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Features of ion mobility spectrometry hardware-software complex

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Abstract. The ion mobility spectrometer (IMS) is a complex hardware and software device for gaseous analysis. The article describes bipolar IMS control system. The paper lists the main requirements in electronic units, the modes of their operation, the ranges of normal operation and the algorithm for handling emergency situations. The main electronics include: a unit for collecting and processing spectrometric data, an ion source control unit, a gate control unit, high-voltage generators, an ion mobility spectrometer control and synchronization system. The structure of additional electronics includes: control unit of actuating devices, air conditioning system, self-diagnostics and protection system. This article may be useful to designers of complex electronic analytical systems.

1. Introduction

The key task in design of modern inspection equipment is the detection of ultra-low trace amounts of explosive, narcotic, toxic [1-4] and other hazardous substances is. Nowadays there is an active fight against smuggling of drugs and explosives. Moreover, there is a need for simultaneous detection of substances of various classes in a number of tasks [5, 6]. Thus, one of the crucial requirements of modern inspection technology is the simultaneous detection of a wide range of substances.

Currently, following methods are most frequently used for the detection of prohibited substances: chromatography [7, 8], mass spectrometry [9] and ion mobility spectrometry (IMS) and detection by trained dogs [10-15]. The method of ion mobility spectrometry allows you to collect sufficiently complete information about the composition of impurities in a gaseous medium, with relatively small size, equipment weight and energy consumption requirements. On the basis of their characteristics, ion mobility spectrometers are considered the most promising and versatile class of instruments in inspection systems. Therefore, ion mobility spectrometers are widely used in electronic checkpoints in enterprises [16–18].

The principle of IMS is based on the separation of ions by time of flight in a gaseous medium in a constant electric field. The resulting time-of-flight spectrogram, in which the peaks of substances can be distinguished, characterizes the presence of ions with a certain mobility. The magnitudes of the mobility of the ions of the test substance, reduced to standard values of temperature and atmospheric pressure, make it possible to identify the composition from tabular values recorded in the database of substances of the instrument.

The purpose of simultaneous detection of substances of different classes requires joint detection of ions of both positive and negative polarity. Therefore, the task of developing a bipolar high-resolution

ion mobility spectrometer for the express detection of ultra-small quantities of substances and its control system is a topical issue.

2. Experimental equipment

The electrical circuits in the device of the ion mobility spectrometer can be divided into two groups - main and additional electronics. Within the main electronics category the following are included: a collection unit for processing spectrometric data, a unit for the control of the ion source, a gate control unit, high voltage generators, a control and synchronization system of the ion mobility spectrometer. The category of additional electronics includes the following: a control unit for executive devices, an air conditioning system, as well as a self-diagnosis and protection system.

The synchronization system provides the generation of pulses with a given time structure within the scope of the spectrometric cycle. The sequence of events is shown in Figure 1.

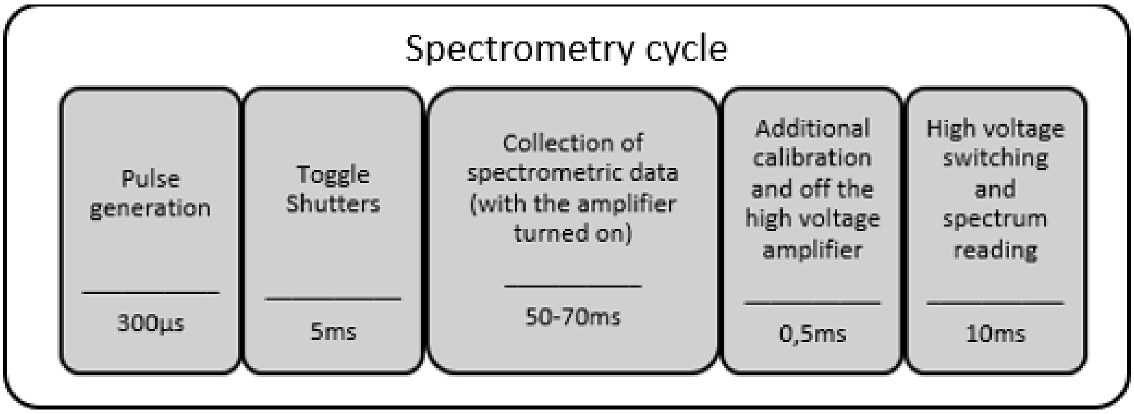

Figure 1. Structure of the spectrometric cycle.

