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ISSN 0350-350X
GOMABN 50, 3, 187 -214
Izvorni znanstveni rad / Original scientific paper
UDK 665.622.048.3 : 66-503.56 : 66.012.122

SOFT SENSORS APPLICATION FOR CRUDE DISTILLATION UNIT PRODUCT QUALITY ESTIMATION

Abstract
Fractionation product properties of the crude distillation unit (CDU) need to be monitored and controlled through feedback mechanism. Due to the inability of on-line measurement, soft sensors for product quality estimation are developed. Soft sensors for kerosene 95% distillation point are developed using linear and nonlinear identification methods. Experimental data are acquired from the refinery distributed control system (DCS) and include on-line available continuously measured variables and laboratory assays. In present work development of AutoRegressive Moving Average with eXogenous inputs (ARMAX), Nonlinear AutoRegressive model with eXogenous inputs (NARX) and Hammerstein-Wiener (HW) model are presented. To overcome the problem of selecting the best model parameters by trial and error procedure, genetic algorithms were used for determining the best model parameters. Based on developed soft sensors it is possible to estimate fuel properties continuously by embedding model in DCS on site as well as applying the methods of inferential control.

Introduction

Process industry is nowadays faced with the ever-growing requirements for product quality enhancement. Hence, there is a need for the continuous monitoring of large number of process variables and properties. In various process plants there are variables that are difficult to measure online (viscosity, density, boiling point, color, etc.) or it is only possible to get infrequent laboratory measurements. Those properties are often of great importance for process industry because they may have high influence on the final product quality. Laboratory analyses can be time consuming and influenced by human factor. Solution of this problem can be found in application of the soft sensors – estimators that estimate infrequent-measured variables on the basis of easy measured variables, such as temperature, pressures, flows, etc. (Dam and Saraf, 2006). As DCS is installed in most chemical plants, many process variables can be measured and stored in real time (Ma et al., 2009).

That historical database enables engineers to build soft sensors with the goal to produce real-time reliable estimates of unmeasured data.

Typical soft sensor design procedure follows the next steps (Fortuna et al., 2007):

1. Selection of historical data from plant database
2. Outlier detection, data filtering
3. Model structure and regressor selection
4. Model estimation
5. Model validation

Step 3, i.e. selection of the proper model structure is crucial for the soft sensor performance (Kadlec et al., 2009). Since that processes of interest have mostly dynamic behavior, selection of proper regressor order and delay is important too.

Soft sensor model development

Linear and nonlinear autoregressive types of dynamic models are often used for developing soft sensor model. The autoregressive models attempt to predict an output $y(t)$ of a system based on the previous outputs $y(t-1)$,y(t-2),... and current and previous inputs u(t), $u(t-1)$, u(t-2),.... Set of parameters need to be adjusted in order to obtain the best performance of each models. To overcome the problem of selecting the best model order and delays of each input and other configurable parameters, in an ad hoc manner, genetic algorithms are used for determining the best set of parameters. Applied procedure is shown on the example of ARMAX model, nonlinear ARX model and Hammerstein-Wiener model.

Model identification

One of the most used linear dynamic model which enables modelling of additive disturbance is ARMAX model:

$$\mathbf{A}(q)y(k) = \mathbf{B}(q)u(k) + \mathbf{C}(q)e(k)$$

where: $y(k)$ is output at time k and $u(k)$ is input at time k. q is time-shift operator.
e is the white-noise disturbance value.

$$\mathbf{A}(q) = 1 + \mathbf{A}_1 q^{-1} + \mathbf{A}_2 q^{-2} + \ldots + \mathbf{A}_{\mathrm{na}} q^{-\mathrm{na}}$$

$$\mathbf{B}(q) = \mathbf{B}_1 q^{-nk} + \ldots + \mathbf{B}_{nb} q^{-nb\text{-}nk+1}$$

$$\mathbf{C}(q) = 1 + \mathbf{C}_1 q^{-1} + \mathbf{C}_2 q^{-2} + \ldots + \mathbf{C}_{\mathrm{nc}} q^{-\mathrm{nc}}$$

Parameters *na*, *nb* and *nk* are defined in Table 1. Parameters A, B and C are determined by nonlinear least squares method. Block diagram shown on Fig. 1 represents the ARMAX model structure. Block diagram shown on Fig. 2 represents the structure of a NARX model.

