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Development of Soft Sensors for Crude Distillation Unit Control

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Abstract: Soft sensors for distillation end point (D95) on-line estimation in crude distillation unit (CDU) are developed. Experimental data are acquired from the refinery distributed control system (DCS) and include on-line available continuously measured variables and laboratory assays. Soft sensors are developed using different linear and nonlinear identification methods. Additional laboratory data for model identification are generated by Multivariate Adaptive Regression Splines (MARSplines). The models are evaluated based on Route Mean Square (RMS), Absolute Error (AE), FIT and Final Prediction Error (FPE) criteria. The best results are achieved with Box Jenkins (BJ), Output Error (OE) and Hammerstein–Wiener (HW) model. Based on developed soft sensors it is possible to estimate fuel properties in continuous manner and apply inferential control. By real plant application of developed soft sensors considerable savings could be expected, as well as compliance with strict law regulations for product quality specifications.

1. INTRODUCTION

Strict product quality requirements and pollutant emission norms impose a need for the effective measurement and process control in industry plant therefore, large number of process variables need to be monitored using appropriate measuring devices. As the main problems occurring is a big price of analyzers and unreliability of on-line instrumentations.

Soft sensors are focused on assessing the system state variables and products quality, thus replacing the physical senses and laboratory analysis. The application of soft sensors for estimating non available or hard-to-measure process variables is extremely interesting in the process industry, where there are usually a large number of values measured continuously and quickly, and these may serve as input signals for the soft sensor (Bolf et al., 2008). They can work in parallel with real sensors, analyzers, measuring devices, allowing fault detection schemes devoted to the sensor's status analysis to be implemented (Kadlec et al., 2009; Buceti et al., 2002). Furthermore, they can take the place of sensors which are down for maintenance, in order to keep control loops working properly and to guarantee product specification without undertaking conservative production policies, which are usually very expensive (Fortuna et al., 2007).

In the last decade, soft sensor applications for the CDU product properties have been studied extensively (Rogina et al. 2011; Napoli et al. 2010; Yan 2008; Badhe et al. 2007; Schladt et al. 2007; Dam et al. 2006; Chatterjee et al. 2004; Liau et al. 2004; etc.).

In the most industrial applications the soft sensor design procedure based on data-driven approaches follows the sequence of the stages shown on Fig. 1.

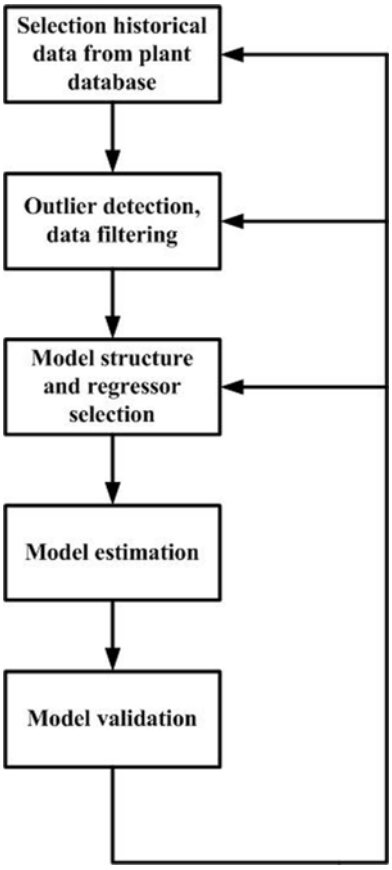

Fig. 1 Block scheme of the soft sensor identification procedure

1.1 Linear model identification

Basic linear model of dynamic systems with additive disturbance (Ljung, 1999) is given by:

$$y(k) = G(q)u(k) + H(q)\xi(q) \tag{1}$$

where: q is time-shift operator; y is output signal and u is input signal,

$$G(q) = \sum_{k=1}^{\infty} q(k)q^{-k} \tag{2}$$

is system transfer operator,

$$H(q) = I + \sum_{k=1}^{\infty} h(k)q^{-k} \tag{3}$$

is disturbance transfer operator and ξ is noise signal.

