

Detection of benzene series by two-dimensional FAIMS technique

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Abstract—Benzene, toluene, p-xylene, m-xylene and o-xylene are harmful to human body seriously, moreover, p-xylene, m-xylene and o-xylene are isomers, which are difficult to distinguish by commonly used spectrum analysis techniques, such as mass spectrometry. In this article, they were detected by using high field asymmetric waveform ion mobility spectrometry (FAIMS). The resolution of detecting samples was optimized by two dimensional scanning concerning the compensation voltage in combination with high dispersion voltage. FAIMS has good solution to identify them. According to the experimental results, we obtained two-dimensional spectra. By fitting of equations about electric field intensity, we worked out second-order and fourth-order coefficient of ion mobility nonlinear function, which is useful to establish characteristic FAIMS spectra of the benzene series compounds.

Keywords—high field asymmetric waveform ion mobility spectrometry (FAIMS); benzene series compounds; isomers

I. INTRODUCTION

Benzene and benzene series are colorless or light yellow transparent oily liquid. They are easy to be volatile vapor and they are flammable and poisonous. Benzene, toluene, and xylene are homologue and they are coal tar fractional distillation product or petroleum cracking product. In the field of indoor decoration, multi-purpose toluene and xylene have replaced benzene as solvent or diluent in many kinds of plastic paint coating and waterproof materials. Shenzhen Consumer Council released the results of a survey indicating that more than 40% of the newly decorated houses, whose pollution level was over standard. To some extent, after decoration, benzene and benzene series contained in paint exceed too much, which leads to the excess of pollution level. Benzene series compounds are harmful to human body seriously, and they have been confirmed currently by the World Health Organization (WHO) as strong carcinogen. Currently, the benzene and benzene series can be detected by gas chromatography (GC) and mass spectrometry (MS), however, GC is not suitable for rapid detection, while MS is not capable of distinguishing isomers.

FAIMS (High field asymmetric waveform ion mobility spectrometry) is a newly developed technology for rapid compounds detection as well as isomers identification^[1]. It is a trace detecting technology that separates and identifies different ions of substances under atmosphere^[2]. Compared with the traditional mass spectrometry and chromatography, the sensitivity of FAIMS is higher and the analysis is faster^[3]. Comparing to traditional IMS (ion mobility spectrometry), FAIMS is lighter and it has higher resolution^[4]. Because different ion drift rate of detected objects changing with the high voltage field strength are diverse from each other, we can achieve two-dimensional spectra of target analytes by scanning compensation voltage and high dispersion voltage, so as to improve the resolution^[5,6]. By using two dimensional scanning FAIMS technique, we detected the some common volatile pollutants such as benzene and benzene series successfully.

II. FAIMS PRINCIPLE

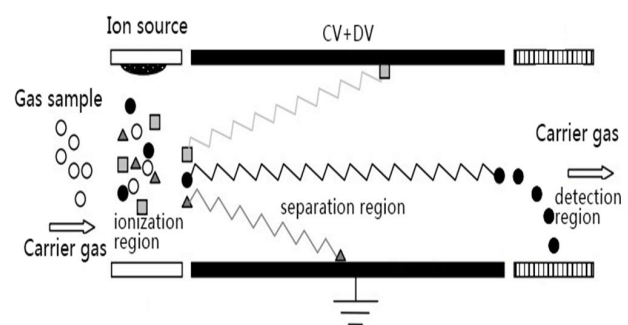


Fig.1. Scheme of the ions movement in FAIMS chip

A schematic of the FAIMS chip is shown in fig.1 and consists of ionization region, separation region and detection region. Ion separation region is composed of two pieces of opposite electrode. Ions are transported longitudinally through a drift tube by a carrier gas stream^[7]. An asymmetric radio-frequency (RF) electric field is produced by applying a

dispersion voltage between two parallel electrodes. The RF electric field causes the ions to oscillate in a direction perpendicular to the carrier gas flow during ion transport through the drift tube^[8]. Only ions with a total transverse displacement less than the drift tube height can reach the detection region. All other ions colliding with the electrodes are neutralized and are removed from the detection region by the gas flow^[9]. If a dispersion voltage and a compensation voltage are applied with proper magnitude and polarity, a certain kind of ions will be able to travel between the two electrodes and reach the detection region. Under the effect of the RF electric field, occurring in the tube, the ions of different types drift with different velocities in a direction perpendicular to the flow of the drift gas and are separated^[10]. By varying voltage, the ions of all types in detected samples can be recorded, and the dependence of the ion current on the compensation voltage, thus the spectrum can be obtained. The characteristic features of the ion separation in FAIMS, where the position of each type of ions in the spectrum is determined by ion mobility nonlinear function, which is a significant factor of ion mobility. The mobility of an ion in an electric field can be described mathematically as:

$$K = K_0 \left(1 + \alpha_{(E/N)} \right) = K_0 \left(1 + \sum_n \alpha_{2n} (E/N)^{2n} \right) \quad (1)$$

