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Soft Sensors for Diesel Fuel Property Estimation

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Virtual soft sensors are developed for properties estimation of diesel fuel as the crude oil column side product. Because of the growing standards for the fuel quality and needs to produce various gradations of diesel fuel, frequently laboratory testing and quality controls of the products are necessary. On the basis of available continuous temperature measuring of particular process streams, soft sensors for estimating end boiling point (D95) of diesel fuel have been developed. Linear and nonlinear soft sensor models have been built using linear regression and artificial neural networks. Statistical data analysis has been carried out and the results were critically judged.

1. Introduction

From industrial facilities are expected to have greater efficiency and compliance with prescribed laws that impose hard limits to the quality of products and emissions of pollutants. For this reason there is a need for an effective measurement and process control, which imposes the need to monitor a large number of process variables using appropriate measuring devices. The main problems are big price, and unreliability of on-line measuring instruments and analyzers.

Soft sensors, as part of virtual instrumentation, are focused on assessing the system state variables and quality products by applying the model, so replacing the physical senses and laboratory analysis (Bolf et al., 2008, 2009).

There are numerous reasons why soft sensors should be applied in industry. They become standard tools showing tendency to change their role from the regulatory one within open control loop towards playing the role of a sensor in control loop. Fields of application characteristically include substitute for measuring devices, reducing need for measuring equipment, sensors validity evaluation, failure detection, and diagnostics (Fortuna, 2007; Kadlec et al., 2009).

Based on the available continuous measurement of process streams the soft sensors have been developed to estimate the distillation end point of diesel fuel. Experimental data were collected on refinery crude distillation unit. Several linear and nonlinear models of soft sensor are developed using a linear regression analysis and artificial neural networks.

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2. Diesel Fuel Production in Crude Distillation Unit

Diesel fuel is a mixture of kerosene fraction, light gas oil fraction, and heavy benzene, containing mainly hydrocarbons C_{10} to C_{12} from the alcane (parafine), cycloalcane (cycloparafine, naphtene), and aromatic hydrocarbons groups. It is used to fuel diesel engine with internal combustion, where the ignition takes place by self-combustion of compressed fuel and air compound. Its important properties include: density, distillation curve, cetan number (cetan index), filterability, ignition point, viscosity, aniline point, corrosion tendency, and sulphur quantity. One of the key properties is distillation end point (Cerić, 2006).

Heavy naphtha, kerosene, and light gas oil fractions are used for blending of diesel fuel; these are being drained away as side fractions of crude distillation column. Section of the column with diesel fuel products is given in Figure 1. Based on the analysis of the process and process expert knowledge the following variables are used for soft sensor development:

T_{CT} - column top temperature, TRC-6104

T_{HN} - heavy gasoline temperature (36th tray), TR-6196

T_{K} - kerosene temperature (23rd tray), TR-6197

T_{LGO} - the light gas oil temperature (19th tray), TR-6198

T_{HGO} - the heavy gas oil temperature, TR-6199

T_{PA} – pump around temperature, TRC-6103.

All the temperatures are functions of side product flow rates and operating conditions.