Somewhat changed variant of Final Impulse Response (FIR) model is OE model:

$$y(k) = \frac{B(q)}{F(q)}u(k) + \xi(k) \tag{4}$$

where:

$$B(q) = I + B_1 q^{-1} + B_2 q^{-2} + ... + \mathrm{B}_{nb} q^{-nb\text{-}nk+1} \tag{5}$$

is polynomial matrix over q^{-1},

B_i is the matrix of dimensions $n(\hat{y}) \times n(\hat{y})$, nb is the number of past input delays and nk is time delay,

$$F(q) = I + F_1 q^{-1} + F_2 q^{-2} + ... + F_{nf} q^{-nf} \tag{6}$$

F_i is the matrix of dimensions $n(\hat{y}) \times n(\hat{y})$, nf is maximal number of past model prediction delays.

In order to obtain a BJ model that can describe the disturbance properties, OE model can be expanded with a parametric disturbance matrix:

$$y(k) = \frac{B(q)}{F(q)}u(k) + \frac{C(q)}{D(q)}\xi(k) \tag{7}$$

where:

$$C(q) = I + C_1 q^{-1} + C_2 q^{-2} + ... + C_{nc} q^{-nc} \tag{8}$$

C_i is matrix dimensions $n(\mathrm{y}) \times n(\xi)$, nc is the number of past delays of model prediction errors,

$$D(q) = I + D_1 q^{-1} + D_2 q^{-2} + ... + D_{nd} q^{-nd} \tag{9}$$

is polynomial matrix over q^{-1};

D_i is matrix dimensions $n(\hat{y}) \times n(e_s)$, nd is maximal number of simulated model prediction errors.

1.2 Nonlinear model identification

While linear model structure is fully defined by chosen regressors, nonlinear model structure additionally depends on nonlinear function characteristic.

It is quite common situation that while the dynamics itself can be well described by a linear system, there are static nonlinearities at the input and/or at the output. A model with a static nonlinearity at the input is called Hammerstein model, and model with the output nonlinearity is Wiener model. (Ljung, 1999).

Block diagram on Fig. 2 represents the structure of a Hammerstein-Wiener model:

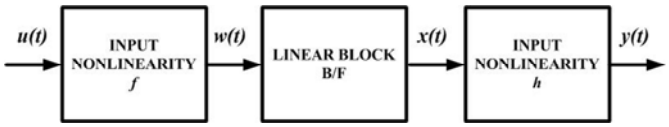

Fig. 2 Structure of Hammerstein-Wiener model

$w(t) = f(u(t))$, is a nonlinear function transforming input data $u(t)$. $w(t)$ has the same dimension as $u(t)$.

$$u(t) = \frac{B}{F}w(t) \tag{10}$$

is a linear transfer function. $x(t)$ has the same dimension as $y(t)$, where B and F are similar to polynomials in the linear OE model.

For ny outputs and nu inputs, the linear block is a transfer function matrix containing entries:

$$y(k) = \frac{B_{j,i}(q)}{F_{j,i}(q)} \tag{11}$$

where $j = 1, 2, ..., ny$ and $i = 1, 2, ..., nu$.

$y(t) = h(x(t))$ is a nonlinear function that maps the output of the linear block to the system output. $w(t)$ i $x(t)$ are internal variables that define the input and output of the linear block, respectively.

Nonlinearity of the HW model can be described by neural network. In our research the sigmoid network is given by logsig function:

$$\kappa(s) = \frac{1}{1+e^{-s}} \tag{12}$$

The network is described with:

$$g(k) = \sum_{k=1}^{n} \alpha_k \kappa(\beta_k (x - y_k)) \tag{13}$$

where α is scalar, β is a raw vector such that $\beta(x - \gamma)$ is a scalar, and n is the number of nonlinear units.

2. PROCESS DESCRIPTION

Since the CDU is the first unit in the sequence of refinery processing, it is essential that the quality of fractionation products (unstabilized naphtha, heavy naphtha, kerosene, light gas oil, heavy gas oil and atmospheric residue), be monitored and controlled. This requires that many properties should be measured online so that the unit can be effectively controlled through a feedback mechanism (Lin et al., 2007). Heavy naphtha, petroleum, and light gas oil fractions are used for blending of diesel fuel. These are being drained away as side fractions of distillation column. Very important product property product to measure continuously on-line is distillation end point (D95) (Cerić, 2006). Section of the column with diesel fuel product and variables used for estimation is given in Fig. 3.