The spectrometric cycle begins with the process of generating corona pulses, which continue for 300 µs. After that, the ionic gates begin their work, which are capable of moving, stopping and injecting the ionic clot, depending on the given algorithm. Further, the ion current amplifier is turned on and the collection of spectrometric data occurs (spectrometry). The recording of spectrometric data requires accurate and stable timing for 50-70 ms. After the process of ion mobility spectrometry, the amplifier is turned off and another high voltage level calibration is performed. Then the high voltage polarity is switched for a duration of 10 ms and the spectrometric cycle starts anew. Thus, the basic requirement for a synchronization system is the exact observance of time intervals.

The main requirements of additional electronics are the compatibility of the parameters when operating with the current system, the flexible tunability of the units, the ability to perform diagnostics, as well as self-testing and protection of electronic units.

Since in the classical system each controller was responsible for controlling each unit with its own unique address, then to implement compatibility with such a system it is necessary to leave the logical level unchanged, that is, to apply virtualization of controllers (Figure 2). More powerful hardware resources of the current system allow to combine several controllers into a single more efficient one.

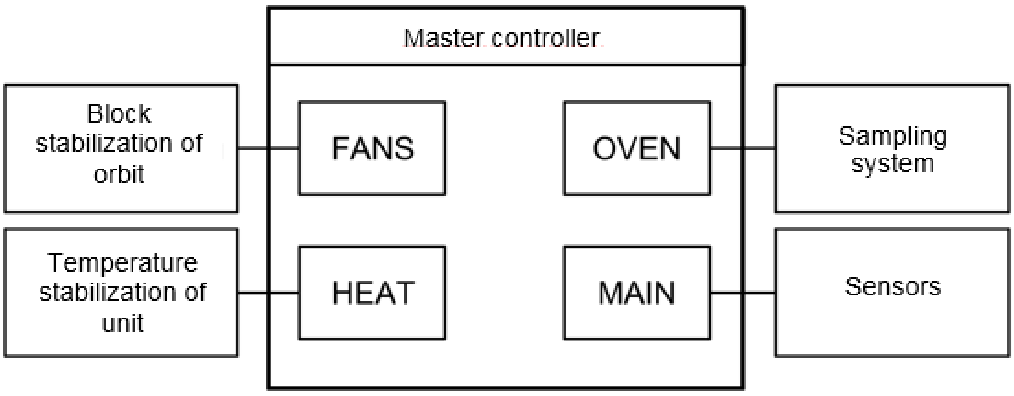

Figure 2. Block diagram of the structure of the master controller.

3. Generation of control signals for the collection of spectrometric data, ion source and gates

The structure of the spectrometric data acquisition unit is shown in Figure 3. To integrate the received data, an accurate countdown is required to avoid distortion of the spectrogram along the horizontal time axis. Therefore, for timing the system of the digitization of spectrometric data is used a timer (TIMER).

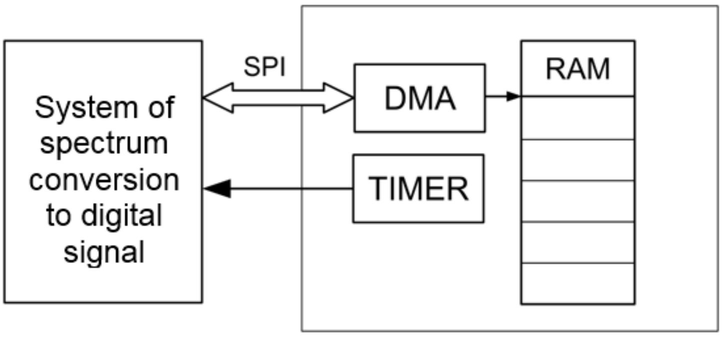

Figure 3. The unit for collecting of spectrometric data.

