Virtual Analyzer of Petroleum Quality Indicators

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***Abstract*— The presence of correlation links between the quality indicators of commercial petroleum products allows to restore the missing values, as well as monitor the correctness of the online monitoring results. In the simplest case, the uncertainty of the process of mixing hydrocarbon solutions is modeled on the basis of a multidimensional Gaussian distribution. The procedure for estimating the controlled parameters of petroleum products based on multivariate statistical analysis of available observations is proposed.**

Keywords*— *virtual analyzer; incomplete data; Gaussian distribution; multidimensional statistical analysis

I. INTRODUCTION

In general, the process of preparation of commodity fuel, dynamic (in-flow) or static (in a tank) mixing of hydrocarbon solutions, which provides an output product with specified quality parameters. At the same time, the dynamic system of mixing in the flow provides significant resource savings and improves the quality of movement, but requires a rather complex adaptive control in compliance with the requirements of commodity standards. On practice, this procedure is complicated by the presence of several levels of uncertainty, the most significant of which is due to a significant spread in the properties of incoming mixing components. The problem is exacerbated by the fact that the standard set of quality indicators of the original components does not fully describe their mixing properties: two sets of components with the same percentage composition (by weight) and the same standard components can lead to mixtures with slightly different properties.

The streaming organization of the mixing process, leads to the need for a consistent correction of the hacking parameters as the results of current analyzes are received (usually incomplete). The effectiveness of this approach can be estimated either by the size of the stock by quality, or by a generalized economic indicator that takes into account the different cost of components.

Efficiency of this approach is reduced due to a slow analysis process involving sampling, sending them to the laboratory and waiting for the results of the measurements, which lasts for several hours. At this time, process control is performed based on assumptions of the general nature, experience and intuition of the staff. As a result, management is conducted with a large margin in quality, which leads primarily to an increase in consumption of material resources and a decrease in profitability [1].

Thereby, one of the obstacles to further improving the efficiency of the technological solutions used is the incompleteness and inadequate efficiency of information on the properties of the main components and, most importantly, the properties of the output products. The problem of operational efficiency is being successfully solved by the introduction of modern on-line analyzers [2]. As one of the means to combat the incompleteness of information in this paper, we propose a procedure for statistical estimation of unobserved physico-chemical indicators based on the results of current analyzes available at each stage.

II. MODEL OF UNCERTAINTY

Probabilistic model for describing uncertainty is based on the hypothesis of the correlation between the parameters of the hydrocarbon mixture being formed. This hypothesis is easily confirmed by an analysis of the formed observations. Since the measured values have different dimensions and different average values, it is necessary to go from the analysis results in real units to dimensionless quantities, in which the measurement unit of each component is taken as an estimate of its standard deviation (sd).

Thereby, as the initial data, matrix Y which dimension $<n \times m>$ is used for the batches analysis of the finished mixture: n – is the number of batches, m – is the number of analyzed indicators. The element y_{ki} element of matrix Y is the result of measuring the j-th index in the k-th batch. Let y – $<1 \times m>$ be the vector of mean

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values of the exponents, $s - <1\times m>$ be the vector of theit sd. Data are normalized by dividing each column of the matrix Y by the corresponding element of the vector s. As a result, we obtain a matrix of analysis results in dimensionless quantities.

Let $S = diag(s)$ – diagonal matrix $<m\times m>$, on which diagonal are the elements of the sd vector *s*, S^{-1} – the inverse matrix towards to C *S*. Then

$$Y_0 = Y \cdot S^{-1}; \quad Y = Y_0 \cdot S. \tag{1}$$

The second of formulas (1) allows us to return from dimensionless quantities to their values in real units of measurement. Y_0 in expression *(1)* – is the matrix $<m\times m>$ of the analysis results of a given batches set of the finished mixture, $y_{0<1\times m>}$ – vector of means, $P_{<m\times m>}$ – covariance matrix. Suppose that the first q characteristics (elements of the vector of analysis results) are observable, and the remaining r - unobservable, $q + r = m$.

This partition generates the corresponding representation block of the matrix Σ and the mean vector:

$$P = \begin{bmatrix} P_{11} & P_{12} \\ P_{12} & P_{22} \end{bmatrix}, \quad y_0 = [y_{01}^T, \quad y_{02}^T]^T. \tag{2}$$

where P_{11} and P_{22} – are the covariance (due to the chosen system of units – correlation) matrixes, respectively, of observed and non-observed analysis results components, P_{12} – mutual covariance (correlation) matrix of observed and unobserved components.

