Mathematical model of radiation interaction with gas

O. V. Osadchuk[a], D. P. Dudnyk[a], R. V. Krynochkin[a], W. Wojcik[b], A. Iskakova[c]
[a]Vinnitsa National Technical University, 95 Khmelnitske Sh., Vinnitsa 21021, Ukraine;
[b]Lublin University of Technology, Nadbystrzycka 38A, 20-618 Lublin, Poland;
[c]Kazakh National Technical University after K. I. Satpaev, Satpaeva 22, Almaty, Kazakhstan

ABSTRACT

The paper presents a mathematical model of radiation interaction with gas. Transfer function of an optical gas concentration sensor is presented here.

Keywords: Radiation, infrared spectroscopy, absorption coefficients.

1. INTRODUCTION

Sensors can receive, record, process and transmit information about the status of various systems. It can be information about the physical condition, chemical composition, shape, location, or the dynamics of the system under study. There are various types of sensors, the principles of which are based on certain physical or chemical properties or processes.

Compact, hand-held analyzers, in most cases are implemented using non dispersive optical methods for measuring the concentration of gases in the wavelength range of 3 - 5 microns, which corresponds to the average infrared range[1]. The advantages of using optical devices of this class, compared with their counterparts based on electrochemical and catalytic principles are high speed, selectivity, resistance to harsh environmental conditions, as well as a long period of work.

Sensors are designed to determine chemical composition of gas mixture. They are widely used, due primarily to the control of combustion processes in order to save energy and reduce pollution. It is also important to control noxious gases at work and at home. In practice, to determine the concentration of gas it is necessary to have adequate mathematical model that could provide a possibility to calculate the parameters of the sensor at a design stage.

2. THE MAIN PRINCIPLES OF INFRARED SPECTROSCOPY

While developing optical gas sensors at first one has to determine transfer characteristic of an optical channel, to determine relationship between concentration of the unknown gas and the change of radiation intensity and the influence of external parameters.

Absorption is a phenomenon of losing energy of light wave passing through matter. According to the classical theory the absorption take place due to the fact that the atoms and molecules of gases have natural frequencies of oscillations which are typical to each gas, and the absorption occurs whenever the oscillation system and incident radiation are in resonance. Thus the absorption spectrum is determined by the dependence of the absorption coefficient of the substance on the wavelength of radiation that passes through the substance. The absorption coefficient determines how deeply radiation of a certain wavelength can leak into substance before it is completely absorbed. Thus the absorption coefficient depends on the chemical nature of the substance and the wavelength of radiation that passes through it [2,3].

General law determining bond intensity radiation with a wavelength λ, that has passed through a medium with the desired gas concentration C in the path length l and the spectral absorption coefficient $\alpha(\lambda)$ is called the law of Bouguer-Lambert-Beer:

$$I(C,\lambda) = I_0(\lambda)e^{-\alpha(\lambda)lC} \quad (1)$$

*gurvasia@rambler.ru; phone 0972961642

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Using (1) we express the desired concentration of gas:

$$\ln\left(\frac{I_0}{I}\right) = \alpha(\lambda) l C. \tag{2}$$

3. MATHEMATICAL MODEL OF INTERACTION OF OPTICAL RADIATION WITH GAS IN THE OPTICAL SENSOR

Any optical gas sensor contains such basic elements as the radiation source, cell, filters that produce the required spectrum, which coincides with the absorption spectrum of the analyzed substance, receiver of measured data and recording unit, which makes the selection and processing of information signal. An optical gas concentration sensor is a serial connection of the listed items.

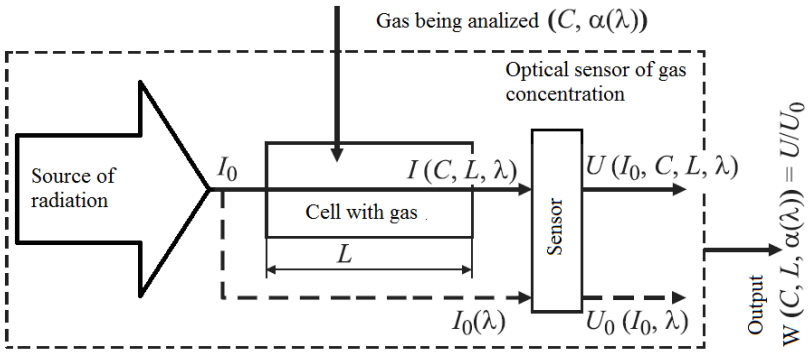

Figure. 1. Structural scheme of the optical sensor of gas concentration.

