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# Rapid method for accurate peak position extraction in high-field asymmetric ion mobility spectrometry

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ABSTRACT

High-field asymmetric waveform ion mobility spectrometry (FAIMS) enables precise identification of substances through fingerprint spectra obtained by multi-cycle scans at different separation voltages (DV) and nonlinear functions. To improve the scan speed of compensating voltage (CV) in multi-cycle scanning, the challenge arises in peak position shifts. This article proposes a method to accurately determine peak positions regardless of scan speed by exploiting the symmetric features of spectra obtained through positive and negative CV scans. The proposed method enables extremely fast scan speeds. A custom-built FAIMS system was used to verify the correlation between peak shifts and scan speed, the symmetry of spectra peaks under positive and negative CV scan modes, and the peak positions and solution errors of nonlinear functions by using benzene, styrene, acetone, toluene, m-xylene, and hydrogen sulfide as experimental samples. The results demonstrate the widespread occurrence of peak shifts, with peak deviations reaching as high as 2.49% even in slow scans of 0.75 V/s. As scan speed increases, peak position deviations gradually increase, with the maximum deviation reaching 46.83% at a scan speed of 30 V/s. By applying the proposed averaging method, peak positions of the six substances were obtained within the scan speed range of 30 to 0.75 V/s. Compared to traditional methods, the maximum peak position error using the averaging method was reduced by approximately 87.5%, and the spectrum acquisition time was reduced by 85%. The use of the averaging method reduced the calculation error of the alpha function by 88% and decreased the acquisition time by 80%. The research findings of this study offer a solution for the accurate determination of peak positions in FAIMS under fast scanning.

## 1. Introduction

High-field asymmetric waveform ion mobility spectrometry (FAIMS) is an instrument that operates at atmospheric pressure and can be easily integrated with microelectromechanical systems (MEMS), enabling features such as miniaturization of sensors and ion separation capabilities of the instrument [1–3]. FAIMS has advantages such as ease of miniaturization, high sensitivity, and two-dimensional identification. It has been successfully applied in the detection of environmental pollutants, explosives, and hazardous chemicals [4–7].

FAIMS is the only ion mobility spectrometer that operates under high electric field conditions. It utilizes the nonlinear variation of ion mobility (K) with high field conditions to achieve ion separation and detection. Under high electric fields, the ion mobility (K) is described by Eq. (1):

$$K = K_0 \left[ 1 + \sum_{n=1}^{\infty} \alpha_{2n} \left( \frac{E}{N} \right)^{2n} \right]$$
$$\approx K_0 \left( 1 + \alpha_2 \left( \frac{E}{N} \right)^2 + \alpha_4 \left( \frac{E}{N} \right)^4 \right) \quad (1)$$

where $K_0$ is the ion mobility coefficient at low fields, $E$ is the electric field strength, $N$ is the gas number density, and $\alpha(E/N)$ is the alpha function describing the nonlinear variation of ion mobility with $E/N$. $\alpha_2$ and $\alpha_4$ are the expansion terms of the alpha function, with higher-order terms typically neglected. Based on this alpha function, spatial separation of different ions can be achieved by applying an asymmetric high-frequency high-amplitude electric field, as shown in Fig. 1. The voltage generating this separation electric field is called the Dispersion Voltage (DV). By superimposing a low-frequency low-amplitude scanning voltage on the separation electrode, the selection of outgoing ions can be achieved. This voltage is referred to as the compensation voltage (CV). Under predetermined DV conditions, the ion current intensity (I) and CV form the FAIMS spectrum. The FAIMS spectra at different DVs constitute the fingerprint spectrum for ion identification. The expansion coefficients of the alpha function, $\alpha_2$ and $\alpha_4$, can be obtained based on this fingerprint spectrum, representing the identification parameters of substance ions.

The acquisition time for a single FAIMS spectrum range from a few seconds to several tens of seconds [8]. However, it takes several min-
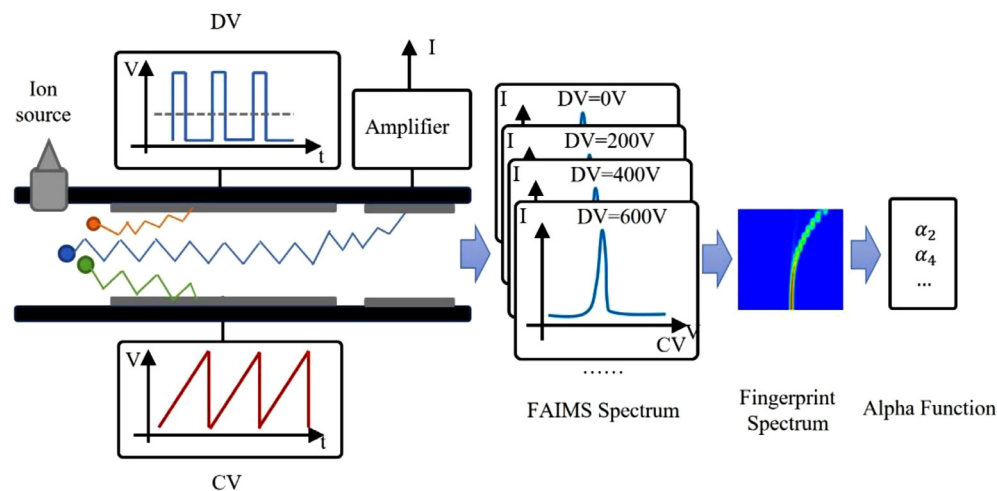
**Fig. 1.** Principle of FAIMS device.