Then for the optimal linear mean square reconstruction of vector z_{02} $<1\times q>$ unobservable characteristics by vector z_{01} $<1\times p>$ observed the following multiple regression [3]:

$$z_{02} = E\{z_{02}\} + P_{12}^T P_{11}^{-1}(z_{01} - E\{z_{01}\}),$$
$$E\{z_{01}\} = y_{01}, \quad E\{z_{02}\} = y_{02}. \tag{3}$$

This approach has the advantage that the matrix Σ_{12} and vectors y_{01}, y_{02} are statistically evaluated and remembered once at the stage of processing the results of output product analysis. For each specific recovery session of missing analysis results, Σ_{12} simply regroups: rows and columns corresponding to the observed characteristics are collected in the upper left corner of the matrix, unobserved - in the lower right corner. The resulting estimate is unbiased. The covariance matrix of estimation errors has the form:

$$P_R = P_{22} - P_{12}^T P_{11}^{-1} P_{12}, \tag{4}$$

its diagonal elements are the variances of the estimation errors by components (in dimensionless quantities). This approach can be applied extensively, considering all the analysis results and the corresponding data on the mass percentage composition of mixture as a single vector of characteristics. In this case, there is a single complete scheme for estimating all the missing characteristics from the set of observables.

III. VISUALISATION OF CONTROL PROCESS

Technical calculations and visualization of evaluation results are carried out by means of a software virtual analyzer [4–6]. Visualization involves reducing the dimension of being solved problem. Analysis results of physicochemical mixture properties in dimensionless quantities can be orthogonalized and two uncorrelated principal components explaining the maximum achievable part of the total data array scattering under study. In this case, any result of the analysis will be represented by a point on the plane of the principal components in the generalized phase space.

At the same time, the tolerance limits, defined by the standard of commercial output, are transformed into point boundaries for these main components. This allows to monitor the flow mixing process, displaying the motion of phase vectors in this plane and visually comparing the estimates with the real results of current analyzes.

This view is extremely clear, but unfortunately, it suffers from incompleteness (to reflect 97.5% of information, you need to have not 2 but 6 factors) and does not have a visual physical interpretation. Nevertheless, it is very convenient, for example, for training technical staff.

IV. EXPERIMENT RESULT

As initial data, the analysis results of physical and chemical properties of summer low-sulfur diesel fuel diesel fuel (DT) finished batches at a particular oil refinery are considered. They are collected in a matrix: its lines are the analysis results of these lots of DT in the following order: (1) flash point, C0; (2) kinematic viscosity, c; (3) cloud point, 0C; (4) pour point, 0C; (5) limiting filterability temperature, 0C, (6) Mass fraction of sulfur, mass%; fractional composition: (7) the beginning of boiling, 0C; (8) 10%, 0C; (9) 50%, 0 ° C; (10) 90%, 0 ° C; (11) 96%, 0C.

Analysis of correlation matrix parameters resulted in the conclusion that the recovery of the missed parameters with an error of 3.7% is possible with the use of five combinations of characteristics, the main components. The greatest accuracy of recovery is achieved by using the following physicochemical parameters in order of increasing sum of correlation coefficients squares: sulfur mass fraction, fractional composition 50%, pour point, flash point, fractional composition 96%. Using only two main components (main factors), an explanation of 78.3% of the available scattering is achieved, which makes it possible to obtain visualization on the plane of various processes associated with the mixing of petroleum products. In the case of using a set of observable parameters, consisting of the flash point, the mass fraction of sulfur, the fractional composition (5 indices), the scores of the unobservable indicators are: pour point and filterability limit of – 0.095 ° C, cloud point – 0.0547 ° C, kinematic viscosity: – 0.095.

V. EXAMPLE OF DATA RESTIRATION

Table 1 gives incomplete data on the physicochemical parameters of several control mixtures and the statistical

estimates of the missing indicators constructed using the above method.

TABLE I. RESULTS OF INDICATORS LINEAR STATISTICAL ESTIMATION

Parameter	Measure	Value	Measure	Value	Measure	Value
1	79	79.5	73	75	84	81.5
2	4.6	4.8	4.3	4.41	5.20	5.3
3	-8	6.2	-8	-7.7	-5	-4.6
4	-10	9.8	-16	-14.7	-12	-13.5
5	-8	-6.3	-8	-7.6	-5	-4.6
6	0.04	0.042	0.043	0.044	0.044	0.045
7	206	201	200	201	207	203
8	229	232	223	223.0	236	234
9	271	273	267	269	276	276
10	332	333	329	329.1	335	336
11	352	353	350	351	354	354

VI. CONCLUSION

As a result of research, the following conclusions can be drawn:

1. These results demonstrate the possibility and effectiveness of multidimensional statistical analysis methods based, generally speaking, on the assumption of Gaussianity and uncorrelatedness, for modeling the uncertainty conditions in which petroleum products are mixed.
2. An approach based on approximate estimation of non-observed indicators based on available ones is used at the level of understanding of the basic regularities by all qualified technologists.

In this paper, a theoretical basis has been obtained for the automated generation of such estimates and for monitoring their accuracy.

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