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Finite-element analysis of a miniaturized ion mobility spectrometer for security applications

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ABSTRACT

A miniaturized Planar Field Asymmetric Ion Mobility Spectrometer (P-FAIMS) has been simulated in N_2 at ambient pressure using COMSOL Multiphysics software. Micro-IMS is based on ion gas-phase separation due to the dependence of ion mobility with electric field. Ions are selected by a DC voltage characteristic of each kind of ion. The average kinetic behaviour of ions in high electric fields conditions is well known but not the chemical reactions and physical collisions related with. The aim of this work is the modelling of the average kinetic behaviour of different kind of ions in a P-FAIMS taking into account the main factors involved in their movement. Three different compounds, with high impact on security applications, have been studied: an explosive 2,4,6-trinitrotouluene $(TNT{-}H)^-$, a volatile organic compound Ac_2H^+ and a chemical warfare agent simulant $DMMPH^+$ that emulates gas sarin. Displacement simulations along the P-FAIMS of theirs vapour phase ions have been done at different values of drift electric field amplitude to gas number density (E/N) ratio. Ions were selected between the ones present in the literature that covers the previous applications and the ones with more reliable experimental data of the main parameters involved in the definition of ions mobility needed for their analysis. Results show that simulations of ions behaviour in a P-FAIMS are possible with COMSOL Multiphysics software and that the time and intensity at which ions are detected are in good agreement with an experimental data in the literature.

1. Introduction

Recently, the European Security Research and Innovation Forum (ESRIF) [1] defined several priority areas concerning the protection of citizen and infrastructures. Among these priorities, detection of explosives, chemical warfare agents and contamination of large infrastructures are areas under development in which the micro- and nano-technologies can carry out a fundamental role.

Ion mobility spectrometry (IMS) is an analytical technique based on ion separation in gaseous phase due to an electric field. The IMS technology has fundamental advantages when compared to other sensor techniques as high resolution (∼ppbv) and fast measurements (∼ms). Additionally, ionization and characterization of the sample in IMS instruments occurs at ambient pressure [2], allowing a smaller analytical unit, lower power requirements, lighter weight and easier use for field applications. Current IMS has a typical chamber volume about 40 cm^3 minimum, but due to the trend toward reducing weight, volume and power consumption, miniaturizations of ion mobility spectrometer, are being explored [3–6]. These advantages make IMS a rapidly advancing technique with a wide spectrum of applications, including detection of narcotics, chemical warfare agents and explosives [7].

FAIMS (Field Asymmetric IMS) uses an electric field E perpendicular to ions displacement to separate and select them. This is allowed taking advantage of the slightly dependence of the ion mobility with strong fields. Using an adequate alternating $E(t)$ field the ions are displaced of their main path depending of their mobility dependence to the electric field, and only one type can reach the detector [3–6]. FAIMS technology uses two main electrodes configurations: cylindrical (C-FAIMS) or planar (P-FAIMS). In this work we focus on the planar configuration as it is going to be easier to fabricate the device once simulated.

In this work the modelling with Multiphysics Finite Element Analysis Simulation Software (COMSOL Multiphysics) of a micro Planar High-Field Asymmetric Waveform Ion Mobility Spectrometer (P-FAIMS) for security applications is presented. As representative examples of target compounds in vapour phase, simulations are done for three different kind of ions: (1) an explosive: 2,4,6-trinitrotouluene (TNT) for the negative monomer ion; (2) a chemical warfare agent simulant: dimethyl methylphosphonate (DMMP) that simulates gas sarin, for the positive monomer ion; and (3) a health risky volatile organic compound: acetone (Ac),

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for the positive dimer ion. The main advantage of P-FAIMS is that it is a powerful tool for detection of positive and negative ions at the same time.

2. P-FAIMS working principle

In presence of an electric field, ions with different collision cross-sections temporally separate based on the frequency of ion–neutral interactions. The continual micro-scale acceleration and scattering collisions deceleration of ions results in a constant average velocity, the drift velocity v_d (m/s), that is directly proportional to the magnitude of the applied electric field strength $E(t)$ (V/cm) [2]:

$$v_d(t) = K \cdot E \tag{1}$$

where K (cm^2/V s) is the ion mobility coefficient. This parameter, which can be seen as the drift velocity normalized to field, is characteristic of each ion and each medium, and is the basis for its identification. The mobility for a given ion at constant temperature and pressure, within a gas, with molecules density N (cm^{-3}) and, under the influence of an electric field E, can be assumed to be constant if E/N expressed in Townsend (1 Td = 10^{-17} Vcm^2), is less than 20. However, if E/N exceeds 40 Td, the mobility varies and can be expressed as [8]:

$$K\left(\frac{E}{N}\right) = K_0 \times \left[1 + \alpha\left[\frac{E}{N}\right]\right] \tag{2}$$

where for low electric fields $\alpha(E/N) \cong 0$, then $K(E/N) = K_0$ is the ion mobility at low electric field at a fixed N and $\alpha(E/N)$ describes the ion mobility dependence on high electric fields at a constant drift gas density N and at normal pressure and temperature (1 atm, 300 K) [2]. Mason and McDaniel [9] determined that $\alpha(E/N)$ can be expressed as a polynomic function composed only by even terms, where $\alpha_2, \alpha_4, \ldots \alpha_{2n}$ are coefficients of the expansion of $\alpha(E/N)$. The number and values of coefficients may vary to fit experimental accuracy, but the majority of authors only calculate it until second term (α_2, α_4). Eq. (3) is a convenient mathematical expression for the alpha function [10]. K_0, α_2 and α_4, are characteristic of each ion and are obtained experimentally.

$$K\left(\frac{E}{N}\right) = K_0 \times \left[1+\alpha\left[\frac{E}{N}\right]\right] \approx K_0 \times \left[1+\alpha_2 \times \frac{E^2}{N^2} + \alpha_4 \times \frac{E^4}{N^4}\right] \tag{3}$$

When the electric field exceeds 10,000 V/cm ($E/N \sim 40$ Td) the mobility of some ions varies (Fig. 1). There is not a comprehensive model to explain such complex dependence of coefficient mobility against the electric field. There are just certain hypothetical models which are based on the Mason Schamp equation.

