OPTIMIZATION OF THERMOOPTICAL GAS ANALYZER CHARACTERISTICS

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The operating principle is examined for a thermooptical gas analyzer. The problem of multiparametric optimization of the analyzer operating mode is solved for a mixture of nitric oxide + air.

Determination of the quantitative composition of gas mixtures is based on the measurement of some physicochemical parameter of the mixture. The more strongly the magnitude of the parameter depends on the mixture composition, the more accurately is the gas content measured therein. The difference rather than the absolute value of the mixture monitoring parameter is determined in order to increase measurement accuracy in the majority of gas analysis methods. Thus, the difference between the refractive indices of the standard gas and the test mixture is recorded in the refractometer method. The thermooptical analysis method [1] assumes the creation of a gradient in the index of refraction directly in the mixture being analyzed by the superposition of stable external fields, in time, on the volume being monitored. Their selection should be dictated by reasons of expediency. In this case, hydrodynamic and thermal fields were utilized simultaneously. Realization of the method is sufficiently simple here. The gas mixture being analyzed was set into motion along the axis of a cylindrical tube whose walls were heated. It is known that in this case [2] a fully developed temperature profile is established for a sufficiently long tube length:

$$\frac{T-T_0}{qR/\lambda}=\frac{4z/R}{\mathrm{Re}\,\mathrm{Pr}}+\bar{r}^2-\frac{1}{4}\bar{r}^4-\frac{7}{24}. \tag{1}$$

Now, if a beam is started along the channel axis, its trajectory is then determined in a cylindrical coordinate system by a system of differential equations [3]:

$$\frac{d^2\bar{r}}{d\bar{\tau}^2}-\bar{r}\left(\frac{d\theta}{d\bar{\tau}}\right)^2=-\frac{1}{2}\,\frac{\varepsilon_0-1}{T_0}\,\frac{qR}{\lambda}\,(2\bar{r}-\bar{r}^3), \tag{2}$$

$$2\bar{r}\,\frac{d\bar{r}}{d\bar{\tau}}\,\frac{d\theta}{d\bar{\tau}}+\bar{r}^2\,\frac{d^2\theta}{d\bar{\tau}^2}=0, \tag{3}$$

$$\frac{d^2z}{d\bar{\tau}^2}=-\frac{1}{2}\,\frac{\varepsilon_0-1}{T_0}\,\frac{qR}{\lambda}\,\frac{4}{\mathrm{Pr}\,\mathrm{Re}}. \tag{4}$$

As is seen from (2)-(4), the beam trajectory will depend on both the magnitude of the external force fields, i.e., on the heat flux and gas flow velocity in the channel, which enters into the Reynolds number, and on the physical characteristics of the gas mixture, which can be combined in the parameter

$$W=\frac{\varepsilon_0-1}{\lambda\,\mathrm{Pr}\,\mathrm{Re}}, \tag{5}$$

which is the ratio between the gas mixture optical and thermophysical characteristics.

Therefore, for constant external force fields the radiation characteristics at the exit from the channel with the gas mixture will be determined single-valuedly by the parameter (5), which is, in turn, associated with the gas composition of the mixture.

The measurement cuvette depicted schematically in Fig. 1 was the fundamental experimental gas analytic apparatus, which included an optical bench with a radiation source, an LG-78 laser, an apparatus to fasten and adjust the measurement cuvette and the sensor optical beam width at the exit from the cuvette or the angle of arrival. Moreover, a flow rate booster with a rheometer to feed the gas mixture to the cuvette and a stabilized voltage source to heat the cuvette walls were part of the apparatus.

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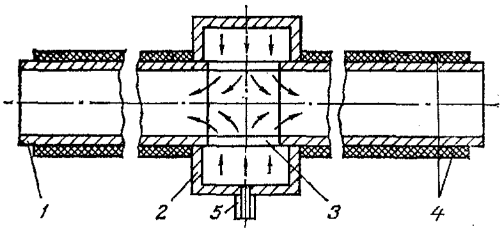

Fig. 1. Measurement cuvette: 1) cylindrical channel; 2) apparatus for gas mixture insertion; 3) porous insert; 4) heater; 5) connecting pipe.