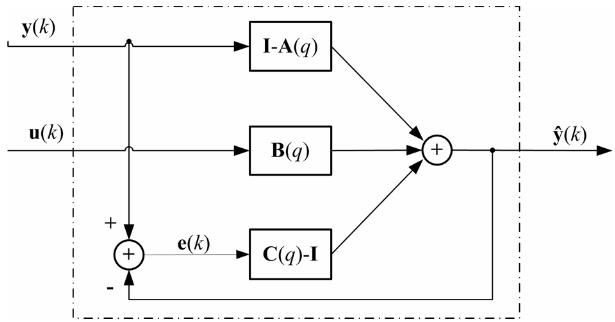

Figure 1: Block diagram representing the ARMAX model structure

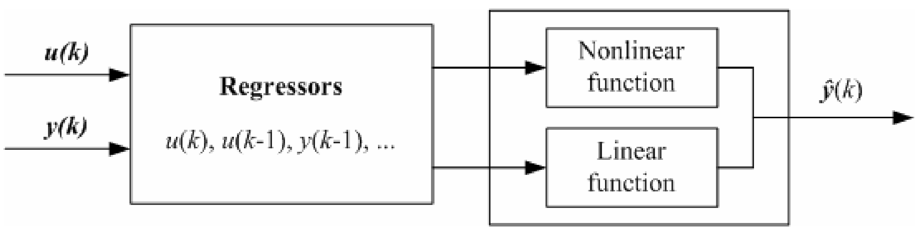

Figure 2: Block diagram representing the structure of a NARX model

NARX model is derived by applying nonlinear regression over the past measured input and output samples.
NARX model predictor is given by:

$$\hat{y}(k) = f_{\mathrm{N}}\left(y(k - 1),...,y(k - na),u(k - nk),...,u(k - nk - nb + 1)\right)$$

NARX model structure enables appliance of static neural networks for approximation of nonlinear function f_{N}. Most nonlinearity estimators represent the nonlinear function as a summed series of nonlinear units, such as tree-partition networks, wavelet networks, multi-layer neural network or sigmoid functions. In our research as a nonlinear estimator the sigmoid network is used. Sigma function is given by form:

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

The network is presented with equation:

$$g(x) = \sum_{k=1}^{n} \alpha_k \kappa\left(\beta_k\left(x - \gamma_k\right)\right)$$

where β_k is a row vector such that $\beta_k\ (x - \gamma_k)$ is a scalar, and n is a number of units.

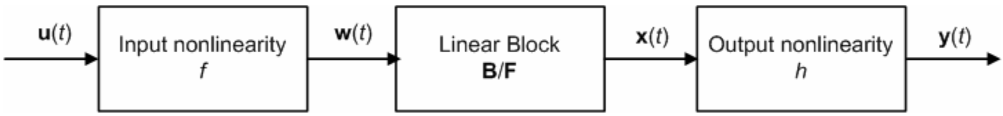

Figure 3: Block diagram representing the structure of a HW model; where:

• w(*t*) = *f*(u(*t*)) is a nonlinear function transforming input data u(t). w(*t*) has the same dimension as u(*t*).
• x(*t*) = (**B**/**F**)w(*t*) is a linear transfer function. x(*t*) has the same dimension as y(*t*).
where **B** and **F** are polynomials of the linear Output-Error model:

$$\mathbf{B}(q) = \mathbf{B}_1 q^{-nk} + \ldots + \mathbf{B}_{nb} q^{-nb\text{-}nk+1}$$
$$\mathbf{F}(q) = \mathbf{I} + \mathbf{F}_1 q^{-1} + \mathbf{F}_2 q^{-2} + \ldots + \mathbf{F}_{\mathrm{nf}} q^{-\mathrm{nf}}$$