utes or even longer to form a complete fingerprint spectrum, which does not meet the requirements for rapid detection in field conditions. Simply increasing the scan speed leads to peak shifts in mass spectrometry methods [9–11], which is unfavorable for peak position-based feature recognition. To improve the detection speed of FAIMS, Li [12], Liu [13], and others have used two complete spectra obtained from pre-scanning to predict the potential positions of characteristic peaks at different separation voltages, and they actively reduce the CV range to shorten the acquisition time of the fingerprint spectrum by an order of magnitude. However, this method assumes that all ions exhibit spectral peaks at high DV, which is not consistent with actual situations and may result in missed characteristic peaks and incorrect predictions of peak trends for substances with multiple peaks. In similar analysis techniques such as mass spectrometry and chromatography, the phenomenon of scan speed induced peak distortion and peak position shifts has been extensively studied [9–11]. However, the impact of scan speed on FAIMS peak positions has not been reported, and no methods have been provided to address or eliminate peak position shifts in other spectrometer devices.

In FAIMS spectra, the abscissa CV reflects the scan speed. CV scanning can be performed in either positive slope scan mode or negative slope scan mode, making it possible to obtain two spectra that are symmetric about the original peak positions. Based on this, we propose a method to rapidly obtain accurate peak positions from spectra using the symmetry of positive and negative CV scans. We acquired FAIMS spectra of various substances, different DVs, and positive/negative scan modes, and studied how scan speed affects FAIMS peak positions, the symmetrical properties of positive/negative scans, how accurate the positive/negative scan averaging method is, and the errors in the alpha function using this method.

## 2. Experimental

### 2.1. Instrument and reagent

This study utilized a custom-built FAIMS system, consisting of an analyzer, a vacuum ultraviolet lamp ionization source, a separation voltage module, a compensation voltage module, and a weak signal amplification module. The dimensions of the detection electrode in the analyzer were 30 mm, with 0.5 mm between the upper and lower plate electrodes. The ionization source used was a 10.6 eV vacuum ultraviolet lamp from Germany's Helium Lamp Company. The separation voltage ranged from 0 V to 1400 V, with a frequency of 1 MHz. The compensation voltage scanning range was −30 V to +30 V. The weak signal amplification module employed a femtoampere level input bias current operational amplifier ADA4530. The amplifier is configured in negative feedback amplification mode with feedback electrons of approximately 10 G ohms. The flow rate of the gaseous samples was controlled using

**Table 1**
Initial sample concentration and diluted concentration.

| No. | Compound | Initial concentration (mg/m³) | Diluted concentration (mg/m³) |
|-----|----------|-------------------------------|-------------------------------|
| 1 | Benzene | 31.95 | 1.07 |
| 2 | Styrene | 42.60 | 1.52 |
| 3 | Acetone | 23.75 | 2.38 |
| 4 | Toluene | 37.68 | 3.77 |
| 5 | M-xylene | 106.17 | 10.6 |
| 6 | Hydrogen sulfide | 13.94 | 2.79 |

a G300C Mass Flow Controller (MFC) from Gist Instruments. Nitrogen gas was purchased from Nanjing Special Gas Co., Ltd., with a purity of 99.999%. Standard sample gases, including benzene, styrene, acetone, toluene, xylene, and hydrogen sulfide, were obtained from Wuhan Newrad Special Gas Co., Ltd., and their initial concentrations are shown in Table 1.

### 2.2. Methods

The FAIMS experimental apparatus is shown in Fig. 2.

The standard sample gas is controlled by Mass Flow Controller 1, while nitrogen gas is controlled by Mass Flow Controller 2. By adjusting the flow rates of Mass Flow Controller 1 and Mass Flow Controller 2, the total flow rate entering the FAIMS chip is maintained at 3 L/min, and the samples are diluted to the specified concentration. The diluted concentrations of each sample are shown in Table 1.