Among which, K is ion mobility, K_0 is low electric field ion mobility, $\alpha_{(E/N)}$ is the ion mobility nonlinear function, α_{2n} is $2n$ -order nonlinear coefficient. K_0 is independent of electric field and it is a constant. Ion mobility is the product of the ion mobility coefficient in a weak field ($K \equiv K_0$) and a factor containing the increment of mobility, normalized by the mobility coefficient, that is, function. The compensation voltage required depends on the ion's α_{2n} , dispersion voltage, furthermore known as the temperature, the pressure, the gas flow rates, and the analyte concentration. The position and height of FAIMS spectra are two characteristic values. Considering the relationship between the dispersion voltage and compensation voltage, equations set are obtained, moreover, the second -order (α_2) and forth-order (α_4) nonlinear function coefficient are achieved^[11]. Spectra analysis is based on spectra's characteristics value and nonlinear function coefficients.

III. EXPERIMENT

A. Instrumentation

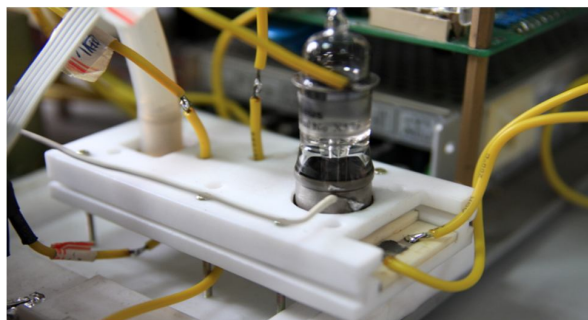


Fig.2. FAIMS chip

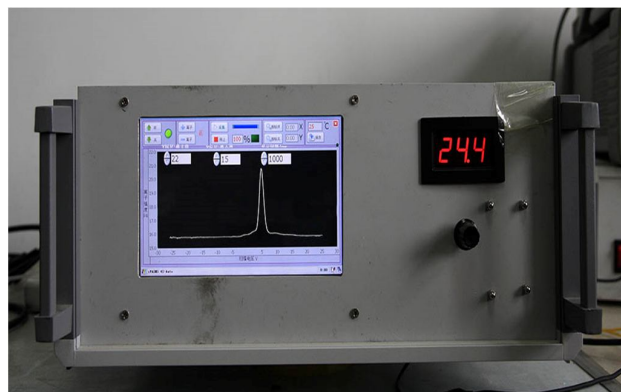


Fig.3. FAIMS instrument

The FAIMS chip and the detection instrument were developed, which were shown in fig.2 and fig. 3 respectively. Sample ionization was accomplished using ultraviolet lamp. The FAIMS chip was made by thick film technique. The gap between two electrodes was 0.5mm. Stepping with 100 V, dispersion voltage took six values ranging from 900V to 1400V, with frequency of 1MHz and variable duty factor. Compensation voltage was swept from -30 to +30 V, and the carrier gas flow rate was 300 L/h.

B. Sample generation and gas supply

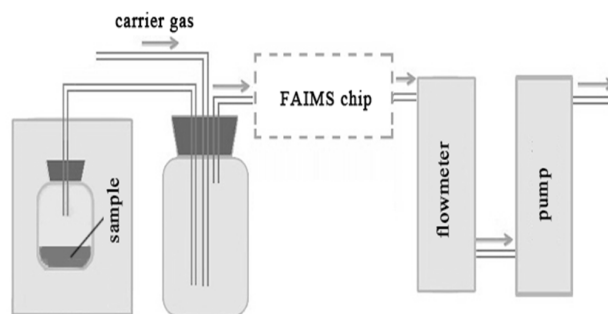


Fig. 4. Scheme of sample injection and gas connections

Scheme of sample injection and gas connections was shown in fig.4. Samples were placed in glass container which was kept in a thermostated container. The carrier gas flow rate was in the control of the pressure regulating valve and it could be measured by flowmeter. The carrier gas was pumped into the entrance of the other container, which was connected to sample's container. Gas outlet jointed the drift tube. In this way, samples' vapor and carrier gas were combined, then, samples were transmitted to the drift tube.

C. Samples

The samples tested in this work were benzene, toluene, p-xylene, m-xylene and o-xylene. They were from the National Medicine Group Chemical Reagent co., LTD. (Shanghai). Pure carrier gas for the experiment was from Nanjing Shang Yuan industrial gas plant, the purity of nitrogen was 99.99%.