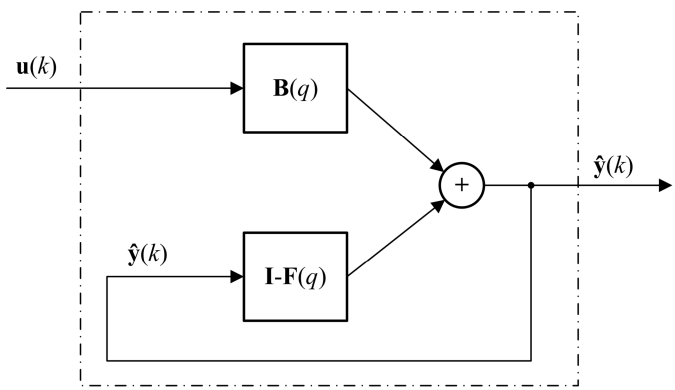

Figure 4: Block diagram representing the structure of an Output Error model

The nonlinear function in HW model can be presented as a summed series of nonlinear units, such as tree-partition networks, wavelet networks, multi-layer neural network, piecewise linear or sigmoid functions. In our research as a nonlinear estimator the piecewise linear function is used.

After choosing model structure, optimal configurable parameters values of ARMAX, NARX and HW model are determined by genetic algorithms in MATLAB Genetic algorithms and Direct Search Toolbox.

Genetic algorithm is optimizing technique that is used for finding global minimum of the function. The evolution starts from a population of randomly generated individuals. In each generation, the fitness function of every individual is evaluated, multiple individuals are stochastically selected from the current population based on their fitness and modified (recombined and mutated) to form a new population. The new population is then used in the next iteration of the algorithm. Commonly, the algorithm terminates when either a maximum number of generations has been produced, or a satisfactory fitness level has been reached.

Process description

The CDU processes the crude oil entering a refinery. Since the CDU is the first unit in the sequence of refinery processing, it is crucial that the quality of fractionation products (unstabilized naphtha, heavy naphtha, kerosene, light gas oil, heavy gas oil), is monitored and controlled (Cerić, 2006; Chatterjee and Saraf, 2004). Heavy naphtha, kerosene, and light gas oil fractions are further use for blending of diesel fuel. Thereby, very important product property is 95% distillation point (D95) of kerosene. 95 % distillation point of the product refers to temperature when 95 % of the product is vaporized when distilled using ASTM D-86 procedure. Section of the column for diesel fuel production with variables used for soft sensor development is given on Fig. 5.

The following variables have been chosen as the input variables of soft sensor model for the estimation of 95% distillation point of kerosene product:

- column top temperature, TR-6104;
- kerosene temperature – 23rd tray, TR-6197;
- light gas oil temperature – 19th tray, TR-6198;
- heavy gas oil temperature–14th tray,TR-6199;
- pumparound temperature, TR-6103 and
- pumparound flow rate, FI-6130.

Soft sensor model development

31898 samples of each input variable are collected from the DCS system, with sampling time of 5 min (Fig. 6). The laboratory assays of output i.e. kerosene 95% distillation point (T95) are carried out four times a day.

Statistical analysis of relevant inputs and their correlation with T95 are presented in Table 1. Data preprocessing included detecting and outlier removal by 3 sigma method and generating additional output data by Multivariate Adaptive Regression Splines algorithm (Salvatore et al., 2009). Data were also detrended (offset or trend were subtracted from data signals).

MATLAB System identification toolbox and Genetic algorithm and Direct Search toolbox routines were used through this work. Data from historical database was divided into two sets: 60% for identification (estimation) data set and 40% for validation data set. After the model structure is chosen, optimal model parameters need to be determined. Configurable parameters and parameter ranges of proposed ARMAX, NARX and HW model are shown in Table 2.