The IMS data is received via the SPI interface using the Direct Memory Access (DMA) controller. This allows for the increase of the performance of the controller by means of using hardware. The construction of the spectrometric data acquisition unit is shown in Figure 4.

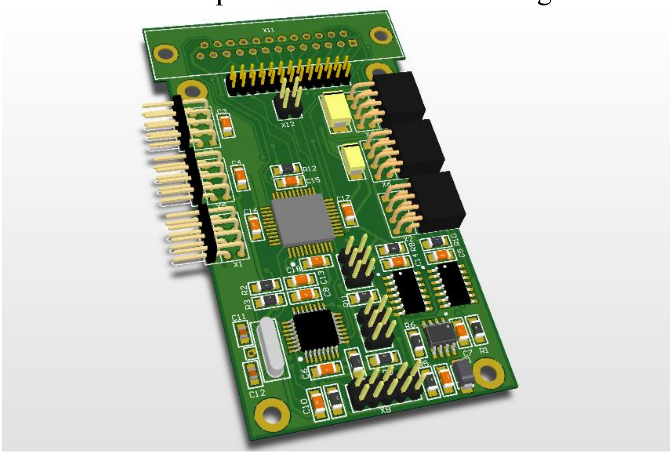

Figure 4. Design of the collection unit of spectrometric data.

To improve the detection parameters, it is necessary to create certain conditions in the ionization chamber so as to maintain the set temperature, humidity, pressure, among other parameters. Therefore, a number of sensors are installed inside the device, which must be cycled. The device makes use of digital sensors of temperature, pressure, humidity and other values with an I2C interface. This interface is used in order to save hardware because only one microcontroller is necessary for the control of a whole set of devices and the serial data bus for communication uses only two bidirectional communication lines (SDA and SCL). Additionally, the standard provides for "hot" connection and disconnection of devices during the operation of the system. The structure of the unit for sensor questioning is shown in Figure 5.

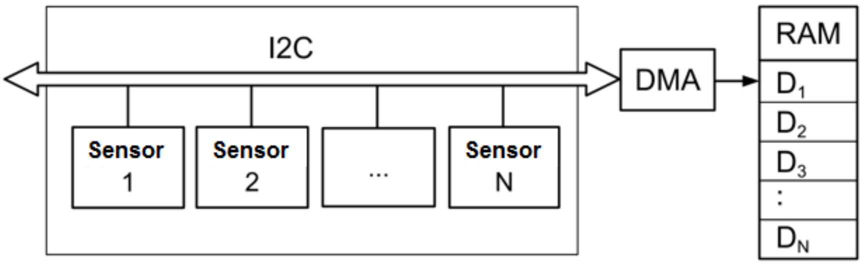

Figure 5. The structure of the unit for sensor questioning.

The controller of the direct memory access (DMA) allows to transmit information that is received from the sensors, bypassing the processor. The use of this mechanism can significantly heighten the transmitting capability and increase productivity. For this is sufficient to take the initial measure: to determine the type of transmission, provide the initial address and size of the data massive.

As in the system are used sensors of differing types, it is necessary to work out an algorithm of the data gathering and a system of the parameters for the microcontroller. The set of the parameters is given in Table 1.

Table 1. Setting parameters for the information gathering of sensors.

