ASTM-D86 of product streams have been developed. Three soft sensors are separately designed in an offline manner for each product quality with steady-state data of the column. The performance of proposed soft sensors is evaluated through testing data and also by online implementation in simulated control system. The prediction results, after tuning controller parameters, show excellent agreement with quality predictions from the rigorous model. Based on developed soft sensors, it is possible to estimate product properties in a continuous manner with minimum delay compared to laboratory ASTM analysis and apply perfect control as well as compliance with product quality specifications.

1. Introduction

Crude distillation unit (CDU) is one of the most important units in the refineries, which separates the preheated crude oil into respective product fractions like naphtha, kerosene and gas oil, *etc.* The stringent quality control requirement in a highly competitive market, makes it essential that all the necessary product properties such as Reid vapor pressure (RVP) for volatile products, flashpoint for light distillates, pour point for heavier fractions, *etc.* are monitored online and kept under control. These product properties are generally not available online and usually measured in an offline manner with intervals of 8–24 h, which may lead to improper control performance. Therefore, the product properties are conventionally controlled using the range of boiling points. There are three types of boiling point analysis, namely ASTM[1]-D86 (Engler), ASTM-D158 (Saybolt) and true boiling point (TBP). The ASTM-D86, among the methods, is the standard test method for distillation of petroleum products at atmospheric pressure [1]. However, changing the product properties within the same boiling interval by external factors (*e.g.* feed characteristics) can result in non-uniformity of product quality. Thus, an inferential sensing-based control strategy is tenable, which needs less manual effort and maintenance cost [2,3].

The soft sensor is a key technology to infer the important quality variables, which are difficult-to-measure online. However, the soft sensor is accurate enough; the predicted qualities can then be used as a feedback for automatic control and optimization purposes. However, there are still many problems with the existing estimators that require the development of new techniques. Nowadays, data-driven soft sensors such as partial least squares (PLS) [4,5], artificial neural networks (ANN) [6,7], support vector regression (SVR) [8,9] have gained much popularity in the industrial processes.

In relation to the use of data-driven soft sensors for estimation of product properties in CDU, many studies have been done in recent decades. To handle the strongly correlated process variables in CDU, the principal component analysis (PCA) and PLS approaches have been used. Wang et al. [10] developed a PLS-based soft sensor and applied to an industrial CDU. The ASTM 90% distillation temperature (D90) of product streams and 14 process variables are considered as the quality index and predictors, respectively. Nevertheless, the PCA and PLS can only extract linear

* Corresponding author.
E-mail addresses: b.bidar@pgs.usb.ac.ir (B. Bidar), a.khalilipour@eng.usb.ac.ir (M.M. Khalilipour), fshahraki@eng.usb.ac.ir (F. Shahraki), sadeghi@eng.usb.ac.ir (J. Sadeghi).

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Nomenclature

$\mathbf{A}_{i,t}$	the ith locally constant SDPs
$\hat{\mathbf{A}}_k$	the state vector in polynomial Spline at the kth sample
$\mathbf{A}_t$	state vector
$a_{i,t}$	the ith SDP in the regression model
e_t	white noise
$\mathbf{I}$	identity matrix
K	kernel function
L_c	concentrated likelihood function
N	number of data points in time series
ns_i	number of state that the ith SDP is a function of them
$\mathbf{P}_k$	covariance matrix of SDP estimation
p	number of all parameters of the model in $\mathbf{A}_t$
p_i	number of parameters in $\mathbf{A}_{i,t}$
q	local polynomial order
$q_{j,i}$	local polynomial order of the ith SDP with respect to $x_{j,i,\,t}$
R_k	variance of prediction noise normalized by σ^2
$\mathbf{S}_{i,t}$	Spline function of ith SDP
t	sample time
$\mathbf{U}_k$	LIV matrix at the kth sample
$\mathbf{U}_{m,k}$	LIV correspondent to the mth regressor at the kth sample
$\mathbf{W}$	local weighting matrix
$x_{j,i,\,t}$	the jth element of ith vector of states
$\mathbf{y}$	the time series vector
y_i	the ith output in $\mathbf{y}$
y_t	output
$\mathbf{Z}_k$	regressor defined for polynomial Spline
$\mathbf{z}$	vector of regressors
$z_{i,t}$	regressor correspondent to the ith SDP
$\mathbf{0}$	zeros vector
Δ	distance between two knots
ε_k	prediction error
$\lambda_{j,i}$	bandwidth correspondent to $x_{j,i,\,t}$
σ^2	variance of error