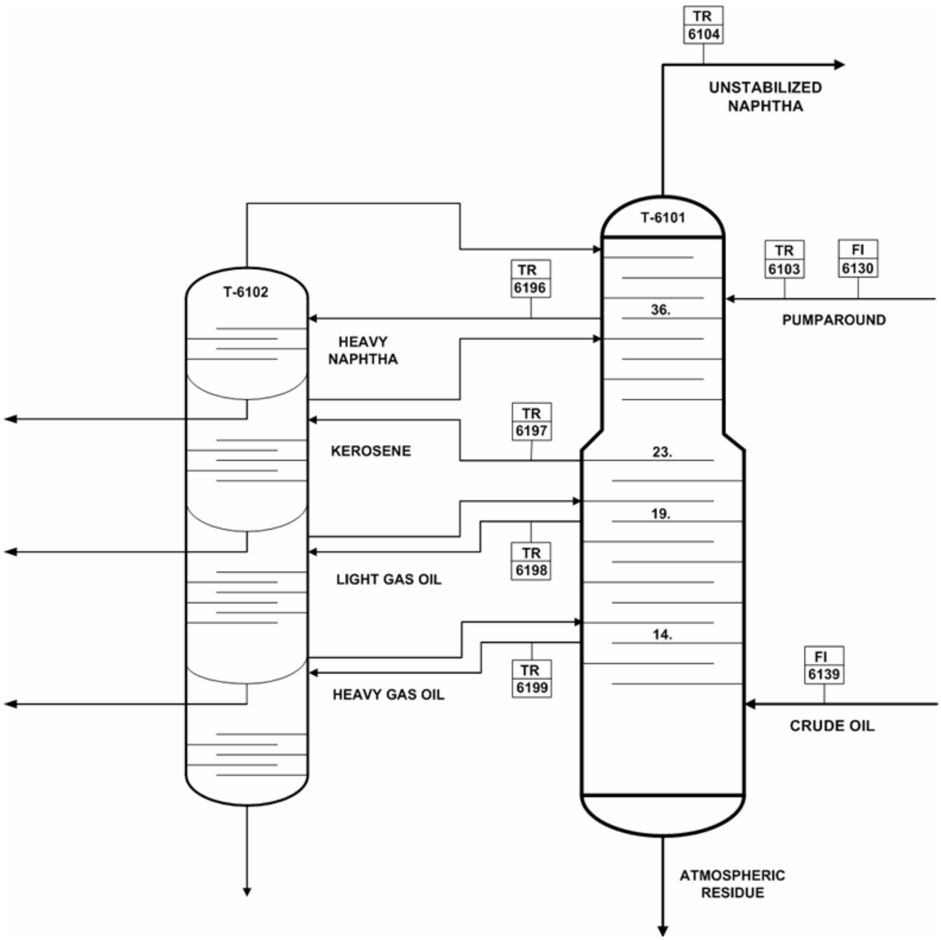

Figure 5: Crude distillation column section

Minimal and maximal configurable parameters values are chosen on the basis of rational complexity of model structure and rational calculating time. Genetic algorithm features have been chosen based on preliminary investigation and experience. In proposed genetic algorithm, in each generation 16 individuals have been created with a crossover procedure, 8 individuals have been created with a mutation procedure, and 1 individual is elite individual (individual with the lowest value of fitness function from previous generation). Search space of configurable parameters for ARMAX model is equal to: $8*8^6*6^6*8 = 7{,}83*10^{11}$.

Search space of configurable parameters for NARX model is equal to: 8*8^6*6^6*12 = $1,17 \cdot 10^{12}$. HW model is the most complex of proposed models, since that 25 parameters need to be determined. Search space of parameters for HW model is equal to: 8^6*6^6*6^5*12^7 = $3,41 \cdot 10^{21}$.