The dispersion field is set to vary from 0 V/cm to $2.8 \times 10^5$ V/cm in increments of $2 \times 10^4$ V/cm. At each separation voltage, spectra are acquired with a CV scan speed from 30 V/s to 0.75 V/s. The CV scan mode includes both positive scan mode (−30 V to +30 V) and negative
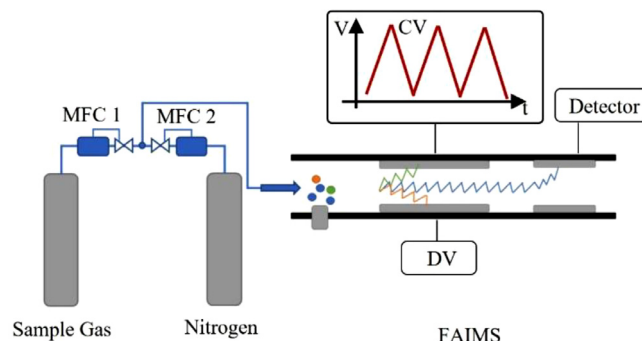


**Fig. 2.** FAIMS Experimental setup diagram.

**Table 2**
Key scan parameter values.

| Item | Value |
| --- | --- |
| Dispersion field strength ($\times 10^4$ V/cm) | 0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28 |
| Scan speed (V/s) | 30, 15, 10, 7.5, 6, 5, 4.29, 3.75, 3.33, 3, 2, 1.5, 1.2, 1, 0.86, 0.75 |
| Scan mode | Positive mode ($-30$ V $-$ $+30$ V), Negative mode ($+30$ V $-$ $-30$ V) |

scan mode (+30 V to −30 V). Specific separation field and scan speeds are listed in Table 2.

## 3. Results and discussion

### 3.1. Scan speed effect on peak position accuracy

The fingerprint spectra and characteristic peaks of each substance with a scan speed of 0.75 V/s are shown in Fig. 3. At a separation field of $2 \times 10^5$ V/cm, all six substances exhibit significant peak separation. The farthest deviated peak at this voltage is identified as the characteristic peak and is indicated by a blue arrow in the figure.

The separation field was set to $2 \times 10^5$ V/cm, and the spectra of characteristic peaks in positive and negative scan modes for the six substances were displayed at scan times of 30 V/s, 15 V/s, 10 V/s, 7.5 V/s, 6 V/s, 3 V/s, 1.5 V/s, 0.75 V/s, as shown in Fig. 4.

The positions of characteristic peaks in both positive and negative scan modes were extracted for all scan speed. The peak positions obtained in both modes were averaged, and the results are shown in Fig. 5.

From Figs. 4 and 5, it can be observed that when the scan speed is changed, the positions of characteristic peaks obtained in positive and negative scan modes for benzene, styrene, acetone, toluene, m-xylene, and hydrogen sulfide show significant differences. As the scan speed

decreases, the characteristic peaks obtained in both modes gradually converge towards the average value. By calculating the error of peak positions in the positive scan mode using the average value as a reference, it can be determined that at a scan speed of 30 V/s, the errors for benzene, styrene, acetone, toluene, m-xylene, and hydrogen sulfide are 23.4%, 22.1%, 46.8%, 23.1%, 22.9%, and 26.4% respectively. Even at a scan time of 0.75 V/s, the errors for the six substances are still 1.0%, 0.7%, 2.5%, 0.7%, 1.0%, and 2.0% respectively.

The peak position deviations are caused by the lower bandwidth of the equivalent RC circuit composed of the FAIMS analyzer and signal amplification system when the scan speed is fast, leading to the filtering of the high-frequency components in the signal [14,15]. In the home-made FAIMS circuit, the main resistor is the negative feedback amplifier resistor with a resistance size of 10 GΩ ($10^{10}$ Ω), and the capacitance is composed of the FAIMS detection electrode capacitance and parasitic capacitance, which is about 10 pF ($10^{-11}$ F), so the cutoff frequency of the system is about 1.6 Hz. The half-peak width of the signal acquired in this experiment is basically around 2 V, as shown in Fig. 4. The half-peak width under different scanning speed is about several seconds. The bandwidth of Gaussian signal is about equal to 0.44 divided by the half-peak width [16]. Therefore, the bandwidth of Gaussian signal under different scanning speeds in the experiment is about 0.1–10 Hz. The bandwidth of the Gaussian signal is exactly similar to the allowable bandwidth of the amplification system. Therefore, when the scanning
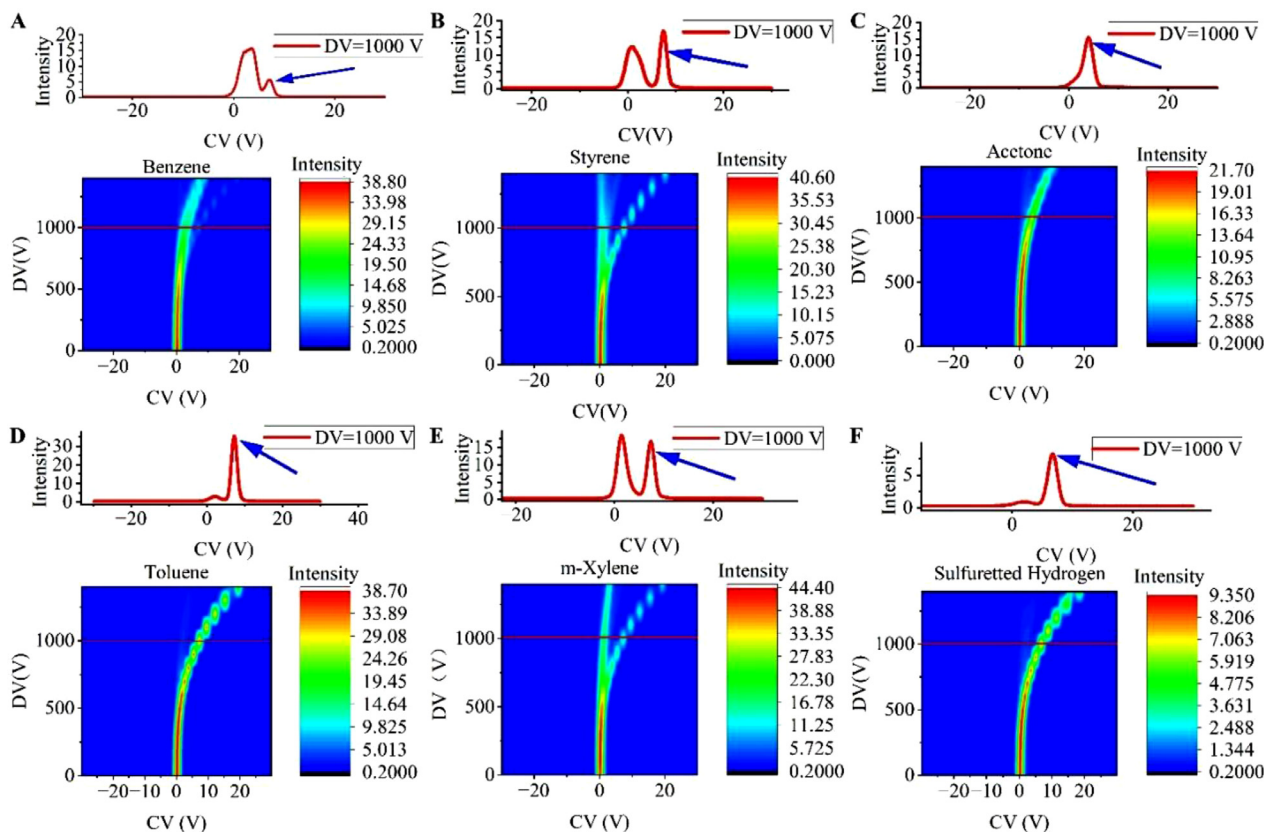