Based on the PLS and PCA analysis and process expert experiences, the following variables have been proposed as potential input variables to infer distillation end point:

- column top temperature (T_{TOP}), TR-6104;
- kerosene temperature – 23rd tray (T_K), TR-6197;
- light gas oil temperature – 19th tray (T_{LGO}), TR-6198;
- heavy gas oil temperature–14th tray (T_{HGO}),TR-6199;
- pumparound temperature (T_{PA}), TR-6103 and
- pumparound flow rate (F_{PA}), FI-6130.

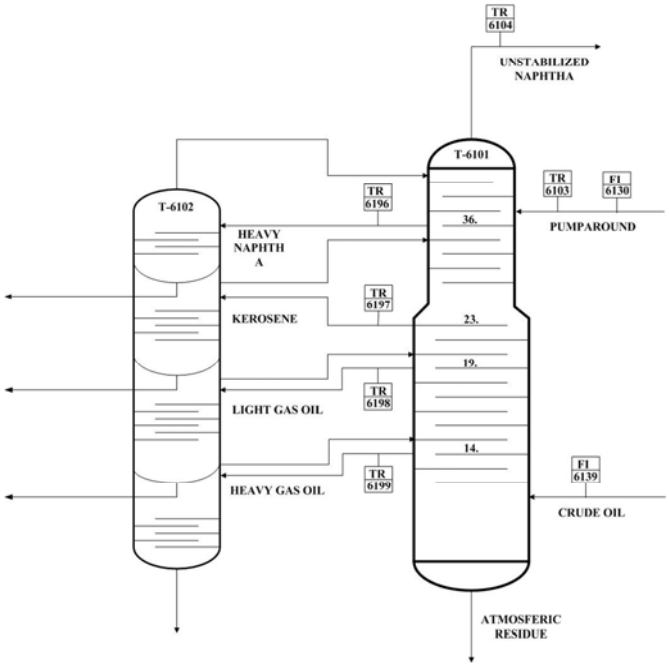

Fig. 3 Crude distillation column section with diesel fuel products

3. SOFT SENSOR MODEL DEVELOPMENT

Data from the real plant have been obtained in the period from January 2009 to October 2009 in a way to involve different process regime according to the different season, and therefore different quality requirements for diesel fuel. The laboratory analyses of the product quality (D95) are carried out four times a day.

Data preprocessing included detecting and outlier removal, generating additional data by Multivariate Adaptive Regression Splines (MARSplines) algorithm (Salvatore et. al., 2009), detrending and filtering data have been performed. According to Shannon's sampling theorem chosen sampling time was 5 min.

MARSplines algorithm operates as multiple piecewise linear regression, where each breakpoint estimated from the data defines the "region of application" for a particular (very simple) linear equation. (Hastie et al., 2001). The MARSplines algorithm builds models from two-sided truncated functions (basis functions) of the predictors *(x)* with the following form:

$$(x-t)_+ = \begin{cases} x-t & x > t \\ o & else \end{cases} \tag{14}$$

The MARSplines for a dependent variable y, and M terms, can be summarized as:

$$H_{km}(x_{v(k,m)}) = \prod_{k=1}^{K} h_{km} \tag{15}$$

where x is the predictor in the *k'th* of the *m'th* product. For order of interactions $K=1$ the model is additive, and for $K=2$ the model pairwise interactive.

The model structure selection step is strongly influenced by the purpose of the soft sensor design. In that important step model structure was chosen, loss function was defined and optimal model structure parameters were determined by some optimization methods (Gauss-Newton, Adaptive Gauss Newton, Levenberg Marquardt, Gradient Search, Partial Least Squares).

Models were evaluated based on RMS, AE, FIT and FPE values (Matlab, 2009) defined by:

$$RMS = \sqrt{\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{n}} \tag{16}$$

$$AE = \left| \hat{y}_i - y_i \right| \tag{17}$$

$$FIT = 1 - \frac{\sqrt{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}}{\sqrt{\sum_{i=1}^{n} (y_i - \bar{y}_i)^2}} \cdot 100 \tag{18}$$

where y is the measured output, $\hat{y}$ is the simulated or predicted model output, and $\bar{y}$ is the mean of y. 100% corresponds to a perfect fit, and 0% indicates that the fit is no better than guessing the output to be a constant ($\hat{y} = \bar{y}$).