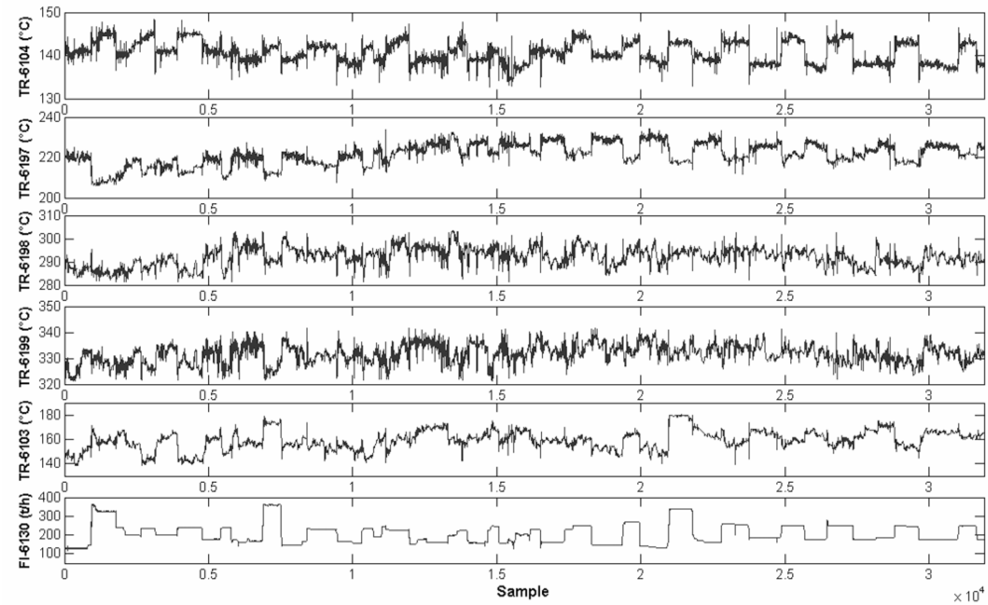

Figure 6: Input variables

Table 1: Statistic parameters of input variables

Input variables	Mean	Median	Min	Max	R with T95
Column top temperature (TR-6104), °C	140,72	140,61	132,64	148,42	-0,70
Kerosene temperature (TR-6197), °C	221,48	221,41	206,33	234,38	0,77
Light gas oil temperature (TR-6198), °C	292,08	292,37	281,19	303,34	0,56
Heavy gas oil temperature (TR-6199), °C	331,64	331,87	321,42	341,72	0,74
Pumparound temperature (TR-6103), °C	159,37	159,48	138,91	180,15	0,35
Pumparound flow rate (FI-6130), t/h	206,56	190,25	116,70	365,06	-0,71

Table 2: Configurable parameters of ARMAX, NARX model and HW model

Parameter label	Parameter meaning	Minimal value	Maximal value
na	No. of past output terms used to predict the current output.	1	8
nb	No. of past input terms used to predict the current output (there are six nb in this model according to six inputs).	1	8
nk	Delay from input to the output in terms of the number of samples (there are six nk in this model according to six inputs).	0	5
nc	No. of past values of the prediction error (only for ARMAX model).	1	8
nf	No. of past prediction output used to predict the current output. (only for HW model)	1	5
n	No. of nonlinear units of sigmoid network (only for nonlinear ARX model).	1	12
np	No. of piecewise units (only for HW model). There are seven np in this model according to six inputs and one output.	1	12

Models are primarily evaluated based on *FIT* and *FPE* value. *FIT* is calculated, as follows:

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

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 is also used for evaluating models. According to Akaike's theory, the most accurate model has the smallest *FPE* (Ljung, 1999; Matlab, 2009). *FPE* is defined by the following equation:

$$FPE = V\left(1 + {}^{2d}\!/_{N}\right)$$

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:

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

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

Since that preliminary investigation showed that *FIT* and *FPE* are non-correlated, but both are frequently used for model evaluation, the aim was to estimate optimal model parameters with the multi-objective function which simultaneously finds model with maximal *FIT* and minimal *FPE*. In this work, weighted sum (scalarization) method is used which is classic method for the integration of several criteria. Each criterion is assigned a weighting value, and the objective (fitness) function is a linear combination of all weighted criteria. Fitness function (*y*) used in this work is defined as follows:

$$y = (100 - FIT) + 10 \cdot FPE$$

Root mean square error (*RMS*) and absolute error mean (e_{MAE}), as frequently used criteria for model evaluation, are also presented in the results.

$$RMS = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_{\exp,i})^2}{n}}$$

e_{MAE} is absolute error mean:

$$e_{MAE} = \frac{1}{n}\cdot\sum_{i=1}^{n}\left|\hat{y}_i - y_{\exp,i}\right|$$

Results and discussion

ARMAX model properties are shown in Table 3.

Table 3: ARMAX model properties

ARMAX GA	
FPE	1,574
FIT	82,893
RMS	2,405
e_{MAE}	1,860
fitness function, *y*	32,843

All results were calculated for validation data set. ARMAX model parameters of the best achieved model are presented in the following matrix form:

na = [7]
nb = [6 1 7 7 7 8]
nk = [0 1 0 0 0 0]
nc = [8]

Fig. 7 shows comparison between simulated and measured output for validation data set. It can be noticed that the model output matches the validation data very well.

