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Analysis of Information Characteristics Objects of Chemical Technology

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ABSTRACT: In order to introduce generalized assessments of the degree of perfection of technological schemes of chemical-technological systems, the basic information characteristics of chemical-technological systems that can be determined from the statistical processing of random functions of the output coordinates of these systems are considered. The methods of calculation information characteristics object Chemical Technology on thermodynamic analysis operation example monoethanolamine separating gas purification at a chemical plant.

KEYWORDS: entropy, amount of information, monoethanolamine purification, differential entropy, spectral density.

I. INTRODUCTION

Recently, there was a need to introduce generalized assessments of the degree of perfection of technological structures of chemical technology objects and their control systems. Information assessments provide the most general approach to quantitative and qualitative research of complex technological processes.

II. PROBLEM DEFINITION

The object of chemical technology (Figure 1) can be considered as an information system that performs the transformation

$$Y(y_1, y_2, \dots y_m) \to X(x_1, x_2, \dots x_n) \quad (1)$$

Here X (x_1, x_2, ... x_n) is a vector of random time functions that characterizes the output coordinates of the object; Y (y_1, y_2, ... y_m) is a vector of random time functions that characterizes external and internal disturbances and control actions.

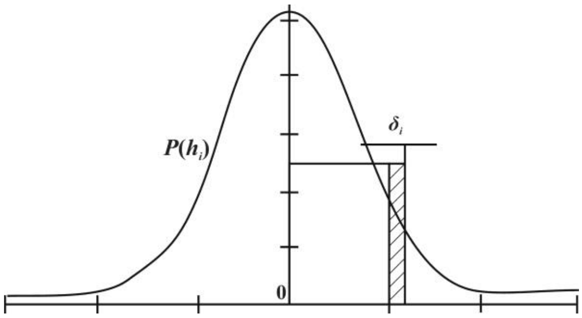

Figure 1. Information on the state of the object of chemical technology

The form of this transformation (in the general case of a nonlinear one) depends on the physicochemical features of the process and the technological structure and connections imposed on the control process [1]. Obtaining an analytical form of the connection between the input and output vectors, when a process that goes beyond one device is considered, in most practical cases it is difficult even with the help of mathematical modeling. At the same time, these

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data are initial for the design, management and optimization of chemical-technological processes. The decision of this problem greatly facilitates the knowledge of the information characteristics of already existing chemical industries.

The main information characteristics of the chemical-technological process are:

- the entropy of the output vector - X (x_1, x_2, ... x_n) as a measure of possible deviations of the process from a given regime, i.e., a criterion for the quality of the process and its organization;

- speed and sign of the change in entropy in time in stationary and non-stationary modes, with and without control, as a measure of its stability and a general criterion for assessing the quality of management;

- the amount of information that carries the output signals: in any of the possible modes, as a measure of the complexity of the object of chemical technology and the basis for calculating the control system; throughput ability of the object through the channels of disturbing and control actions, allowing to justify the choice of means and schemes of automation.

III. DECISION METHOD

Let us consider in more detail the information characteristics of chemical technology objects and describe the methodology for calculating them using the example of information analysis of the separation of monoethanolamine treatment (MEAO). Any of the output coordinates of the process is physically a signal that carries information about the state of the object for n samples over time (see Figure 2).

$$I = -n\sum_{i=1}^{n} P(h_i)\delta \log_2[P(h_1)\delta]. \tag{2}$$

This signal removes the uncertainty of the information about the object by the value of ΔH of the entropy, which is numerically equal to the amount of semi-information ΔH=1. For the case of n-independent coordinates of the system

$$H = \sum_{i=1}^{n} H_i \tag{3}$$

If the number of signal quantization levels is sufficiently large, then

$$I = -n\int_{-\infty}^{\infty} P(x)\log_2[P(x)\delta_x]dx \tag{4}$$

Andsince $I = nH$ then for the entropy of the quantized signal

$$H = -\int_{-\infty}^{\infty} P(x)\log_2[P(x)\delta_x]dx \tag{5}$$

Most of the processes of chemical technology proceed relatively slowly (excluding the points of critical regimes), that is, their signals have a continuous character with a shift to the low-frequency part of the spectrum. In this case, one can not give preference to any of the quantization criteria by level. Therefore, it is more convenient to process the records of realizations obtained as a result of an industrial experiment with quantization only in time.