Akaike's Final Prediction Error (FPE) criterion provides a measure of model quality by simulating the situation where the model is tested on estimation set and validation set. According to Akaike's theory, the most accurate model has the smallest FPE. (Ljung, 1999; Matlab, 2009).

Akaike's Final Prediction Error (FPE) is defined by the following equation:

$$FPE = V\left(\frac{1 + 2d}{N}\right) \tag{19}$$

where V is the loss function, d is the number of estimated parameters, and N is the number of values in the estimation data set.

The loss function V is defined by the following equation:

$$V = det\left(\frac{1}{N} \sum_{1}^{N} \varepsilon(t, \Theta_N)(\varepsilon(t, \Theta_N))^T\right) \tag{20}$$

where θ_N represents the estimated parameters and ε is output model error.

4. RESULTS AND DISCUSSION

Laboratory data were equidistantly collected by regular laboratory assays which are conducted four times a day. For this reason MARSpline method has been done. Data collected from DCS were synchronized regarding particular time delays and sampling system location. The extreme values were eliminated from the data using the three-sigma method (Licitra et al., 2000).

Based on PLS and PCA analysis the following variables have been chosen as the model inputs: T_{TOP} , T_K , $T_{LG\,O}$, T_{HGO} , T_{PA} and F_{PA} . Variables with the greatest influence on D95 are the temperature of light gas oil, heavy gas oil, kerosene temperature and the pumparound temperature.

Real plant data were divided into two sets: 70% data for modeling (estimation) and 30% independent data for validation purpose. Over than a ten types of models have been developed. The most of them are linear: Finite Impulse Response models (FIR), AutoRegressive model with eXogenous inputs (ARX), AutoRegressive Moving Average with eXogenous inputs (ARMAX), BJ, OE, State Space models etc. The rest of them are nonlinear: NFIR, NARX and HW models with peacewise linear, sigmoid, wavenet and other types of networks.

From variety of developed models the best achieved results are shown. Their optimal model structure parameters are determined by Least Square method.

Optimal structure of the BJ model comprises 2 past delays of each 6 inputs, 2 past delays of model prediction errors, 2 past delays of simulated model prediction errors, 1 past model prediction delays and time delay of 5 minutes, as shown in Table 1. The model shows very high FIT coefficient and very low RMS, FPE and absolute deviation from experimental data. Also, the average absolute deviation of the laboratory-determined distillation end point temperature is around 2°C which is approximately in the range of measurement uncertainty. From Fig. 4 excellent correspondence between measured and the one-step ahead model prediction data can be seen.

Optimal structure of the OE model consists of 2 past delays of each 6 inputs, 6 past model prediction delays and the time delay of 5 minutes, as shown in Table 1. OE model structure does not include past outputs for estimating the model outputs. Model shows high FIT coefficient and low RMS, FPE and absolute deviation from experimental data. Dynamic responses on Fig. 5 exhibit very good correspondence between measured and the one-step ahead model prediction data.

Hammerstein-Wiener model consists of linear dynamic block and two nonlinear static blocks, i.e. input and output static nonlinearities. Parameters of nonlinear HW model are *nb*, *nf*, *nk* and the number of nonlinear blocks (*n*).

Linear block of the model is a matrix of the transfer functions containing 1 past input delay, 3 past model prediction delays and the time delay of 5 minutes. HW model also does not use past real-process outputs for estimating the model outputs. The structure of the model's input and output nonlinear parts comprises sigmoid network, as shown in Table 1.

Static nonlinearities of all 6 inputs is presented by sigmoid network with 10 units. HW model shows satisfactory FIT coefficient and acceptable RMS, FPE and absolute deviation from experimental data. Dynamic response shown on Fig. 6 shows satisfactory correspondence between measured and the one-step ahead model prediction data.