**Fig. 3.** FAIMS fingerprint spectra and characteristic peaks for a scan time of 80 s. (A) Benzene; (B) styrene; (C) acetone; (D) toluene; (E) *m*-xylene; (F) sulfuretted hydrogen.
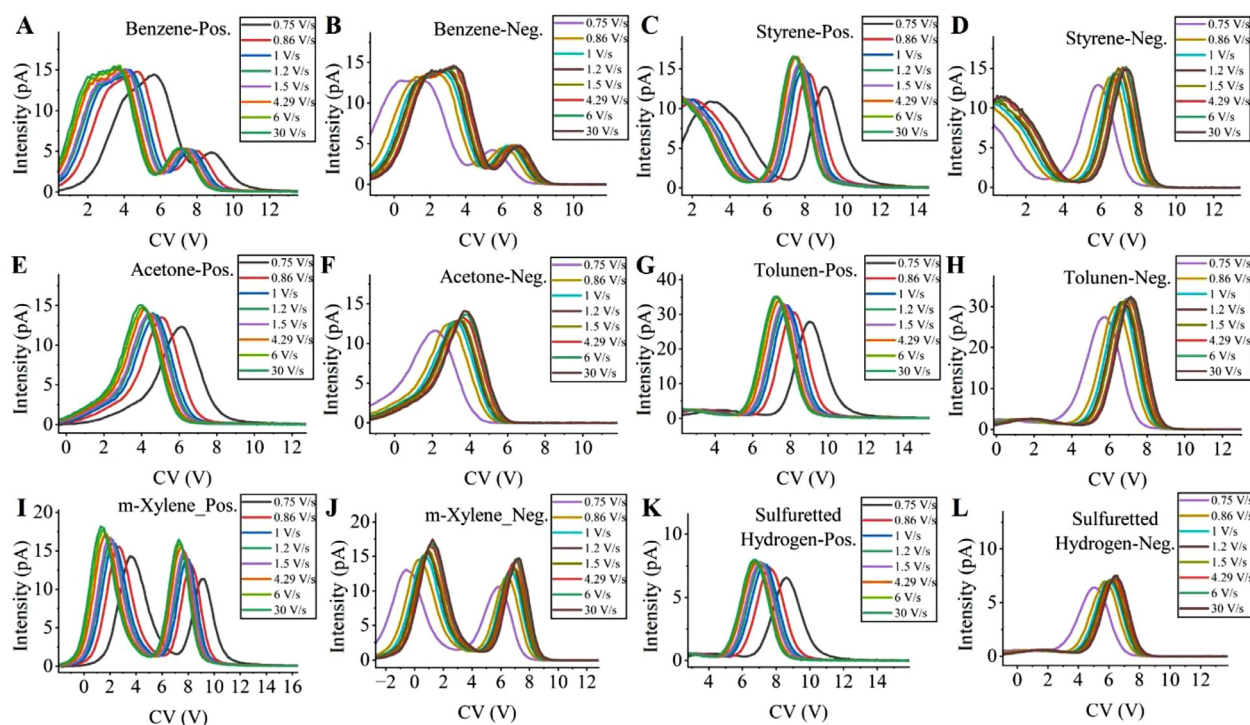
**Fig. 4.** FAIMS spectra at dispersion field of $2 \times 10^5$ V/cm and scan speed 0.75–30 V/s. (A) Benzene, positive scan mode; (B) benzene, negative scan mode; (C) styrene, positive scan mode; (D) styrene, negative scan mode; (E) acetone, positive scan mode; (F) acetone, negative scan mode; (G) toluene, positive scan mode; (H) toluene, negative scan mode; (I) m-xylene, positive scan mode; (J) *m*-xylene, negative scan mode; (K) sulfuretted hydrogen, positive scan mode; (L) sulfuretted hydrogen, negative scan mode.
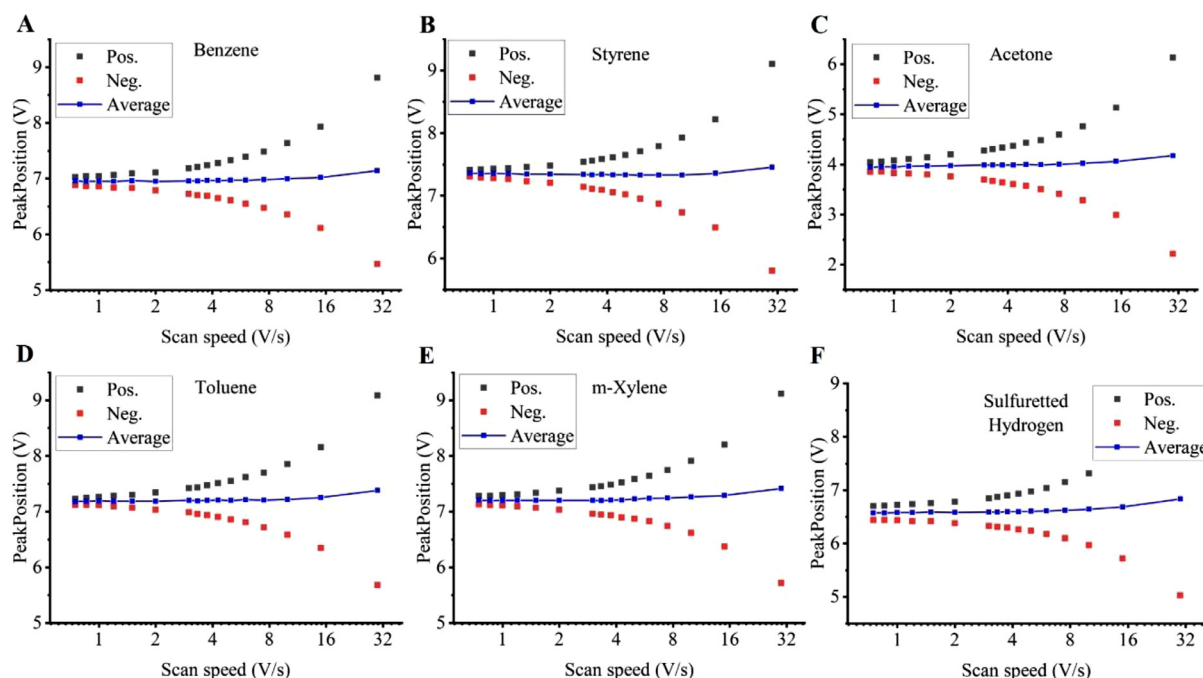