Obviously, the transition from a discrete random variable to a continuous one is possible by reducing the quantization step to 0 with an unlimited growth in the number of possible values of the quantized signal, since

$$m = \left[\frac{2X_{max}}{\delta_x} + 1\right], \tag{6}$$

$$m \to \infty \; npu \;\; \delta \to 0$$

A direct limit transition with δ_x → 0 by formula (5) leads to the value of the entropy of the process, which is equal to infinity. Nevertheless, for continuous random variables, it is possible to obtain a number of relationships that also make it possible to successfully study the information properties of both continuous and discrete signals.

After simple transformations, formula (5) can be rewritten in the form

$$H(x) = -\left[\int_{-\infty}^{\infty} P(x)\log_2 P(x)dx + \log_2 \delta_x\right]. \tag{7}$$

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The first term depends only on the type of distribution, that is, all quantized signals with the same probability distribution of occurrence of their levels can have different entropies only due to different quantization steps. The considered integral is called the differential entropy

$$h_x = \int_{-\infty}^{\infty} P(x) \log_2 P(x) dx \quad (8)$$

$$H(x) = h(x) - \log_2 \delta_x . \quad (9)$$

When imposing restrictions on the accuracy of the measurement, additional uncertainty is introduced by reducing the different gradations of the signal Hy (x)

$$H_y(x) = h_y(x) - \log_2 \delta_x \ (10)$$

Obviously, the amount of information in Y (t) is equal to the amount of information of the source X (t), minus the loss in the discriminator.

Corresponding entropies will be connected $H(y) = H(x) - H_y(x)$or on the basis of (9) and (10)

$$H_y = h(x) — h_y(x) \quad (11)$$

or in expanded form

$$H(y)=\int_{-\infty}^{\infty} P(x) \log_2 P(x)dx+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(x,y) \log_2 \left[\frac{P(x,y)}{P(y)}\right] dxdy=$$

$$=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(x,y) \log_2 P(x)dxdy+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(x,y) \log_2 \left[\frac{P(x,y)}{P(y)}\right] dy;$$

Because

$$\int_{-\infty}^{\infty} P(x,y)dy = P(x)$$

In the end

$$H(y) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(x,y) \log_2 \left[\frac{P(x,y)}{P(x)P(y)}\right] dx\, dy. \quad (12)$$

The relation (12), which determines the entropy of the source for a given accuracy of the measurement of the signal, does not depend on the quantization step, and consequently it will also hold for δ_x = 0.

The amount of information produced by the source of continuous signals with limited accuracy of their measurement will be expressed as

$$I = n[h(x) - h_y(x)]. \quad (13)$$

Information systems of chemical industries in real conditions most often deal with correlated signals that are close in character to normal distribution. Therefore, it is of interest to obtain expressions for determining the information characteristics of normally distributed correlated signals. For an uncorrelated normally distributed signal (one-dimensional probability density)

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma_x} \cdot e^{-x^2}/2\sigma_x{}^2$$

after integration into

$$h(x) = \int_{-\infty}^{\infty} P(x) \log_2 P(x) dx$$

gives the value of differential entropy

$$h(x) = \log_2 \sigma_x \sqrt{2\pi}\, e. \qquad (14)$$

For a correlated signal

$$h(x) = \log_2 \left[\sigma_x \sqrt{2\pi e(1-r^2)}\right] \qquad (15)$$

where r is the correlation coefficient [3].

The entropy value for a given mean squared error σ_p at the source output can be found

$$H(y) = h(x) - max h_y(x)$$

$$\max h_y(x) = \log_2 \sigma_p \sqrt{2\pi}\, e$$

whereσ_p — the mistakes differ.

