

Spectrometer for Toxic Gases Detection with Pyroelectric Multispectral Detector

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Abstract:

The aim of the paper is to present results of design spectrometer for toxic gases detection with pyroelectric multispectral detector. Sensing of toxic gases is very important in many applications. Automotive, defense, aerospace, agriculture, chemical industry, medicine, environmental, food and drink are many important markets for chemical and biological sensors. Principle of designed spectrometers is the interaction of the infrared radiation with studied gases. In the case of photon absorption, we are talking about infrared absorption spectroscopy. In our case, near-infrared spectrum is used.

Anotace:

Článek se zabývá návrhem spektrometru pro detekci plynů s pyroelektrickým vícespektrálním detektorem. Detekce toxických plynů je velmi důležitá v mnoha oblastech jako v automobilovém, leteckém, chemickém a potravinářském průmyslu, zemědělství, lékařství, životním prostředí. Navržený spektrometr je založen na principu interakce plynu a infračerveného záření. V případě absorpce fotonu mluvíme o infračervené spektrometrii. V našem případě je využito blízké infračervené spektrum.

INTRODUCTION

Molecular spectroscopy is an important class of spectroscopic methods, which can be used for analysis of organic and inorganic substances. The essence of spectroscopic methods is monitoring of the interaction of radiation with an unknown substance for the purpose of its identification, studying its structure or to determining its concentration. Infrared spectroscopy is based on the absorption of infrared radiation by molecules of substances.

Total energy of molecule is increased by the absorption of a photon and molecule passes into excited state. The energy difference between the excited energy level E_i and basic energy level E_j must be equal to the received quantum radiation according to the equation

$$E_i - E_j = h \cdot \nu \quad (1)$$

where h is Planck constant and ν is frequency of radiation. The absorption of radiation is reflected by a change in the charge distribution of the molecule in the excited state (change in the dipole moment of the molecule). The absorption of electromagnetic radiation is accompanied by a change vibrational and rotational state of molecule. Amount of nearby potential energy of electron transitions in molecules is large. This means that we do not differentiate rotational and vibrational lines, but we view them as band. These bands are characteristic for each molecule in a certain wavelength region. [1, 2]

IR spectroscopy is utilized in the analysis of trace impurities in the pure gases well as in the analysis of gaseous mixtures concentrated in industry and the environment. It is typical for gaseous samples that in the spectrum vibrational and rotational transitions are clearly observable. Wave number of spectral bands is not shifted due to environment. Both properties are the result of low gas density and consequently gas molecules are not influenced by the surrounding molecules. The spectrum of gaseous mixtures is simple sum of individual constituents [3].

While qualitative analysis determines what substances are found in the sample, quantitative analysis determines the amount of substances. For quantitative evaluation the Lambert-Beer law is used

$$A = \varepsilon \cdot c \cdot l \quad (2)$$

where A is the absorbance, c is the concentration, l is the pathlength and ε is the molar absorptivity [1, 2]. For the absorbance we can write

$$A = \log \left(\frac{I_0}{I} \right) \quad (3)$$

where I_0 is the intensity of the light entering the sample, I is the intensity of the light transmitted by the sample [1].

DESCRIPTION OF THE SPECTROMETER

The designed spectrometer was designed for detection of hydrocarbons (HC), carbon monoxide and carbon dioxide. The spectrometer is composed of the four-channel pyroelectric detector InfraTec GmbH with temperature compensation, MEMS infrared source, multiplexer and differential amplifier. Figures 1, 2 show designed spectrometer. Modulation frequency of infrared source is 3Hz because of the use pyroelectric detector. Gas is pumped into the cuvette by a micropump. Each sensor of the detector (Fig. 3a) is provided with a filter in the absorption band of the gas. Tab. 1 shows detected gases and used filters and Fig. 3b) their transmission spectra. Reference channel serves for correction of radiation fluctuation. Signals for each channel are switched by multiplexer and amplified with shift of DC level to 1,5V for processing by microcontroller.

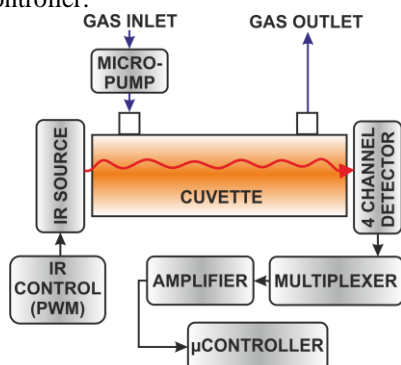


Fig. 1: Block diagram of the spectrometer

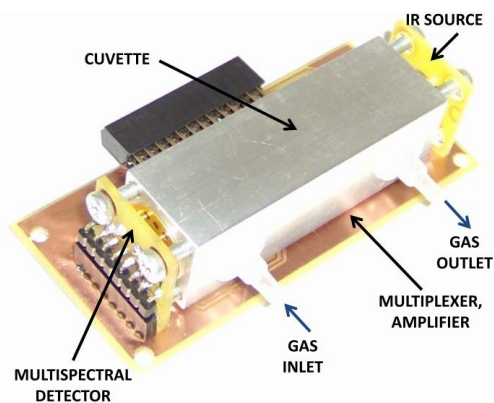


Fig. 2: Realized spectrometer

Tab. 1: Detected gases and filters

Gas	Filter-center wavelength/bandwidth
CO	4.66 μm / 180nm
HC	3.40 μm / 120nm
CO ₂	4.26 μm / 180nm
Reference	NBP 3.95 μm / 90nm