**Fig. 5.** Peak position and average value at dispersion field of $2 \times 10^5$ V/cm and scan speed 0.75–30 V/s. (A) Benzene; (B) styrene; (C) acetone; (D) toluene; (E) m-xylene; (F) sulfuretted hydrogen.

speed is high and the bandwidth of the Gaussian signal exceeds about 1.6 Hz, the peak produces a significant distortion. Currently, when the scan speed of the equipment is in the range of 4.3–60 V/s [8,17], peak positions often have significant errors, which make it harder to identify the types of substances based on FAIMS spectra that depend on peak positions [6,18-21].

### 3.2. Accurate peak position acquisition based on averaging method

The exact peak position is calculated by averaging the peak position in positive and negative scan mode. For the first test, appropriate scan parameters are determined by pre-experimentation. The parameters include CV range, separated electric field value, and characteristic peak.
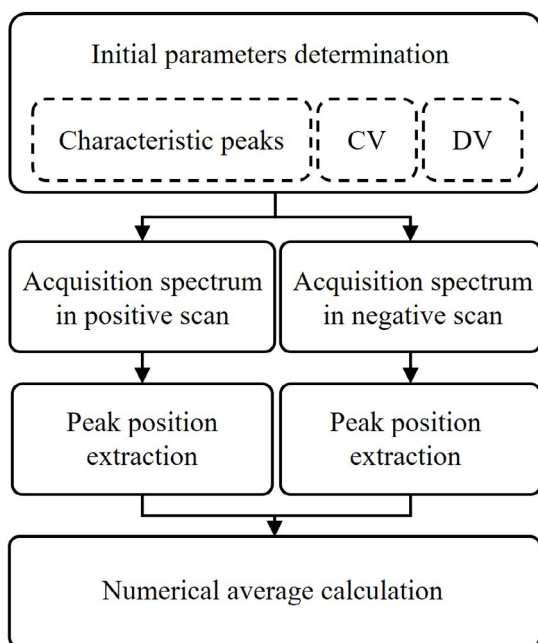
**Fig. 6.** Flow chart of the averaging algorithm.