Then

$$H(y) = \log_2[\sigma_x \sqrt{2\pi e(1-r^2)} - \log_2 \sigma_p \sqrt{2\pi e} = \log_2 \frac{\sigma_x}{\sigma_p} \sqrt{1-r^2}. \qquad (16)$$

The total amount of information from the object for independent coordinates is expressed as[4]

$$I = h \sum_{i=1}^{m} H_i(y). \qquad (17)$$

For the rate of change of entropy

$$v(t,\tau) = \frac{\Delta H_T(x,t,\tau)}{T}, \qquad (18)$$

Where ΔH_T is the entropy increment over the time interval T = (t-τ).

In the special case, if the derivative of the entropy with respect to time in a system not subject to the action of noise is always negative, then there is a general entropy stability[5]

$$\mathrm{H} = \frac{dH}{dt} = -\frac{\Delta d}{dt} \int_{-\infty}^{\infty} P(x) \log_2 P(x) dx.$$

If H is alternating, but the absolute value of the entropy of the process is bounded by some finite number N, then the process is non-divergent[6].

The effectiveness of management can be assessed by the ratio[7]

$$\eta(t,\tau) = \frac{H_0(t,\tau) - H_1(t,\tau)}{H_0(t,\tau)}. \qquad (19)$$

Here: H_0 (t, τ) is the entropy of an uncontrolled process.

The percentage of carbon dioxide in the purified gas is continuously recorded on the diagram tape. Thus, in the transformation (1) we have the records of the realizations X (x_1) -defining the output coordinate of the process.

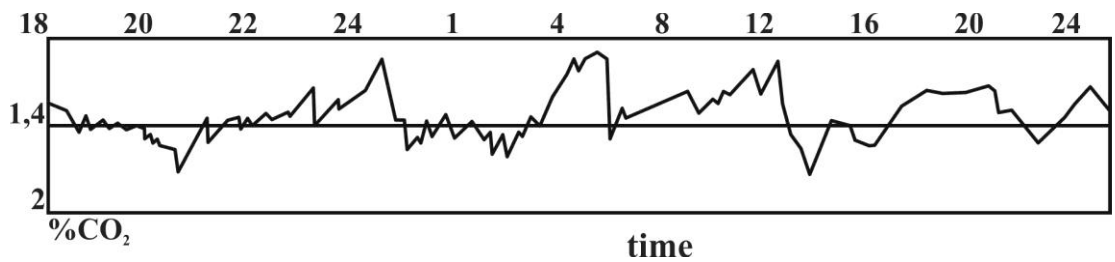

Figure 2. Recording the implementation of the output signal of the monoethanolamine gas purification process

An approximate estimate of the first moments of the distribution of output coordinate realizations for two samples of duration 1 day each, according to the recommendations described in [8], under the condition of normal distribution, gives the value of the mathematical expectation of dispersion and entropy[9]:

1. For the first sample: m_ (x_1) = 1.29%; σ_ (x_1) = 0.39%.

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2. For the second sample: m_ (x_1) = 1.56%; σ_ (x_2) = 0.45%.
The technological norm of the parameter is 1.4%.

Based on the results of an approximate evaluation, we can conclude:

An uncontrolled process is entropy-unstable, dH / dt> 0 σ_ (x_2)>σ_ (x_1), that is, it disorganizes in time.

Quantitatively, the measure of the disorganization of the process is estimated by the positive irreversible increment of entropy ΔH = log_2⁡〖σ_ (x_2) / σ_ (x_2)〗 = 0.06, units / day and rate of entropy change ΔH/Δt=0.06/24 = 2.5 · 〖10〗 ^ (-3) unit / h

3. Within the selected time intervals, the process is not divergent.

It should be noted that the results of an approximate evaluation are obtained for a stationary process regime that is not perturbed by sharp load fluctuations (gas flow)[10].

For an accurate calculation of the entropy and the amount of information, it is necessary to know the correlation function and the spectral density of the process (Figure 5 and Figure 6). They were obtained as a result of processing the record of realizations with a confidence probability (P = 0.9).