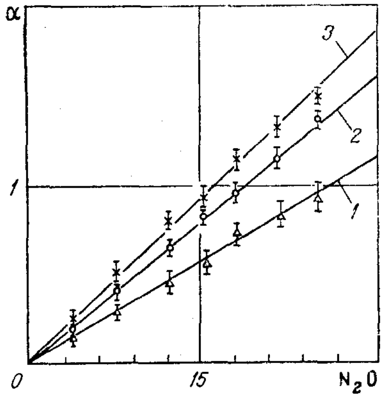

Fig. 2

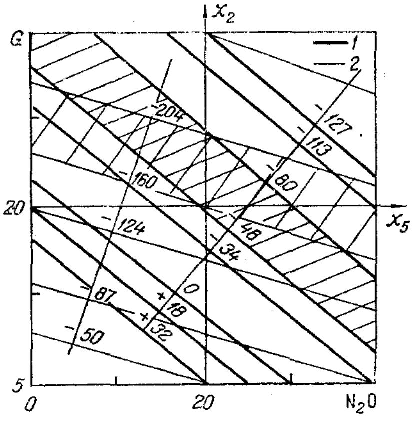

Fig. 3

Fig. 2. Dependence of the angle of beam arrival $\alpha(10^3$ rad), through the cuvette, on the composition (%) of the nitrogen oxide + air mixture for a different heating temperature: 1) $\Delta T = 45°C$; 2) 50; 3) 55.

Fig. 3. Determination of the compromise zone corresponding to 10% accuracy in regulation of the mixture flow rate and cuvette heating temperature: 1) isolines for $\partial Y/\partial x_5$; 2) for $\partial Y/\partial x_2$. G in cm³/sec and N_2O in %.

Preliminary experiments showed that the thermooptical analyzer possesses a linear characteristic in a broad band of concentrations. Results obtained for an air + nitrogen mixture in a N_2O concentration range to 30% are presented in Fig. 2, which indicate a dependence of the analyzer calibration characteristic on the cuvette heating temperature and the gas flow rate. To optimize the gas analyzer apparatus characteristics, an investigation was later performed by the method of experiment planning [4]. Selected as independent factors were: the magnitude of the cuvette wall heating temperature (X_1), the flow rate of the gas mixture (X_2), the heating temperature gradient along the cuvette length (X_3), the length of the heated cuvette (X_4), and the concentration of one of the gases in the mixture (X_5). Selected as the output parameter was the light beam width at the exit from the cuvette (Y). The factors were later made dimensionless and normalized so that the factor space was bounded by a multidimensional cube with vertex coordinates $x_i = |1|$, where

$$x_i = \frac{X_i - 0.5(X_{i\max} + X_{i\min})}{0.5(X_{i\max} - X_{i\min})}. \tag{6}$$

An almost D-optimal plan of type Ha_5 was used to describe the zone of the experiment. It is quite economical since only 27 points exist for the determination of 21 effects (the principal semireplica PFE 2^{5-1}, 10 asterisk points for $x_i = \pm 1$, and the central point).

Realization of the plan permitted obtaining an adequate second-order polynomial model

$$Y = 1074{,}85 - 73.78x_1 - 132.45x_2 - 36.28x_3 - 73x_4 - 94.9x_5 - 54{,}28x_2^2 - \\ - 36.28x_4^2 - 79.56x_1x_2 - 17.13x_1x_3 - 43.19x_1x_4 - 66.19x_1x_5 - 51.81x_2x_4 - 35.56x_2x_5 - 35.19x_3x_4 - 17.81x_3x_5, \tag{7}$$

TABLE 1. Alternative Solutions of Output Parameter Minimization

Number of the version	x_1	x_2	x_3	x_4	Y_{min}	$\frac{\partial Y_{min}}{\partial x_5}$
1	+1	+1	+1	+1	226,94	−214,5
2	+1	−1	+1	+1	830,52	−138,4
3	+1	−1	+1	−1	1025,49	−143,5
4	−1	−1	+1	−1	1094,1	− 10,9
5	+1	−1	−1	−1	1097,45	107,7

whose analysis confirms the deduction made earlier that the characteristic of the thermooptical gas analyzer is linear. Indeed, as a regression analysis showed, the square term $b_{55}x_5^2$ is insignificant. The sufficiently strong dependence of the output parameter on the magnitude of the flow rate (x_2) and the heating temperature (x_1) is also confirmed.

Let us examine the expression for the cuvette sensitivity to a change in the concentration of one of the mixture components (x_5) for which we take the derivative of (7):

$$\frac{\partial Y}{\partial x_5} = -94.9 - 66.19x_1 - 35.56x_2 - 17.81x_3. \tag{8}$$

It is easy to see that $\partial Y/\partial x_5$ depends, at first glance, on the cuvette heating temperature, the magnitude of the mixture flow rate but is independent of the cuvette length (x_4).

