Prospects for the use of security air flow to prevent ion-molecule reactions in the ionization and drift zone in classical IMS

A V Golovin, N V Makarova, A A Poturuy and V V Beliakov

National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe shosse 31, 115409 Moscow, Russian Federation

Corresponding author e-mail address: avgolovin@bk.ru

Abstract. The effective transfer of sample problem is relevant in modern analytical equipment. The paper considered a problem in detection trace concentrations of explosives by Ion Mobility Spectrometry (IMS). The investigation deals with sample adsorption on the walls of transport tubes, the ion drift chamber and the chamber of the ion source in ion mobility spectrometer. The sample losses on inlet channel surface and diffusion through penetrable gas channels are comparable with the quantity of sample itself at the sensitivity level of 10-14 g/cm³. The trinitrotoluene (TNT) sorption in different channel materials depending on their sorption properties is analyzed. A new approach preventing sorption of the substance on the chamber walls by security airflow is presented. The study includes gas flow simulation and experiments of protective gas flow setup.

1. Introduction
Ion Mobility Spectrometry is a widely used method for the detection of explosives and narcotics [1-4]. The method is characterized by the ability to separate ions of isomers, high speed of detection and high level of sensitivity, as well as the combination of usability and low cost. However, the construction of spectrometers has vulnerabilities such as "dead space" problem and adsorption of contaminating substances on the internal surfaces. The gas sample passes through the ion mobility spectrometer (Figure 1), can be adsorbed on the walls of transport tubes, the ion drift chamber and the chamber of the ion source [5-7]. The simulation of gas flow in the chamber of the ion source is considered. It is developed the regulation and diagnostic equipment for the formation of gas streams. A new approach preventing sorption of the substance on the chamber walls by security airflow is presented.

2. Modeling
It is solved an aerodynamic equation for 2D and 3D models of the ion source chamber. The simulation of gas flows is analyzed into the ion source chamber using Comsol Multiphysics package. The equation describes sample transfer probe through a finite volume without mixing gas streams (Figure 2-3). The test substance it is not adsorbed on the walls of the ion chamber due to clean air flow, which ensures the purity of ion drift region and significantly increases the durability of the device and the accuracy of detection of trace explosives and narcotics concentrations. The effect is achieved by using an automated apparatus for experimental testing, including air handling unit, which prevents the gas flow of the substance in contact with the chamber walls.
Experimental testing shows that the system of formation of the gas flow runs successfully. The device allows reducing the pollution of ion source chamber and provides the effective transport of substance flow.

Figure 2. The two-dimensional simulation of gas flow in ion source camera with a complex shape, structure excluding guard stream (left). The two-dimensional simulation of gas flow in ion source camera with complex shape, structure with guard stream (right).

3. Prototyping
The automated device is developed for experimental testing (Fig. 4) including an air flow control unit which does not allow to contact the gas flow of the test substance with the chamber walls.

Figure 3. Structural scheme of a test setup for the study of sample tubes. The airflow diagnostic is performed by an optical method.
The simulation results confirm the effectiveness of the changes in the sample chamber of the ion source configuration. Original structure airflow test particles are adsorbed on the walls of the ion chamber; the system is contaminated and require cleaning, or reduced accuracy in determining the composition of substances. It is, therefore, necessary to develop a system that improves the accuracy and selectivity of the instrument in the analysis of ultra-small quantities of substances. Such a system is an improved structure of the ion source chamber. Due to protection of the flow of clean air test substance, it is hardly adsorbed on the walls of the ion chamber, which ensures the purity of ion drift region and significantly increases the durability of the device and the accuracy of measurements.

4. Experimental data and results
In the first experiments on the creation of a system of formation of the gas flow problem transferring the sample of the test substance over the final volume. The sample did not reach the end of the tube due to the low flow rate. This problem has been eliminated thanks to the selection of the optimum fan speed.

Optimized speed: \( V_{\text{in put}} = 7000 \, \text{rev/min}, V_{\text{out put}} = 11000 \, \text{rev/min} \).

At sufficiently low gas flow rates, the flow is always laminar, but with an increase in speed, it is always a transition to turbulent flow, which is time-dependent and spatially inhomogeneous. The speed of the liquid particles, pressure and other characteristics of the medium are changed in time and space randomly even under constant environmental conditions.

In the experiment by asking a different fan speed, installed on the inlet and outlet of ion drift chamber, manages the primary and secondary air flow, resulting in the separation is achieved introduced air samples and walls of the experimental tube. The flow is laminar. The fans are controlled by the PWM signal from the microcontroller. Results of experimental studies conducted in this work are interesting for further optimization of the ion mobility spectrometer.

5. Conclusion
It is necessary to develop a system to prevent leakage of ion-molecule reactions in the drift zone which increases the accuracy and selectivity devices, ensure purity ion drift region and significantly increase the durability of the device and accuracy. The simulation of gas flows in the chamber of the ion source using the package Comsol Multiphysics. The study developed an automated apparatus for experimental testing, including an air-handling unit which does not allow the gas flow of the substance in contact with the chamber walls. Diagnosis airflows provided by the optical method. In the drift, the chamber is created by the counter ions flow of dehydrated and purified air to prevent leakage of ion-molecule reactions in the drift zone. This stream is formed in a closed air circulation system, including the pump and adsorption trap filled with molecular sieves. The task of sample transfer through a finite volume without mixing gas streams has been solved for 2D and 3D models of the ion source chamber. Results of experimental studies are presented in the paper are interesting for further optimization of the block sampling and testing sample ionization.
The effective transfer of sample problem is relevant in modern analytical equipment. The paper considered a problem in detection trace concentrations of explosives by Ion Mobility Spectrometry (IMS). The investigation deals with sample adsorption on the walls of transport tubes, the ion drift chamber and the chamber of the ion source in ion mobility spectrometer. The sample losses on inlet channel surface and diffusion through penetrable gas channels are comparable with the quantity of sample itself at the sensitivity level of 10-14 g/cm³. The study includes gas flow simulation and experiments of protective gas flow setup.

Acknowledgements
This work was supported by the Competitiveness Program of NRNU MEPhI.

References
[1] Eiceman G A, Karpas Z and Hill H H 2013 Ion Mobility Spectrometry (3rd ed.). (Taylor & Francis Group) p 45-48
[2] Samotaev N, Golovin A, Vasilyev V, Malkin E, Gromov E, Shaltaeva U, Mironov A and Lipatov D 2014 Lecture Notes in Electrical Engineering 268 p 447-451
[3] Laakia J, Kauppila T J, Adamov A, Sysoev A A and Kotiaho T 2015 Talanta 132 889 - 893
[4] Chernyshev D M, Frolov I S, Frolov A S, Mukhanov M S and Sysoev A A 2011 Journal of analytical chemistry 66(13) 5-9
[5] Pershenkov V S, Tremasov A D, Belyakov V V, Razvalyaev A U and Mochkin V S 2006 Microelectronics Reliability 46 641-644
[6] Pershenkov V S, Razvalyaev A U and Tremasov A D 2006 Proc. 25th Int. Conf. Microelectronics (Belgrade) (Art. no. 1651051) p 689-692
[7] Samotaev N, Pershenkov V, Belyakov V, Vasilyev V, Golovin A, Ivanov I, Malkin E and Gromov E 2014 Procedia Engineering 87 436-439