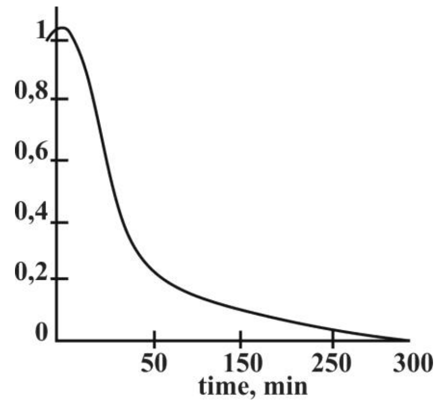

Figure3. Correlation function of the output signal of the MEAO process

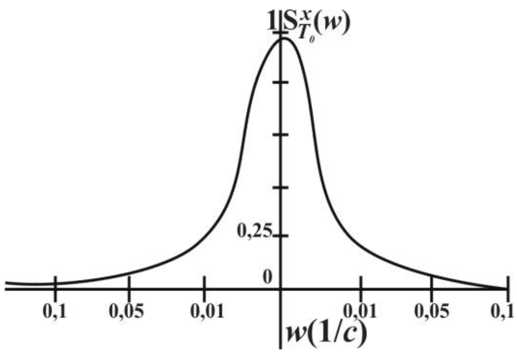

Figure 4. Spectral density of the output signal of the MEAO process

$$\rho|\tau| = 0{,}34\left(30{,}3e^{-0{,}013|\tau|}\right) - e^{-0{,}400|\tau|}, \quad (20)$$

$$S(\omega) = \frac{1}{1{,}49\cdot 10^3\omega^4 + 0{,}23\cdot 10^3\omega^2 + 1}[1/s^2] \quad (21)$$

The specified statistical characteristics of the process make it possible to calculate the information characteristics of the system for a time-quantized output signal.

The graph of the spectral density of the output signal of the MEAO process (Figure 6) is shifted to the low-frequency region and practically does not contain frequencies above F = 1 Hz. Therefore, according to Kotelnikov's theorem[11], the interval of quantization with respect to time can be taken $\Delta t = \frac{1}{2F} = 0{,}5$ s.

For the steady-state mode of the process, we determine the entropy value by one sample, the information capacity of the output signal, and the redundancy caused by the presence of a correlation[12]

$$R = 1 - \frac{H}{H_{max}} = 1 - \frac{H(y)}{H(y)_{max}} \quad (22)$$

where H (y) _max is the entropy of the signal at R = 0.

In the expression for the entropy of the signal, with limited measurement accuracy, there is an error in measuring the signal in the discriminator (Figure 3). The accuracy of the measurement of the output value is due to the sensor error and the accuracy class of the secondary instrument[13]. With a common measurement error, Δ = 2%, σ_x = 0.45, and the instrument scale l = 3, we have σ_P = 3 · 0.02 = 0.06.

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The correlation coefficient is determined from (20) for $\tau = \Delta t$ - the quantization time interval. The results of the calculations are summarized in the table 1.

Table 1.
Results of calculation of information characteristics of MEAO gas.

Correlationcoefficient*r*	Entropy per one count (two-ed.) *H*	Number of information dv./d./min. *S*	Redundancy*R*
Stationary mode			
0,89	5,12	604	0,11
Non-stationary mode			
0,81	18,3	2180	0,18

By results of calculations it can be concluded that the process is characterized by a large residual uncertainty. Strong correlation and redundancy create good prerequisites for stabilizing the process by active management. The value of the information capacity of the signal in non-stationary mode determines the lower limit of the capacity of the control loop.

IV. INFERENCE

The information characteristics of chemical-technological systems can be determined by the results of statistical processing of random functions of the output coordinates of these systems.

By the methods of information theory, it is possible to evaluate the quality of the complex technological complex as a whole, to investigate the nature of the uncontrolled flow of the process and to formulate the requirements for the throughput of the control systems of the technological objects being studied.

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