Then the spectra of positive and negative scan modes at the same scan speed were acquired separately. The peak position information of the characteristic peaks under each mode is extracted. Finally, the extracted peak positions are numerically averaged to obtain the accurate values. The flowchart of the algorithm for the averaging method is shown in Fig. 6.

Peak positions are averaged and plotted in Fig. 5 using blue lines. It can be observed that the peak positions directly extracted from the spectra (represented by the red and black dots) are time dependent. As the scan speed decreases, the extracted peak positions in both positive and negative scan modes gradually approach the average peak position. Meanwhile, the average peak position remains constant across all scan times. Taking the scan time of 0.75 V/s as a reference, the errors between

the peak position average obtained at other scan times and the reference are examined, as shown in Fig. 7.

From Fig. 7, when the scan speed is 30 V/s and 15 V/s, the maximum error in peak positions obtained through averaging is 5.75% for acetone at a scan speed of 30 V/s. The possible reason for the presence of errors when the scan speed is less than or equal to 7.5 V/s is that the scanning speed is too fast, and there may be some synchronization issues between the measurement and control system, resulting in discrepancies between the acquired spectra and the scan signals generated by the system. However, once the scan speed exceeds 10 V/s, the peak positions obtained through averaging remain relatively unchanged. After 10 V/s, the maximum errors in peak positions obtained through averaging for the six substances are 0.61%, 0.42%, 1.85%, 0.56%, 0.82%, and 1.03% respectively. The errors in peak positions obtained through averaging for all substances are lower than the errors obtained by directly extracting peak positions from the spectra at 0.75 V/s. The maximum reduction in peak position errors obtained through averaging across all scan times is approximately 12.5% compared to the direct extraction method. Therefore, by using the averaging method, peak position information that is not influenced by scan speed can be obtained within a certain range. In both positive and negative scan modes, when a scan speed of 10 V/s is used and peak positions are obtained through averaging, they are consistent with the peak positions obtained at a scan speed of 0.75 V/s. However, reducing the scan time to 15% of the original duration.

### 3.3. Non-linear function calculation using averaged peak positions

Based on the peak positions obtained through averaging under the condition of a dispersion field of $2 \times 10^5$ V/cm, the accuracy of calculating non-linear functions using the averaged peak positions was investigated across the dispersion field range of 0 V/cm to $2.8 \times 10^5$ V/cm. The peak positions for the six substances were obtained using both the averaging method and the direct extraction method at all separation voltages within the scan speed range of 30 V/s to 0.75 V/s. The alpha2 and alpha4 functions were calculated, as shown in Fig. 8. Taking the scan speed of 0.75 V/s as a reference, the errors for other scan times were calculated and are presented in Fig. 9.
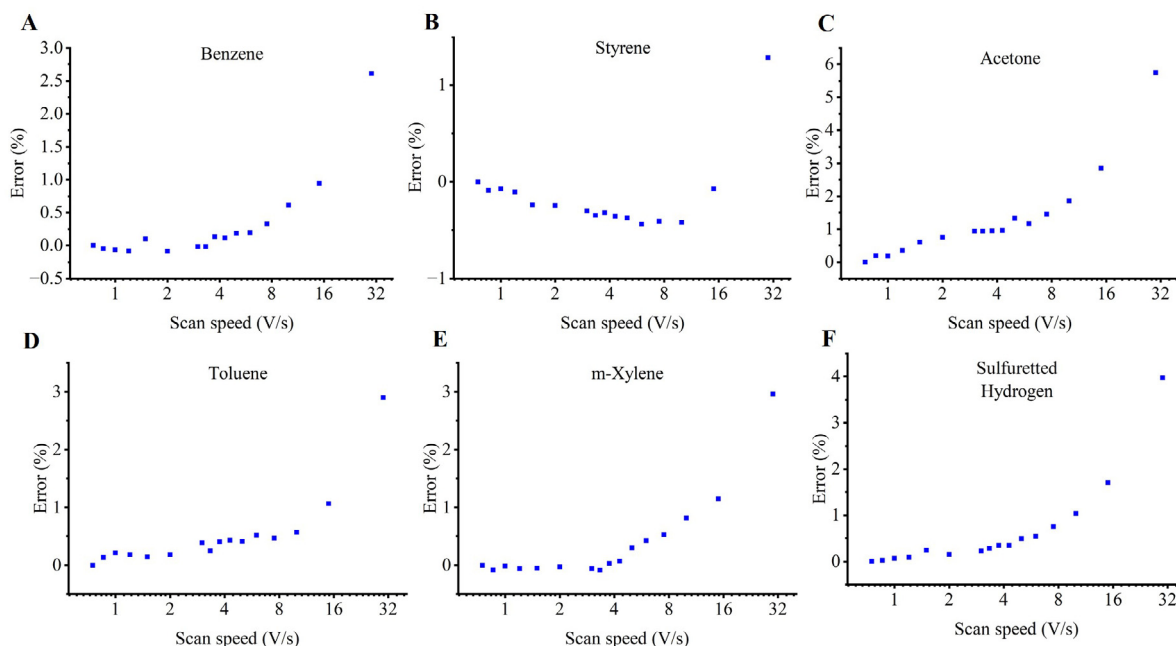