The offered scheme includes a radiation source $I_0(l)$, the area of the gas being analyzed (cell with gas) and the sensing element. While radiation passes through the gas cell it becomes modulated by gas which is being analyzed. Sensor output signal is an electrical signal $U_0(I_0, C, \lambda)$ that depends on the intensity of the incoming radiation $I_0(l)$ and concentration of gas being analyzed *C*. So to determine the parameters of concentration C, you first need to get rid of the in intensity of the incoming radiation $I_0(l)$ from the output signal $U_0(I_0, C, l, \lambda)$. Providing this we thus will remove the need to consider the effects of dispersion and loss of radiation intensity that passing borders of environments. This condition can be achieved in two main ways. The first is the use of additional "reference" channel that will contain gas, which is non-selective for the incoming radiation. Another option is to maintain the value of $I_0(l)$ on a constant, pre-known level determined prior to the measurement, i.e., the previous calibration. The difference between the output signal being exposed to input radiation that has passed through the cell without gas and the signal from radiation that has passed through the cell with gas will give us information about the concentration of the unknown gas.

$$W(C, L, \alpha(\lambda)) = \frac{I(C, L, \lambda)}{I_0(\lambda)} = \frac{U(C, I_0, L, \lambda)}{U_0(I_0, \lambda)} = \exp\left[-\alpha(\lambda) L C\right]. \tag{3}$$

The expression (2) represents the transfer function of the optical gas concentration sensor in case of monochromatic probe radiation and allows to determine the concentration of the unknown gas C. To exclude the impact parameter $I_0(\lambda)$ for an unambiguous determination of the concentration from the value of output signal as the output signal is proposed to consider transmittance function of the cell with gas.

For simplicity, you can consider not the value of the radiation intensity before and after the gas cell, but the value of the output electrical signal from sensor normalized with a certain coefficient.

The quantity $D(l,\lambda,C)$ is called the optical density of the substance. It has the properties of additivity thus optical density of mixture components for which the absorption laws are valid and which do not interact with each other is equal to the sum of the optical densities of the components, in case of constant cell length:

$$D(l,\lambda,C) = l\sum_i \alpha_i(\lambda)C_i, \tag{4}$$

where l - length of cell with gas, $\alpha_i(\lambda)$ - absorption coefficient for *i*-th component, C_i - concentration for *i*-th component.

4. DETERMINATION OF SPECTRAL GAS ABSORPTION COEFFICIENT G

The ability of gas molecules to emit or to absorb in the infrared range caused primarily by so-called vibrational-rotational mechanism of the molecules and it looks like a sequence of almost equidistant from each other spectral lines that define the amount of collisions probability between gas molecules. The spectrum of such structure is described by absorption coefficient of spectral band.

The line intensity is basically the integral of the absorbance over one line:

$$a_i = \frac{1}{cd}\int \ln\left(\frac{I_0}{I}\right)d\nu \tag{5}$$

The *cd* is the concentration distance product, *k* is the wavenumber (spatial frequency. It's easy to calculate the absorption over a bandwidth *dυ* that is wider than the linewidth[4].

To calculate the absorbance over a region that is narrower than the line itself, we need the line shape function. The usual line shape is the Lorentz function:

$$L(\nu,\nu_0,\sigma) = \frac{1}{\pi}\cdot\frac{\sigma_i}{\sigma_i^2 + (\nu-\nu_0)^2} \tag{6}$$

The absorption coefficient of spectral band and under normal conditions is described by the Lorenz function and is expressed by the sum of the coefficients of individual lines:

$$\alpha(\nu) = \sum_{i=1}^{\infty}\frac{a_i}{\pi}\cdot\frac{\sigma_i}{\sigma_i^2 + (\nu-\nu_0)^2}, \tag{7}$$

where ν_0 - resonant frequency, which is independent of pressure or temperature; a_i - line intensity; σ_i - half-width of the line that has temperature dependence proportional to $1/\sqrt{(T/T_0)}$, where T_0 = 296 K.