IV. RESULTS AND DISCUSSION

A. Influence of dispersion voltage on spectrum

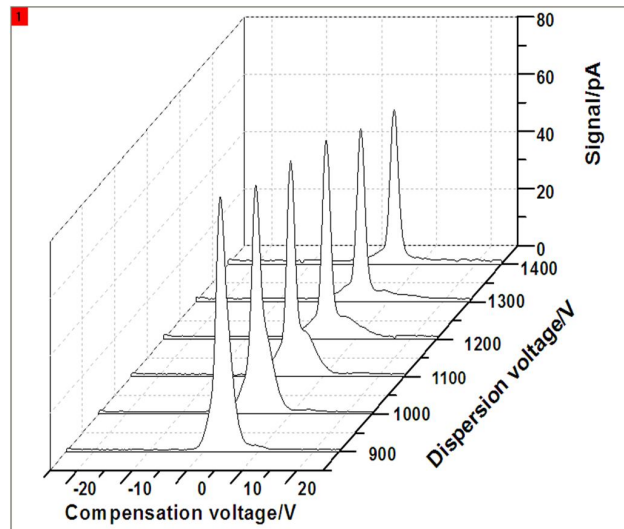


Fig.5. Benzene spectra under different dispersion voltage

As shown in fig.5, sample is benzene under different dispersion voltage. The benzene series after ionization were positively charged. The effect of separation among sample's spectra was observed with the application of the RF field to the drift tube. It was useful to improve the resolution of spectra. Nevertheless, high field would increase the amplitude of ions in the perpendicular direction. In the process of ions flight in the drift tube, electrodes were more likely to neutralize ions which are located at the top electrode edge or bottom electrode edge. In this way, ions passing rate was reduced and the detection sensitivity was decreased. With the increasing of dispersion voltage, the compensation voltage of peak gradually shifted away from 0 V, meanwhile, peak height declined accordingly. Obviously, with increment of dispersion voltage, ions were more difficult to arrive detection region and spectra's height was shortened.

B. Isomers detection

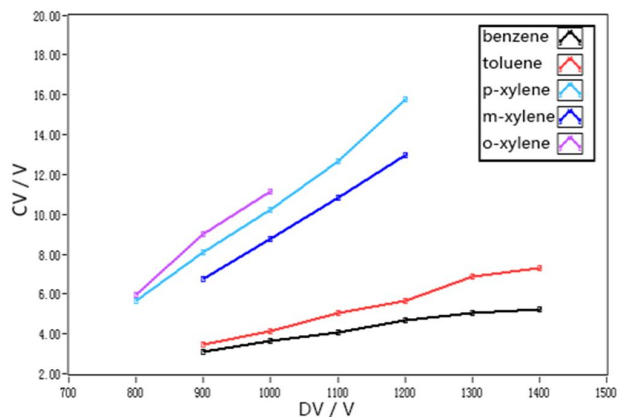


Fig.6. Peak position of benzene series under different DV

As shown in fig.6, o-xylene, m-xylene and p-xylene were isomers. Formula of isomers were identical, however, chemical structure of them were various. As was well-known, distinguishing isomers was difficult for some instruments. For instance, mass spectrometry is considered to be a widely used method which is a combination of high specificity and high sensitivity. Nevertheless, mass spectrum, which was based on measuring charge-mass ratio of ion, was not easy to detect isomers. Facing the issue, FAIMS had a good solution. As shown in figure, under the same dispersion voltage, corresponding compensation voltage of isomer was different apparently. It indicates that FAIMS technique is not only able to distinguish benzene and benzene series, but also capable of identifying isomers. Therefore, we could infer that FAIMS technique had promising application in detecting various kinds of chemicals.

C. Solving nonlinear function coefficient

TABLE I. COEFFICIENT OF ION MOBILITY NONLINEAR FUNCTION.

Sample name	coefficient of nonlinear function.	
	α_2	α_4
benzene	-1.50E-05	1.36E-09
toluene	-1.60E-05	1.18E-09
p-xylene	-3.60E-05	1.94E-09
m-xylene	-3.30E-05	2.33E-09
o-xylene	-3.93E-05	2.03E-09

According to dispersion voltage adopted in the experiment and the corresponding compensation voltage, we obtained five kinds of equations set about benzene and benzene series. We could solve out second-order and fourth-order coefficient of ion mobility nonlinear function, which were shown in table I. These coefficients played an important role in the FAIMS and they laid a solid foundation for the spectra analysis. Depending on detected samples' spectra, we achieved characteristic values, second-order and forth-order coefficients. They were useful for rapid field detection and recognition.

V. CONCLUSIONS

By employing FAIMS' two dimensional scanning technique concerning the compensation voltage in combination with dispersion voltage, the resolution of detection could be optimized. Experiments showed that this technique had a good separation effect on benzene and benzene series. Meanwhile, it was also good at identifying isomers. α_2 , α_4 and characteristics value of spectra were calculated and preserved in database. It was significant for rapid field detection and identification.

ACKNOWLEDGMENT

This work was supported by External Cooperation Program of Chinese Academy of Sciences (No.GJHZ1218) and National Natural Science Foundation of China (No.61004133).

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