Electric Modeling of Charged Particles Trajectories in the Drift Tube of Ion Mobility Spectrometer for Hazardous Industrial Chemicals Detection

Nikolay Samotaev*, Vecheslav Pershenkov, Vladimir Belyakov, Valeriy Vasilyev, Anatoliy Golovin, Igor Ivanova, Evgeniy Malkin, Evgeniy Gromov

*Micro- and Nanoelectronics Department, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe highway 31, Moscow 115409, Russia

Abstract

The problem of hazardous industrial chemicals ions separation with close mobility by IMS method has identified the need of design and drift tube electrical parameters modeling to ensure the ion transport. A simulation of IMS drift tube electric field was performed and the trajectories of the ions in the region of ionization source electrodes, in the ionization region and in the drift region of IMS tube was shown. Obtained results have allowed to estimate influence of inhomogeneity of the field in the drift region on the resolution of the ion mobility spectrometer, as well as to make changes in the parameters of the tube to minimize this impact. Based on the performed modeling have been identified best constructive decisions for the manufacture of drift tubes. On the manufactured drift tube been successfully carried out the experimental detection of hazardous industrial chemicals.

1. Introduction

Main focuses of application for IMS device is detection of explosives (TNT, PETN, RDX, TATP, NG, EGDN and others), identification of narcotics (Heroin, Cocaine, Amphetamine, Methamphetamine, Tetrahydrocannabinol, and others), detection hazardous industrial chemicals (SO₂, NO₂, Cl₂, NH₃ and others) and diagnostic of human

* Corresponding author. Tel.: +7-925-585-8273; fax: +7-499-324-2111.
E-mail address: nnsamotaev@mephi.ru
illness by breath test technology (Volatile organic compounds) [1]. Typical IMS drift tube structure is shown on Fig. 1a. Drift tube consists of ionization chamber, ion source, electrostatic gate, drift tube and collector with signal amplifier. One of the most important IMS part is ion source. Ionization source affects the sensitivity and selectivity of the spectrometer. The second most important part in the IMS device is the drift tube. Parameters drift tube gives resolution and the warm-up time of the device. The lighter the drift tube mains faster warm-up IMS device and reduce power consumption. The longer drift tube hence high resolution. The third most important is sample system. Sample system is most sensitive to the type of application and one construction depending on the type of the detected substance (volatile, liquid or solid components) [2, 3].

Current our work focused on modeling electric fields and trajectories of charged particles in the areas of ionization and drift of ion mobility spectrometer. Design of ion mobility spectrometer requires electrical modeling of the ionization chamber and the drift tube. To ensure losses of an ion current on the way from ion source to collector, geometrical and electrical parameters straw should correspond to the estimated model. For full gathering formed in the ion source is required to calculate the field and set an exact geometrical and electrical parameters, since the distribution density of ions across the collector electrode depends on the density of electrons in the ion source. For calculation of constructive solutions requires the development of mathematical and physical models of the motion of ions and modeling of the processes occurring in the drift tube of ion mobility spectrometer.

2. Modeling

The modeling was carried out with the help of the software, based on the solution of system of equations of Laplace. The calculation principle is to present plot of drift region in the form of a resistive structure, forming a homogeneous region, and setting the initial values of potentials in accordance with geometric dimensions. The potential values for all nodes are calculated by law Kirchhoff, after the construction of equipotential surfaces.

Fig. 1. (a) Structure of IMS device and direction of gas flow and ion flux movement in drift tube; (b) Visual model of the ions movement in ionization chamber.

Along the axis of the drift tube longitudinally located electrodes with linearly varying potential is formed by a homogeneous electric field. Uniformity of field depends on the dimensions and location of the electrodes. The unevenness of the field leads to the fact that the flight time of the ion depends on the distance to the tube central axis. Because of the uneven fields ions of one substance arrive at the collector at different times, that is reducing resolution of IMS (visual model and assembled drift tube is presented in Fig.2b).