The strong dependence on the regime parameters naturally requires strict stabilization. In this connection, the optimization problem was formulated as follows: Find the value or range of variation of the regime parameters for which the minimum cuvette response to heating temperature changes and the mixture flow rate through the cuvette would correspond to the maximum cuvette response to the mixture composition. The solution of such a problem would permit reduction in the requirement of stability in maintaining the operating regime and would thereby simplify the apparatus and its servicing.

The minimal value Y_{min} of the output parameter of the model (7) was sought in the first step of the optimization. The search was performed by the algorithm of the dissociative-step method proposed in [5]. The results are presented in Table 1.

Comparison of the alternative solutions in the quantity Y_{min} shows that the first version has the best reading; however, versions 2 and 3 should not be discarded since they have a $\partial Y_{min}/\partial x_5$ close to first magnitude. Only two regime factors are determined reliably in this stage: $x_1 = +1$ and $x_3 = +1$. It was established earlier that the cuvette length exerts no influence on the response of $\partial Y/\ x_5$, hence it is possible to set $x_4 = -1$, which permits diminishing the cuvette length and the size of the gas analyzer as well.

The expressions for the cuvette response to changes in temperature and mixture flow rate have the form

$$\frac{\partial Y}{\partial x_1} = -73{,}78 - 79{,}56x_2 - 17.18x_3 - 49{,}19x_4 - 66.19x_5, \tag{9}$$

$$\frac{\partial Y}{\partial x_2} = -132.45 - 108.56x_2 - 79.56x_1 - 51.81x_4 - 35.56x_5. \tag{10}$$

After substituting the magnitudes of the factors found, we obtain

$$\frac{\partial Y}{\partial x_1} = -47.77 - 79.56x_2 - 66.19x_5, \tag{11}$$

$$\frac{\partial Y}{\partial x_2} = -160.2 - 108.56x_2 - 35.56x_5. \tag{12}$$

For zero responses $\partial Y/\partial x_i$, the system (11)-(12) has no solution in a factor space with boundaries $x_i = |1|$. Only a compromise solution with assumptions about the allowable magnitude of the equation parameters is possible.

Experimental determination of the mixture flow rate through the cuvette was realized with ±10% accuracy, which corresponded in the encoded variables to $\Delta x_2 = \pm 0.2$. On the other hand, it follows from (8) that the magnitude of the factor x_2 should be closer to the upper level. We assume the allowable diminution in the response $\partial Y/\partial x_5$ should not exceed 20%. This corresponds to the domain of positive values of x_2. If $x_2 = 0$-0.4, then this implies a diminution in $\partial Y/\partial x_3$ of not more than 15%. In this case the system (11)-(12) is easily solved graphically, to give the domain of allowable changes in x_2 and its corresponding concentrations (Fig. 3). The allowable interval of the cuvette temperature change is determined easily from (10): $x_1 = 1-0.35$, which corresponds to $T = 45.2 \pm 4.8°C$ in natural variables. Therefore, the operating regime found for the thermooptical gas analyzer requires ±10% accuracy in maintaining the magnitude of the flow rate and the heating temperature.

NOTATION

T, temperature; q, heat flux; R, channel radius; θ, r, z, coordinates; $\bar{r} = r/R$; ε_0, dielectric permittivity of the gas; σ, arc length; $\tau = \int_0^\sigma \varepsilon^{-1/2} d\sigma$; $\bar{\tau} = \tau/R$; λ, heat-conduction coefficient; Re, Reynolds number; Pr, Prandtl number; x_i, coordinates in factor space.

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EXISTENCE OF A CLASSICAL VARIATIONAL PRINCIPLE FOR NONLINEAR COUPLED HEAT AND MASS TRANSPORT

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Using the example of nonlinear coupled heat and mass transport, we examine whether a functional exists for which the required kinetic equations follow from the condition that the functional be stationary.

In nonlinear problems of heat conduction and coupled heat and mass transport, variational methods are widely used today. These methods are based on variational formulations of the problem, called in physics variational principles.

In the restricted sense, by a variational principle we mean the statement that a certain functional must attain a maximum or minimum [1]. This functional contains all of the defining equations and boundary conditions for the problem. Thus, the equations and boundary conditions follow from the variational formulation as conditions that the functional be stationary (the Euler equations). We will refer to this kind of variational formulation as a classical variational principle. Examples include Hamilton's principle of least action in mechanics [2], Castilyan's principle in the theory of elasticity [3], Fermat's principle in optics [4], and certain variational principles in the classical and relativistic theory of fields.

The classical variational formulations are distinguished by simplicity, generality, elegance, and are of heuristic value as well. However, attempts at obtaining these variational principles by fitting a variational equation to a problem previously formulated in differential form is difficult and not always successful. This is because many differential equations and systems of equations, especially nonlinear ones, do not have classical variational principles.

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