**Fig. 7.** Average method peak position error at dispersion field of $2 \times 10^5$ V/cm and scan speed 0.75 V/s –– 30 V/s. (A) Benzene; (B) styrene; (C) acetone; (D) toluene; (E) m-xylene; (F) sulfuretted hydrogen.
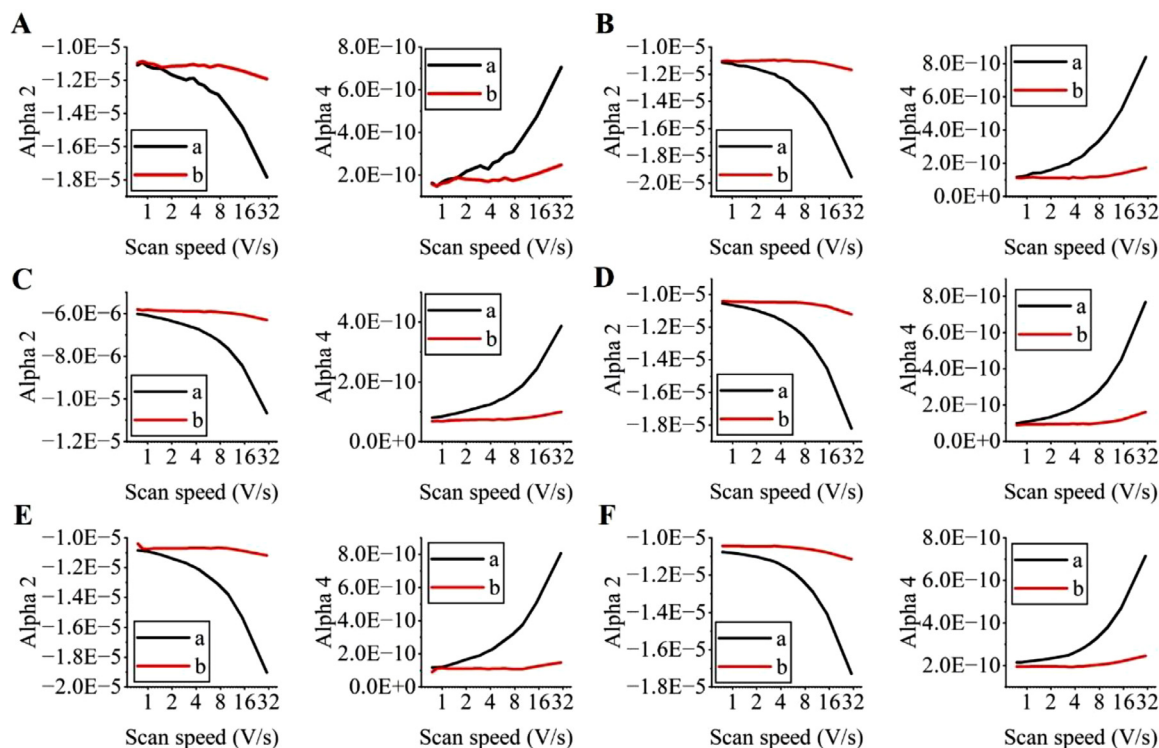
**Fig. 8.** Alpha function (A) benzene; (B) styrene; (C) acetone; (D) toluene; (E) m-xylene; (F) sulfuretted hydrogen. (a) Direct acquisition; (b) averaging method.
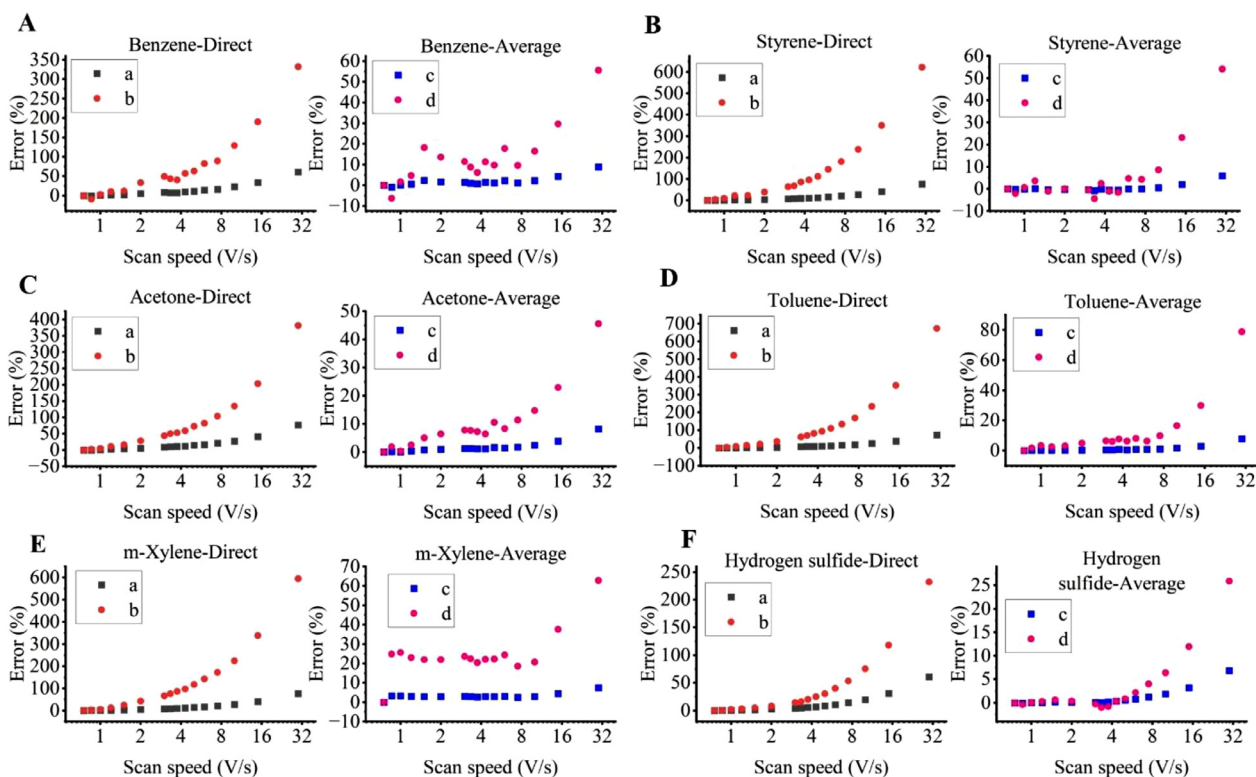