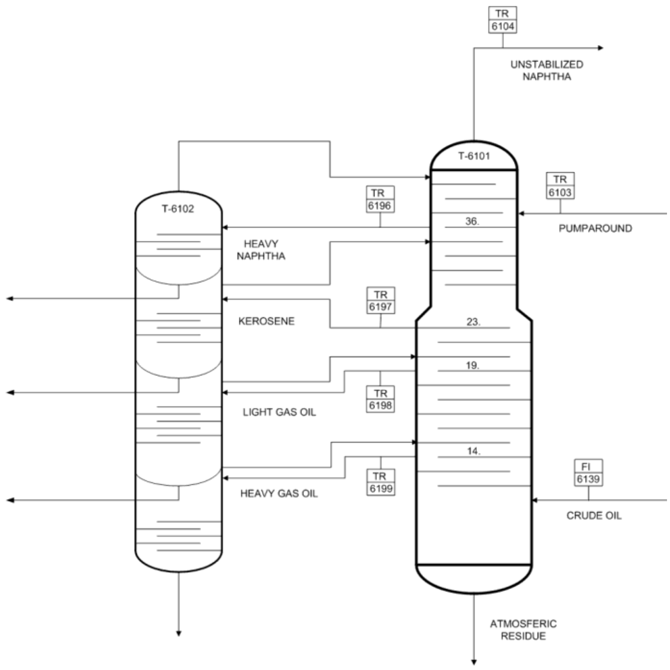

Figure 1: Crude distillation column with diesel fuel products

3. Results and Discussion

3.1 Linear model

At the beginning of the analysis, statistical data processing has been conducted (Statistica, 2006). The data from the plant have been obtained in the period of one year. Laboratory analysis was conducting 4 times a day. The extreme values from the data were eliminated using data filter. The correlation coefficients between the variables have been calculated, Table 1. If the input and output variables are independent correlation coefficient ρ is equal to zero and if they are dependent correlation coefficient is in the range from -1 to 1.

Table 1 Correlation coefficients after removing the extreme values

ρ	T_{CT}	T_{HN}	T_{K}	T_{LGO}	T_{HGO}	T_{PA}	T_{D95}
T_{CT}	1.00	0.71	0.04	0.05	-0.15	-0.15	-0.17
T_{HN}	0.71	1.00	0.62	0.53	0.12	-0.04	0.21
T_{K}	0.04	0.62	1.00	0.73	0.34	0.11	0.61
T_{LGO}	0.05	0.53	0.73	1.00	0.34	0.36	0.71
T_{HGO}	-0.15	0.12	0.34	0.34	1.00	0.16	0.36
T_{PA}	-0.15	-0.04	0.11	0.36	0.16	1.00	0.35
T_{D95}	-0.17	0.21	0.61	0.71	0.36	0.35	1.00

Based on the analysis it was decided to create a linear model with the two most influential input variables (T_K and T_{LGO}).

Table 2 presents statistical parameters of the linear model. Multiple correlation coefficient R represents relatively good correlation, and the value of the coefficient of determination R^2 and adjusted coefficient of determination, which indicate approximatively linear model. F-test rejects the hypothesis that the model has no linear dependence, and with the level of significance (p) which is equal to zero we can 100 % confirm the reliability coefficient of determination. The standard error estimate of parameters has a satisfactory value for the linear model.

Table 2 Statistical parameters of linear model

R	R^2	Corrected R^2	F(2,319)	p	Stand. error
0.72	0.52	0.52	175.21	0.00	10.81

Multiple correlation coefficient, determination and adjusted coefficient of determination values are between 0.5 and 0.6 which are small but indicates that the regression model is partly representative. Parameter p is equal to zero, which tells there is no autocorrelation of error relation..

The resulting linear model has the following form:

$$T_{D95} = -274.11 + 0.64 T_{K} + 1.61 T_{LGO} \tag{1}$$

3.2 Nonlinear model

After performing multiple linear regression analysis, it was determined that due to relatively small multiple correlation coefficient and big standard error it was not possible to realize linear models in real plant environment. So, neural network-based soft sensors were developed.

Neural network based soft sensor models were developed using simulation package (Statistica, 2006). During preliminary tests, some twenty experiments had been carried out where, in reciprocity, the characteristics of differently structured neural networks have been compared: the linear ones, the networks based on the RBF – Radial Basis Function Networks, and the Multilayer Perceptrons (MLP). Each experiment included examining of one hundred neural networks, and twenty best of them were singled out.

The entire data set is divided into three parts by randomization: the train set, the select set, and the testing set, positioned in the 2:1:1 ratio. In order to study the impact of individual inputs to the outputs of model of the software sensor also was carried out sensitivity analysis. Sensitivity analysis showed that it is necessary to consider five of the seven possible inputs for both soft sensors, Figure 2.

The findings showed that the MLP networks have the best characteristics, thus they were chosen to carry on additional researches aimed to improving the model.

During MLP neural networks training, the number of neurons in the hidden layer was varied from 1 to 20 and different learning algorithms were used (back propagation with variations of learning rate and momentum, conjugate gradient descent, Levenberg-Marquardt) as well as pruning and Weigend regularization techniques. Also, the best results were achieved using a combination of back-propagation algorithm in the first, and conjugate gradient descent algorithm in the second stage of neural network training.