To calculate this ratio we have to choose the contour of vibrational-rotational bands. However, taking into consideration the lack of knowledge about the individual characteristics of the individual lines to calculate the absorption coefficient a method of approximate models of the spectra is usually used, which describes the assumptions about the nature of the line location in the band intensity. The most common are such models as the Goody model and Elzasser model. The Elzasser model provides equal intensities of lines a_i, half-width σ_i and the distance between the lines b.

While adopting Elzasser model and assuming that the absorption coefficient to be described by the Lorentz function, but not including the broadening of the line, we can determine the impact of temperature and pressure.

The value of the half-width of the spectral line at pressure P and temperature T can be written as:

$$\sigma(P,T) = \sigma_0\cdot\frac{P}{P_0}\cdot\left(\frac{T_0}{T}\right)^n, \tag{8}$$

where - half-width of the line at normal pressure P_0 = 1 atm. and temperature T_0 = 296 K, n - temperature coefficient[5].

The dependence of the line intensity on temperature and pressure take the form:

$$a_i = a_{i0} \cdot \left(\frac{T_0}{T} \right)^q \cdot e^{\frac{E}{k} \cdot \left(\frac{T - T_0}{T T_0} \right)}, \tag{9}$$

where a_{i0} - line intensity at $T_0 = 296$ K i $P_0 = 1$ atm., q- temperature coefficient, k - Boltzmann constant, E - energy of the lower energy state.

To determine the parameters ν_0 and a_i international databases HITRAN can be used, and the value of the line width is determined from the experimental spectra of gases absorption based on PNNL laboratory data.

Using this approach a graphically designed impact of ambient temperature on the absorption coefficient of CO_2 gas is presented in Fig. 2.

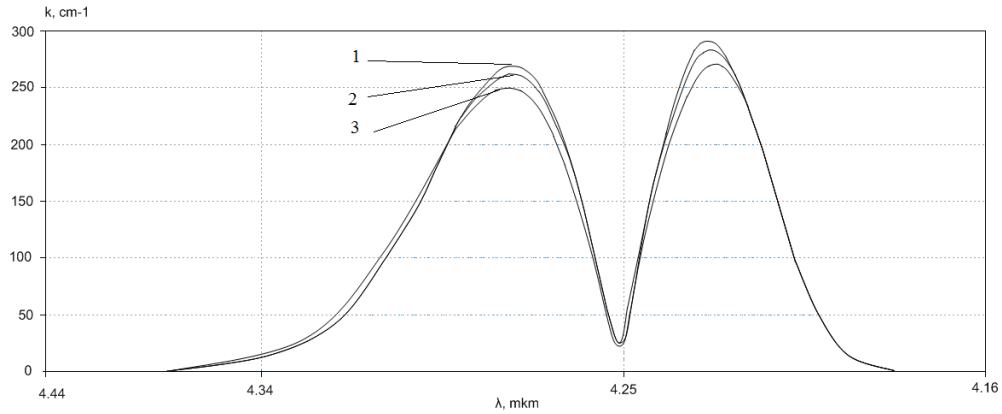

Figure 2. Changing the CO2 absorption coefficient with temperature: 1 – 286 K; 2- 296 K; 3 - 310 K.

CONCLUSION

This work represents both development and the synthesis of the mathematical model of radiation interaction with gas, which can be used to calculate the transmission characteristics of sensors to determine gas concentration, help to assess the expected accuracy and consider the impact of most common external factors such as temperature and pressure. The results of calculations of temperature and pressure effect on the absorption coefficient of CO_2 gas are shown.

The mathematical model can be used as a quality instrument at the early stage of development of optical sensors for different purposes.

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