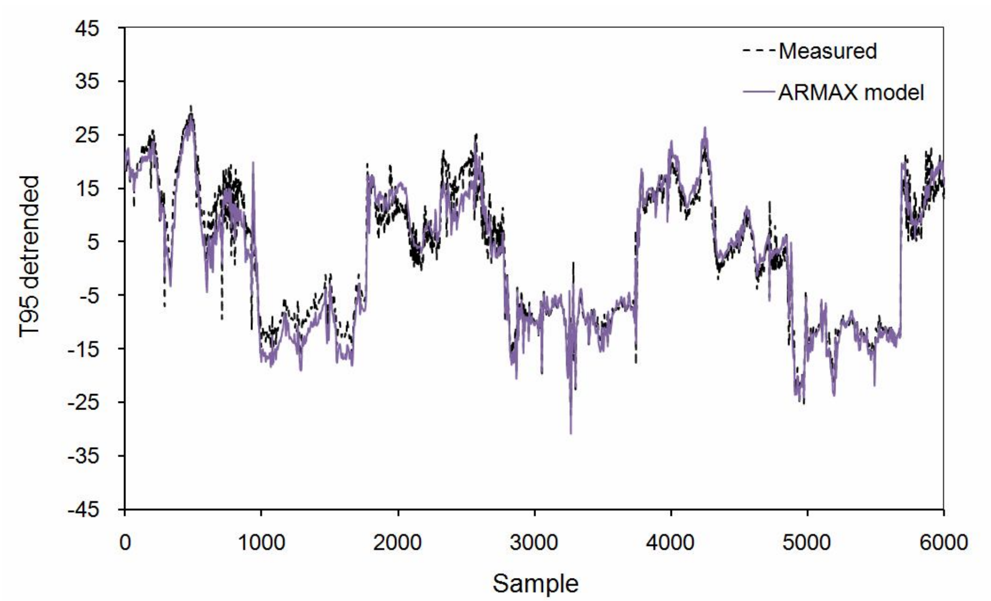

Figure 7: Comparison between measured and ARMAX model output data.

Due to complexity and nonlinearity of the distillation process, NARX model was developed. In the preliminary investigation, among sigmoid net and wave net as nonlinear block of NARX model, better results were achieved with sigmoid net. In this work results of NARX with sigmoid networks are shown. NARX model properties for validation data set are presented in Table 4. NARX model structure parameters of best achieved model are presented in the following matrix form:

na = [6]
nb = [4 5 4 4 7 5]
nk = [1 0 0 0 0 0]
n = [6]

Fig. 8 shows comparison between simulated and measured output for validation data. From graphical comparison, corresponding *FIT*, *FPE* and *RMS* value it can be observed that experimental and model data show satisfactory agreement. It can be noticed that NARX model shows somewhat better agreement with measured output data with lower model order than linear ARMAX model.

Table 4: NARX model properties

NARX model	
FPE	1,010
FIT	83,888
RMS	2,265
e_{MAE}	1,514
fitness function, *y*	26,207

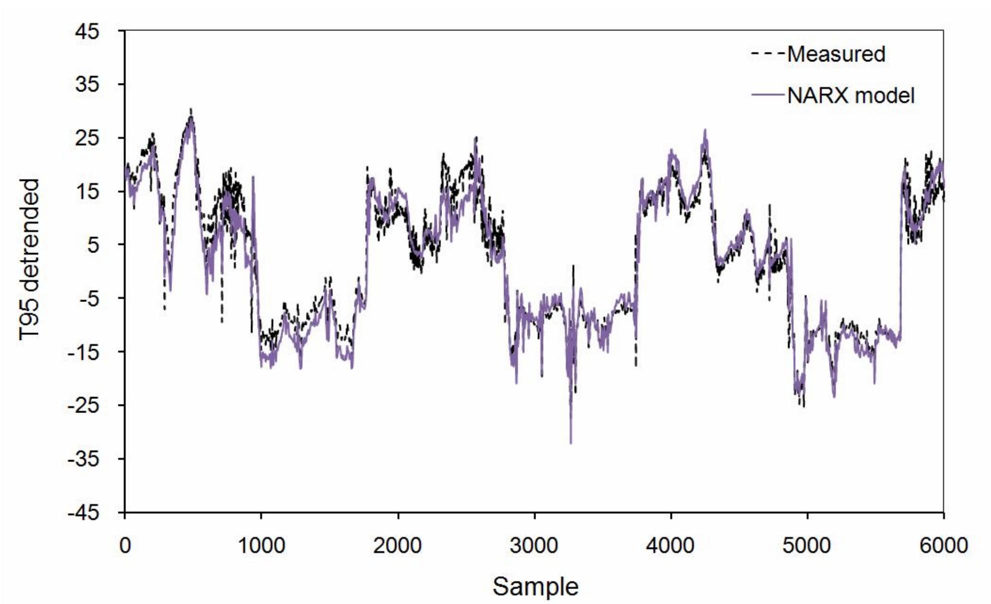

Figure 8: Comparison between measured and model output data, using NARX model with sigmoid network