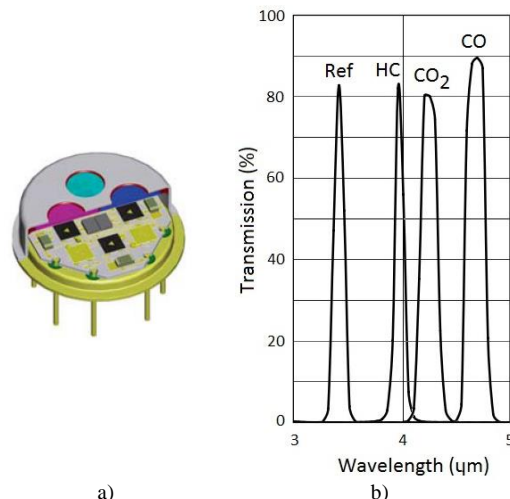


Fig. 3: Four-channel spectrometer a), transmission spectra of filters b) [4, 5]

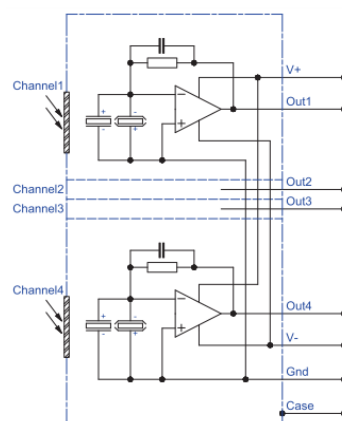


Fig. 4: Electrical circuit of multispectral detector [5]

RESULTS

The designed spectrometer was exposed to different concentration of different gasses in designed measuring apparatus (see Fig. 5). The tested gas was obtained by scrubbing in a bubbler with the measured substance and was mixed with the carrier gas by a mass flow controller to achieve the desired concentration. This mixed gas is forced in a spectrometer. The whole process is controlled by a PC.

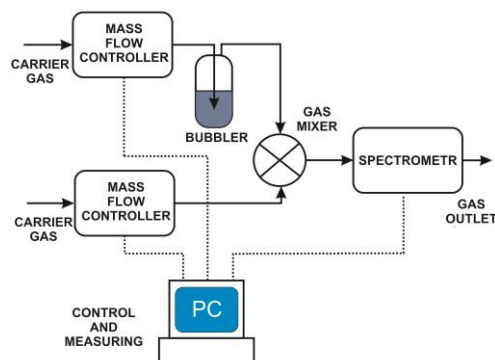


Fig. 5: Block diagram of measuring system

The following figures represent relationship between voltage from detector and concentration of CO₂ (Fig. 6) and absorption of hydrocarbons at concentration 5000ppm and 10000ppm (Fig. 7).

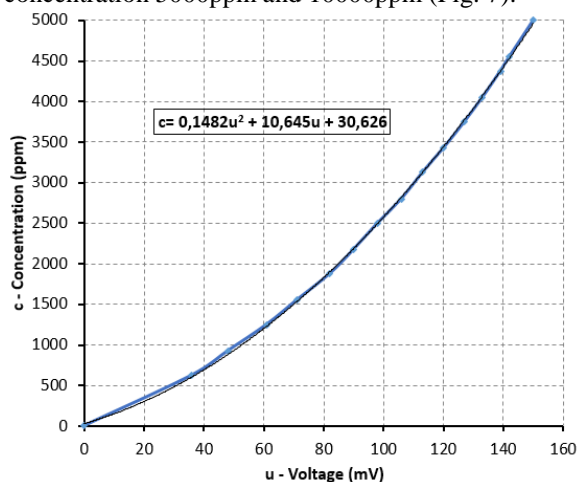


Fig. 6: Relationship between voltage from detector and concentration of CO₂

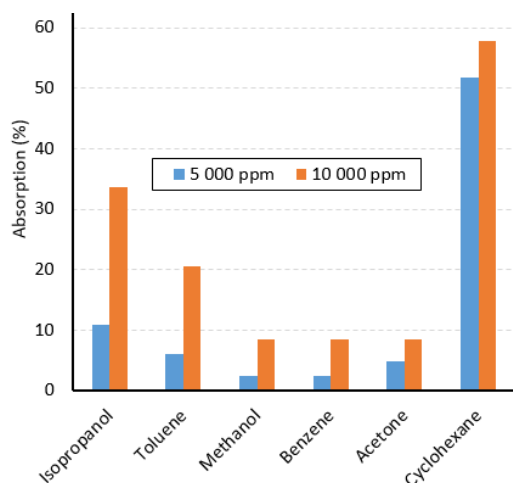


Fig. 7: Absorption of hydrocarbons at 5000ppm and 10000ppm

CONCLUSIONS

In this paper was described spectrometer for detection of toxic gases (CO, hydrocarbons, CO₂) with pyroelectric multispectral detector. It is possible to determine the concentration of several percent. Advantage of the spectrometer are good selectivity and stability over time during the measurement.

ACKNOWLEDGMENTS

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