relationships and cannot handle the dynamic of nonlinear processes. Therefore, Shang et al. [11,12] suggested dynamic PLS-based (DPLS) soft sensor modeling approach with temporal smoothness. They compared different approaches to improve DPLS soft sensors through a CDU. The proposed soft sensors were established to predict the ASTM temperatures by using process variables such as temperatures, pressures, flows, *etc.* Moreover, non-linear extensions of PCA models such as kernel PCA (KPCA) was developed by Li et al. [13] for estimation of dry point and flashpoint of aviation kerosene in the atmospheric distillation column. The results showed that the performance of the model was in good agreement with lab measurements. However it should be noted that the KPCA approach suffers from the difficulty in choosing nonlinear parameters.

The complexity and non-linearity of CDU prohibits the practical use of linear methods and that motivates researchers to consider non-linear soft sensing approaches, such ANN. Dam and Saraf [14] proposed an ANN-based soft sensor for prediction of ASTM temperatures, specific gravities and Flash Points of CDU products. Liu et al. [15] developed and deployed a neural network-based data-driven soft sensor for estimation of ASTM 90% distillation temperature (D90). Rogina et al. [16] also developed neural network-based models such as LNN, MLP and RBF for light naphtha vapor pressure (RVP) estimation. However, ANN demonstrates several drawbacks such as getting stuck in local minima, weak interpretation capability and has difficulty in the optimization of deep structures. To overcome the mentioned issues, deep learning technique was developed and applied to an industrial CDU by Shang et al. [17] in order to build deep NN-based soft sensors. The predictions made by the model match real values better than traditional data-driven modeling approaches such as the single hidden layer neural network, SVM, PLS and NNPLS while the model had a relatively higher training time.

There are many studies that have been applied modified linear and non-linear approaches to CDU soft sensors, *e.g.* evolving fuzzy Takagi–Sugeno models [18,19], modified nonlinear generalized ridge regression (MNGRR) [20], auto-regressive moving average with exogenous inputs (ARMAX), nonlinear auto-regressive model with exogenous inputs (NARX) and Hammerstein-Wiener (HW) models [21] and output error (OE) and neuro-fuzzy models [22].

The literatures disclose the massive use of different modeling methods for estimating quality properties of CDU products. The soft sensor modeling methods for CDU mainly focus on using pressure, temperature, flow rate, *etc.* and the study on using multiple temperature measurements have not been taken into account. The temperature as an accessible and measurable variable is widely used to estimate product qualities in distillation columns [23–25]. This motivates the design of temperature data-driven soft sensors to infer qualities based on the process model and available temperature measurements [26].

Using varying parameter models such as state dependent parameter (SDP) models as a novel data-driven approach to train soft sensor models introduced by Gharehbaghi and Sadeghi [27] and Bidar et al. [28]. The modeling approach incorporates process information into the model while at the same time provides a good explanation of data. In this way, SDP-based soft sensors have shown successful applications for identification and estimation of industrial processes, where SDP method outperforms other traditional data-driven methods like PCR, PLS, ANN, SVR and so on, due to its remarkable ability to describe the behavior of non-linear systems.

In SDP estimations, a state must have two special properties to be called an instrumental variable (IV). Each IV should be correlated with correspondent regressors as much as possible while it should be correlated with the estimated error and other regressors as little as possible. Otherwise, the estimation of each SDP affects the estimation of other SDPs and because they are functions of different state variables, this will cause distortion in the final estimate of SDP. In this case, there is no need to sort after finding the IVs and consequently there is no need for a back-fitting algorithm in order to eliminate the effects of other states and regressors on the estimation of the desired parameter.

With regard to SDP modeling method, this paper presents the design and implementation of a novel data-driven soft sensor using the technique of instrumental variables (IV) to introduce a new method of SDP estimation termed local instrumental variable (LIV). An extensive evaluation of the proposed method to soft sensor design is conducted using a simulated industrial crude distillation unit, and demonstrate its good performance that is comparable to the available Aspen soft sensors. The proposed method is used to predict 95%ASTM-D86 of side products in atmospheric crude distillation unit. The soft sensor model is applied to the Aspen dynamic model of the column using MATLAB-Simulink while the proportional integral plus (PIP) control structure is implemented. The Aspen soft sensors represent the values of ASTM-D86 of side products, which are considered as the reference values for validation of proposed soft sensor. The prediction results of the SDP-based soft sensors are compared with Aspen soft sensors and further validated the soft sensing model when applying it online over simulated unit.