HW model parameters of the best achieved model are presented in the following matrix form:

nb = [1 1 2 2 2 2]
nf = [1 1 2 1 2 2]
nk = [0 0 1 0 0 0]
np = [9 8 9 11 9 10 11]

Figure 9 shows comparison between HW model output data and measured output data. As can be seen from Table 5 and Fig. 9, HW model showed the best performance (the highest *FIT* and the smallest errors) among developed models.

Table 5: HW model properties

HW model	
FPE	1,351
FIT	94,991
RMS	0,684
e_{MAE}	0,265
fitness function, *y*	18,518

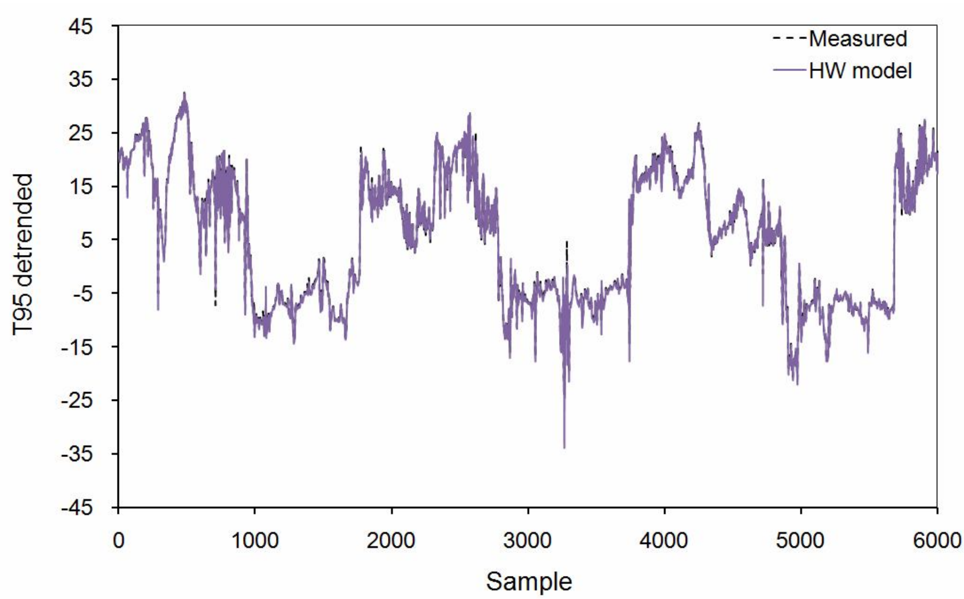

Figure 9: Comparison between measured and HW model output data

From graphical comparison, corresponding *FIT*, *FPE* and *RMS* value it can be observed that model data match with experimental data with high accuracy. The average absolute deviation of HW model (0.3°C) is quite satisfactory for the on-line implementation. Developed code for developing models is quite general and with some modifications it can be easy adapted for development of other autoregressive identification models. In this work, *FIT* and *FPE* were included in fitness function since they are common used measures for model evaluation and comparing the model quality. However, fitness function can be some other measure that is often used for model evaluation, for example (*RMS*). Presented work showed that evolutionary algorithms can be successfully used for tuning NARX, ARMAX and HW model parameters.

Conclusions

In this work, linear and nonlinear dynamic models for the estimation of kerosene 95% distillation point were developed. Chosen linear and nonlinear models showed satisfactory matching with experimental data, thus improved that can be employed as the soft sensors for the on-line estimation of the key product properties of the crude distillation unit. Using the present procedure it was shown that evolutionary algorithms can be satisfactory applied for optimizing configurable parameters of autoregressive models. HW model showed the best performance and can be successfully employed as the soft sensor for the on-line prediction of the kerosene 95% distillation point.

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UDK	kjučne riječi	key words
665.622.048.3	atmosferska destilacija	topping
66-503.56	optimalno vođenje i regulacija procesa	optimal process control and regulation
66.012.122	softwarski senzori za selekciju modela upravljanja procesom	software sensors for process modeling system selection

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Received
04.05.2011

Accepted
06.06.2011.