Sensor number	I2C Address	Qty. of bytes	Address of memory	Type
1	0b10011000	2	(u32)&Temperature3	1
2	0b10010100	2	(u32)&Temperature4	1
3	0b10011100	2	(u32)&Heater1_Temperature	1
4	0b10011010	2	(u32)&Heater2_Temperature	1
5	0b01010110	4	(u32)&Temperature1	2
6	0b01010110	4	(u32)&Humidity1	3
7	0b01010010	4	(u32)&Temperature2	2
8	0b01010010	4	(u32)&Humidity2	3
…	…	…	…	…

The given table of parameters is loaded into the microcontroller. The algorithm consists of the following sequential actions:

- Controller for the direct access to the memory counts the given quantity of bytes by the I2C address.
- The sensor type determines the formula by which are worked out the gathered data.
- Further, the information is recorded by the indicated address of the operating memory.

The electronic subsystem, coming into the components of the equipment, contains a multichannel temperature stabilization unit, which fulfills the following functions:

- Providing of the temperature mode of the sampling device.
- Providing of the temperature mode of the ionic source and gas channel of the sample input.
- Providing of the temperature mode.

Multichannel of the stabilization of temperatures allows providing for the even heating of the various zones of the. In the system are used a total of 9 temperature stabilization channels. For each channel are used separate settings of maximal power (maximal – of the controlling signal, entering the, fulfilled on the basis of the field transistor) and required temperature.

The control devices are divided into three units: heaters of the drift region, heaters of the, pumps. Each unit contains within itself the required quantity of devices and settings.

Air pumps are used for the formation of gas currents in the drift area and during the sample input. The unit for the regulation and stabilization of rotations has the following settings: work mode, starting PWM and the required speed of rotation (rot/min).

4. Monitoring of the parameters of the functioning of the ion mobility spectrometer and protection of the electron units

For the precise detection of substances and elimination of the chance of false alarms is necessary the constant control of an array of parameters and cyclical questioning of the ion mobility spectrometers.

Parameters of the equipment can be divided into several classes:

1. parameters used in ion mobility spectrometry (pressure, temperature, et al);
2. parameters determining the workability of the equipment (humidity, speed of gas currents, et al);
3. parameters of protection.

Monitoring of the atmospheric pressure of the surrounding air allows to provide correcting coefficients in the data processing program, allowing to detect substances by the data introduced into the database outside of the dependence from weather-climactic conditions.

For the channel of sample transfer and drift area the optimal temperature is 100 °C and more. This is provided for by the fact that under such temperatures the main substances under analysis weakly absorb onto inner surfaces, which provides for small losses, fast cleaning and good dynamic properties during the detection of the probe.

The charge of an ionic bunch can be estimated when the area under the spectrum of the ion current spectrum is calculated. This value affects the signal-to-noise ratio, and hence, the detection accuracy.

The device periodically conducts a self-test to check the operability and protection of electronic components. Most parameters have a range of normal operation. If you exceed the range and reach a critical value, you must take the appropriate action. These parameters are given in Table 2.

Table 2. The ion mobility spectrometer protection parameters.

Parameter number	Parameter name	Nominal value	Critical value
1	Consumption current	8 A	14 A
2	Current consumption of high-voltage unit	70 mA	200 mA
3	Current consumption of heaters per channel	1.5 A	2.5 A
4	Value of high voltage	2.2 kV	2.6 kV
5	Voltages on the collector grid	85 V	100 V
6	Temperature of the sampling device	200 °C	230 °C
7	Temperature of heaters	100 °C	115 °C

In dependence of the rank of the event, the executive controller can undertake the following actions:

- signalize to the main program about the mistake;
- block the channel;
- disconnect the device;
- completely turn off the equipment.

5. Conclusion

The article describes control system of bipolar high-resolution ion mobility spectrometer for the express detection of ultra-small quantities of substances. System includes universal microcontroller, multi-threaded control system for electronic nodes of the ion mobility spectrometer with fast polarity switching. The paper presents the algorithms for the operation and interaction of the electronic components of a bipolar ion mobility spectrometer, allowing to increase the detection efficiency of substances.

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