The ion source consists of the sharp electrodes placed on the carrier insulating substrate. It generates a bunch of charged particles in the form of a disk with a diameter of 4 mm and thickness of 1.5 mm, with adjustable time of corona discharge burning. The simulation shows that the motion in the electric field of ionization chamber electrode system transforming the ions bunch form. At the shutter grids its diameter is 8 mm. Visual model of the ions movement is presented in Fig.2a.
Simulations of the electric field dependence of the uniformity in the drift region from the ratio of the electrodes geometric parameters shown in Fig.3. Electrodes drift tubes are made of aluminum or stainless steel rings that form a cylindrical channel transport of ions with diameter from 8 to 24 mm in determining this construction is the width of the electrodes and the thickness of the dielectric gasket between the electrodes used for formation of the closed pressurized volume. To minimize the possibility of uncontrolled accumulation of charge on the dielectric surfaces and improve the uniformity is required to minimize the thickness of the strips, but the reduction is limited to mechanical and electrical strength of the material.

![Fig. 2. (a) Visual model of the ions movement in drift tube; (b) Photo of assembled drift tube.](image)

It is shown that on the distance from the electrode is larger than the width of the electrode, the heterogeneity of the field does not exceed 1%. Defined by the ratio of the geometric parameters of electrodes for the existing pipes, which allowed to achieve the inhomogeneity of the field, less than 1% in the central region diameter 8 mm, this has led to the improvement of the resolution of the spectrometer compared with the earlier design and allowed us to separate the ions with the values of mobility ($K_0$), characterized by less than 1%.

![Fig. 3. (a) diameter 24 mm, width 8mm; (b) diameter 16 mm, width 8mm; (c) diameter 8 mm, width 8mm;](image)

The obtained results have allowed to estimate influence of inhomogeneity of the field in the drift region on the resolution of the spectrometer ion mobility, as well as to make changes in the settings of the tube to minimize this impact.
3. Experimental

In the course of the research assessed the possibility of different TIC detection (SO$_2$, NO$_2$, Cl$_2$), including joint. First experiment was conducted on detection of Cl$_2$ concentration $3 \times 10^{-9}$ g/cm$^3$ and higher, IMS spectra is shown in Fig.4a. Another experiment was conducted on joint detection of SO$_2$ concentration $2.81 \times 10^{-7}$ g/cm$^3$ and NO$_2$ concentrations of $3.3 \times 10^{-8}$ g/cm$^3$. Obtained spectrogram for negative ions is shown in Fig. 4b.

The effect of the heterogeneity of the electric field on ion transport in the drift region of ion mobility spectrometer, to minimize the effect of inhomogeneities in the field of movement of a bunch of ions allowed the spectrometer to separate ions with mobility differ no more than by 1%.

Experimental work with toxic industrial components allow to establish the possibility of detecting them and to determine the thresholds of detection of substances. The ion mobility spectrometer showed confident detection of substances, including joint that meets the conditions for actual device operation.

![Fig. 4. (a) Cl$_2$ ($K_0=2.19$) ion mobility spectra; (b) SO$_2$ ($K_0=2.18$) and NO$_2$ ($K_0=1.98$) ion mobility spectra.](image)

4. Conclusion

The simulation of IMS drift tube electric field was performed and the trajectories of the ions in the region of ionization source electrodes, in the ionization region and in the drift region of IMS tube was shown. Obtained results have allowed to estimate influence of inhomogeneity of the field in the drift region on the resolution of the ion mobility spectrometer, as well as to make changes in the parameters of the tube to minimize this impact. Based on the performed modeling have been identified best constructive decisions for the manufacture of drift tubes. On the manufactured drift tube been successfully carried out the experimental detection of hazardous industrial chemicals.

Acknowledgements

The authors gratefully acknowledge for support experiments part in this work from industrial partner JSC NPP “Delta” (Moscow, Russian Federation) and CEO of LLC “Analit MEPHI” (Moscow, Russian Federation) Konstantin Oblov, personally for support in part of producing mechanical components for drift tubes.

References

[1] H. Borsdorf, T. Mayer, et. al., Recent developments in ion mobility spectrometry. Applied Spectroscopy Reviews, 2011 (46) 472-521
[2] V. Matsaev, M. Gumerov, et. al. IMS Spectrometers with Radioactive, X-ray, UV and Laser Ionization, International Journal for Ion Mobility Spectrometry, 5 ( 2002) 112-114.
[3] N. Samotaev, A. Golovin, et. al. IMS development at NRNU MEPhI. Lecture Notes in Electrical Engineering, 2014 (268) 447-451.