Table 1. Model description

Parameter	BJ	OE	HW
na	-	-	-
nb	2	2	2
nk/min	5	5	5
nc	2	-	-
nd	2	-	-
nf	1	6	3
n	-	-	10
V	1,59	6,06	4,85
FPE	1,59	6,06	4,97
FIT / %	93,51	83,50	81,07
RMS/°C	1,48	2,33	2,74
AE/°C	0,89	1,81	2,15

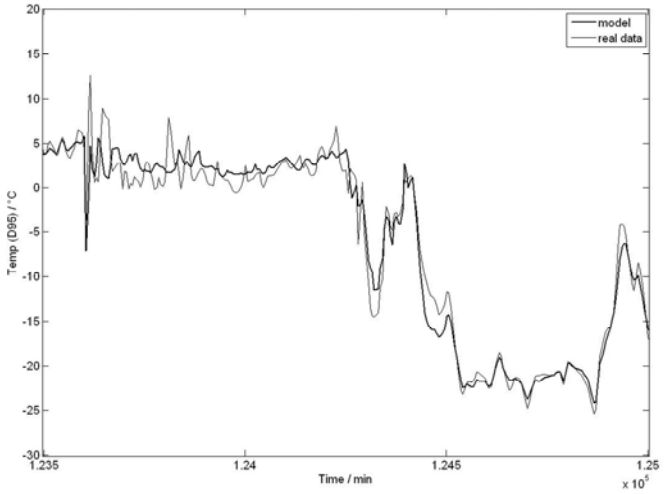

Fig. 4 Comparison between measured and one-step-ahead predicted outputs on validation data for BJ model

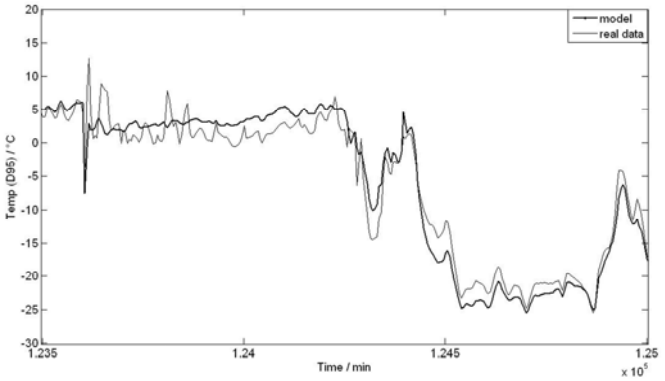

Fig. 5 Comparison between measured and one-step-ahead predicted outputs on validation data for OE model

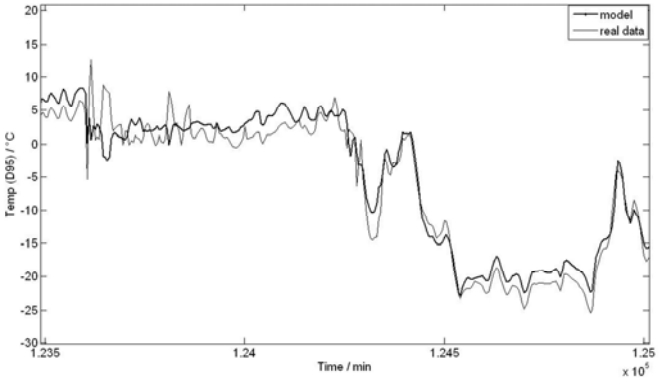

Fig. 6 Comparison between measured and one-step-ahead predicted outputs on validation data for HW model

5. CONCLUSION

Based on continuous temperature and flow measurements of adequate process streams, the dynamic soft sensor models for the estimation of distillation end point were developed. Data were collected from the DCS and laboratory assays. Different dynamic linear and nonlinear models were developed using several identification methods.

FIT, FPE and RMS values were accepted as satisfactory by the plant experts. The average absolute deviations of all model results lie in the acceptable tolerance limits for the on-line implementation. BJ model shows the best performance and can be employed as the soft sensor within the advance process control or for diagnostic purposes. The OE and HW model show somewhat inferior performances but can be still successfully used for prediction of the distillation end point of the crude distillation unit and for advance process control, as well.

6. ACKNOWLEDGMENTS

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