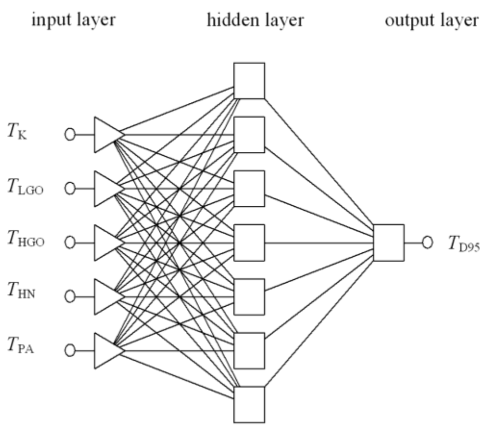

Figure 2: The structure of the neural network model

Multilayer perceptron neural networks has optimal structure of 5-7-1 (five neurons in the input network layer, seven in the hidden layer, and one neuron in the output layer), and are shown in Figure 2.

Table 3 show performances and errors of each data set – the train set, the select set, and the testing set. The performance of the sets equals the ratio of standard deviations, i.e. the ratio of standard error deviation and standard data deviation:

$$performance = \frac{\sqrt{\frac{\sum_{i=1}^{n}(e_i - \bar{e})^2}{n}}}{\sqrt{\frac{\sum_{i=1}^{n}(y_{\exp,i} - \bar{y}_{\exp})^2}{n}}} \quad (2)$$

Error (E) is equal to the difference sum squares between neural network outputs and experimental outputs:

$$E = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_{\exp,i} - \hat{y}_i)^2} \quad (3)$$

Table 3 Parameters of best model performance

T_{D95} (°C)	*Performance of train set*	*Performance of select set*	*Performance of testing set*	*E (train set)*	*E (select set)*	*E (testing set)*
MLP 5-7-1	0.59	0.59	0.58	0.12	0.13	0.13

The best network model has also been trained with the back propagation algorithm in a hundred iteration steps, followed by thirty-three iterations with gradient descent method. The best neural network for each of the models has been chosen using the testing set error criterion. It is taken into account that the train set, the select set, and the testing set performances are at approximately the same level, which indicates that behavior of the neural networks is uniform in each of the three sets.

Table 4 Regression parameters for diesel fuel distillation end point (D95)

T_{D95} (°C)	Train set	Select set	Testing set
$\bar{x}_{\exp}$	322.04	334.48	333.39
$\sigma_{\exp}$	14.80	15.99	16.57
$\bar{e}$	0.11	-1.37	-0.19
σ_e	8.78	9.43	9.69
$\lvert\bar{e}\rvert$	6.78	7.82	7.86
Ratio σ	0.59	0.59	0.58
R	0.81	0.82	0.83

Table 4 shows that absolute error mean for the developed neural network for distillation end point is about 7 °C. Multiple correlations for the neural network are relatively high (0.8). Figure 3 shows the results obtained by neural network model where two most influential variables were taken as inputs (T_K and T_{LGO}).

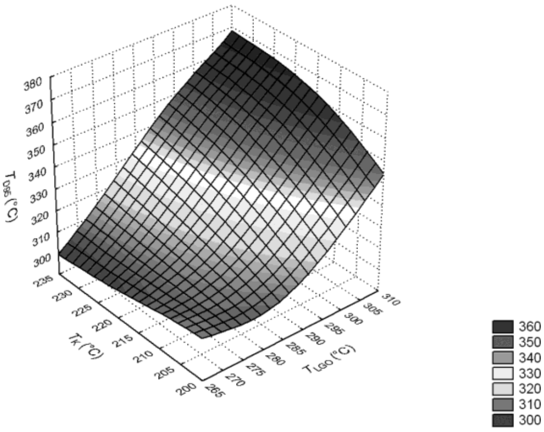

Figure 3: The results obtained using two most influence variables

4. Conclusions

Based on continuous temperature measurement of adequate process streams the soft sensors for estimation of diesel fuel distillation end point were developed. Several soft sensor models were developed using regression analysis and neural networks. Sensitivity analysis showed that the temperature of light gas oil eminently affects the diesel fuel distillation end point.

Based on the result analysis and statistical indicators it can be concluded that models of linear soft sensor satisfy the purpose. Models are suitable for use, but caution is needed due to variability of operating conditions. Nonlinear models applying neural networks give similar results.

Developed soft sensors can be used for continuous estimation of diesel fuel properties, and the methods of inferential control. For this purpose it is necessary to implement one of the dynamic compensation methods.

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