**Fig. 9.** Error of Alpha function (A) benzene; (B) styrene; (C) acetone; (D) toluene; (E) m-xylene; (F) sulfuretted hydrogen. (a) Direct acquisition alpha2; (b) direct acquisition alpha2; (c) averaging method alpha2; (d) averaging method alpha4.

From Figs. 8, 9, it can be observed that the non-linear functions calculated using the averaged peak positions remain stable across different scan times. In contrast, there are significant differences in the non-linear functions calculated using the directly extracted peak positions from the spectra at different scan times. Moreover, as the scan time increases, the values of the non-linear functions calculated using the directly extracted peak positions gradually approach the values calculated using the averaging method.

Among the six substances, the maximum error in the non-linear functions calculated using the averaging method is found in alpha4 for toluene at a scan speed of 30 V/s, with an error of 78.80%. Under the same conditions, the error in calculating the alpha4 function using the directly extracted peak positions from the spectra is 673.59%, approximately 8.5 times larger than the error in the averaging method. Extracting peak positions using the averaging method and calculating non-linear functions significantly reduces the errors.

Using the averaging method to calculate non-linear functions requires a single spectrum acquisition time of 6 s and a total of 12 s for both positive and negative scan modes. To cover the entire voltage range, it would take 180 s. On the other hand, using the direct spectrum extraction method, obtaining similar numerical values would require a single spectrum acquisition time of 80 s and a total of 1200 s to cover the entire voltage range, more than 5 times longer than the averaging method. The averaging method reduces the computation time for calculating non-linear functions while improving the accuracy of the results.

## 4. Conclusions

The real-time and rapid requirements for on-site applications pose higher demands on the scan speed of high-field asymmetric waveform ion mobility spectrometry (FAIMS). This study investigated the impact of different scan speed on peak positions and proposed a speed-independent method for peak position extraction. The results showed that the phenomenon of peak position variation with scan speed was widespread, and simply increasing the scan speed would lead to significant misalignment of peak positions in high-field asymmetric waveform ion mobility spectra. By using the proposed method of averaging peak positions from symmetrical spectra, the accuracy of peak position extraction can be improved, and the time required for peak position extraction can be reduced. The non-linear functions calculated based on the peak positions obtained using the averaging method remain consistent across a wide range of scan speeds. This research provides a fast and accurate method for peak position extraction in on-site detection of high-field asymmetric waveform ion mobility spectrometry. This method can also be used for spectral library construction, enhancing the accuracy of non-linear function calculations, and shortening the library construction time. In this article, only the effect of scanning speed on the position of FAIMS peaks was investigated, and the effect of scanning speed on the peak heights and widths of FAIMS spectra, as well as the method of accurately obtaining the peak widths and heights, need to be further explored.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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