If in a P-FAIMS a radio frequency (RF) high asymmetric electric field is applied between the two parallel plates, while ions are carried between them by a gas flow, they will undergo oscillations perpendicular to gas flow as shown in Fig. 2. One of the plates is grounded and the other is biased at high voltage with an asymmetric waveform, $V_{RF}(t)$, which has to satisfy that its integration over a period has to be zero.

Net motion of the ion between the two plates consists of two components: (1) the longitudinal component due to gas flowing stream; and (2) the transverse component due to the electric field between plates produced by $V_{RF}(t)$ ($E(t) = V_{RF}(t)/g$), a two-harmonics waveform in our case. The asymmetric waveform consists of a positive high-voltage V_H, component lasting for a short period of time t_H and a negative lower-voltage V_L, component lasting for a longer period of time t_L. The field oscillation period T is: $T = t_H + t_L$. The effect of the asymmetric field is to make the ions oscillate along the transverse direction with period T during their motion in the gas carrier stream.

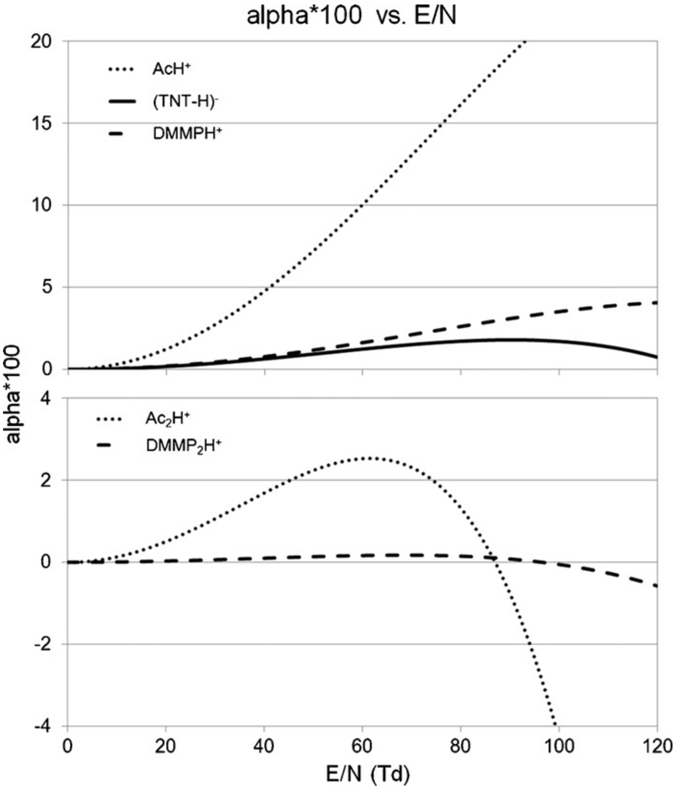

Fig. 1. Plots of alpha parameter related to the electric field drift to gas number density ratio. Top frame is for monomers and bottom frame is for dimers of the analyzed compounds. Abbreviations can be found in Table 1.

$$\Delta z = \int_0^{nT} K\left(\frac{E}{N}\right) \times E\,\mathrm{d}t = n \times \int_0^{T} K_0 \times \left[1+\alpha\left(\frac{E}{N}\right)\right] \times E\,\mathrm{d}t \tag{4a}$$

$$\Delta z = n \times K_0 \times \int_0^{T} \left[1+\alpha\left(\frac{E}{N}\right)\right] \times E\,\mathrm{d}t \tag{4b}$$

$$\Delta z = n \times K_0 \times \int_0^{nT} E\,\mathrm{d}t + n \times K_0 \times \left[\int_0^{T} \alpha\left(\frac{E}{N}\right) \times E\,\mathrm{d}t\right] \tag{4c}$$

If the RF electric field is chose so that his integral along one period is null, then

$$\Delta z = n \times K_0 \times \left[\int_0^{T} \alpha\left(\frac{E}{N}\right) \times E\,\mathrm{d}t\right] \tag{5}$$

Resultant motion of the ion along the drift channel under the influence of electric field and gas flow corresponds to a trajectory that is specific to each ion species. Simulations are done introducing a continuously fixed concentration of ions (obtaining a stream of ions, not ion clouds), just in the middle of the drift channel high, so only ions with a total transverse displacement less than half of the drift channel height can reach the detector (shown in Fig. 2). All other ions colliding with the filter electrodes are neutralized and removed from the drift region by the gas flow.

Selected ions can be kept in the flowing gas by applying particular low DC field ($|E_C| < |E_L| \ll |E_H|$) between the filter electrodes. This DC voltage or compensation voltage (V_C) prevents the ion migration towards either electrode. Thus, a selected ion passes through the filter electrodes and reaches the detector being this V_C voltage a characteristic of each ion species.

Sweeping the compensation voltage produces a high-field equivalent of a mobility spectrum of the different ion species