ARTICLE IN PRESS

Engineering in Agriculture, Environment and Food xxx (2016) 1–12

Contents lists available at ScienceDirect

Engineering in Agriculture, Environment and Food

journal homepage: http://www.sciencedirect.com/eaef

# State of ion mobility spectrometry and applications in agriculture: A review

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ARTICLE INFO

*Article history:*
Received 3 April 2015
Received in revised form
1 April 2016
Accepted 14 May 2016
Available online xxx

*Keywords:*
Volatile organic compounds
Agriculture
Biotic and abiotic plant stress
Post-harvest loss management

ABSTRACT

Ion mobility spectrometry (IMS) has been employed successfully to detect chemicals such as explosives, illicit drugs, chemical warfare agents, pharmaceutical chemicals, and environmental pollutants. However, applications of IMS in pre- and post-harvest agriculture production management has not been explored adequately. Characteristics such as high sensitivity, selectivity, analytical flexibility, field portability, and real-time monitoring abilities offer great potential of IMS applications in agriculture. In this paper, reviewed are the different types of IMS, their working principles, and agricultural applications. Some of the agricultural applications include; detection of contaminants affecting soil and plants, assessing plant stress, and monitoring postharvest agricultural produce quality and safety.

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**Contents**



*Abbreviations:* AIMS, Aspiration ion mobility spectrometry; CD, Corona discharge; DMS, Differential mobility spectrometry; ESI, Electrospray ionization; FAIMS, Field asymmetric ion mobility spectrometry; GC, Gas chromatography; IMS, Ion mobility spectrometry; $K_0$, Ion mobility at standard temperature (273 K) and pressure (1 atm.)($cm^2/(V \times s)$); LC, Liquid chromatography; LC/MS, Liquid chromatography-mass spectrometry; MCC, Multiple capillary column; MESI, Membrane extraction with a sorbent interface; MS, Mass spectrometry; NMR, Nuclear magnetic resonance; NTD, Needle trap devices; SPME, Solid phase micro-extraction; SS-IMS, Subsurface-ion mobility spectrometry; TW-IMS, Travel wave-ion mobility spectrometry; UV, Ultraviolet; VOC, Volatile organic compound.

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http://dx.doi.org/10.1016/j.eaef.2016.05.004
1881-8366/Published by Elsevier B.V. on behalf of Asian Agricultural and Biological Engineering Association.

## 1. Introduction

Pre- and post-harvest crop management is critically important in agriculture worldwide. Proper agricultural produce management through integrated sensing based decision-making will not only result in preventing economic losses to the producers; but also will address aspects of global food security. For example, early detection of plant diseases and disorders (before the onset of disease symptoms) could be vital for implementing proper pest management and disease control strategies. Similarly, rapid sensing for post-harvest food quality monitoring throughout packaging and market supply-chain can reduce the agricultural produce losses and might improve consumer perception. Therefore, academia and industry have put enormous thrust towards development and evaluation of non-contact rapid sensing modules for pre- and post-harvest produce management. Prior and ongoing research suggests that several sensing approaches and techniques have been explored to address this aspect. One such approach is volatile organic compounds (VOCs) or biomarker-based sensing.

Naturally, plants and agricultural produce release key volatiles that can be associated with their morphological and physiological status, which can be affected by abiotic/biotic stress factors and other disorders. These VOCs or the VOC profile can be an indicator of plant or produce condition. VOC-based sensor technologies facilitate non-invasive, real-time detection of biological volatiles can be utilized to prevent the crop losses, improve agricultural management practices, and ultimately provide economic benefits (Sankaran et al., 2010). Dudareva et al. (2006) reviewed a range of volatiles released by the plants under stress such as terpenoids, phenylpropanoids and benzenoids, volatile fatty acids (trans-2-hexenal, cis-3-hexenol and methyl jasmonate), and amino acid volatiles (such as aldehydes, alcohols, esters, acids, and nitrogen- and sulfur-containing volatiles derived from amino acids), which can be used for such applications (Sankaran et al., 2010).

Different techniques have been used to evaluate volatiles qualitatively and quantitatively. Most common techniques of biogenic VOCs determination are based on purge-and-trap or headspace sampling methods, such as solid-phase micro extraction (SPME), followed by gas chromatography-mass spectrometry (GC-MS) analysis (Fellman et al., 1993). However, sample preparation for GC-MS analysis can be time consuming, expensive, and requiring specific skills for proper operation. Thus, such techniques of VOCs monitoring may not be applicable for rapid volatile monitoring in agriculture (Laothawornkitkul et al., 2008; Ciesa et al., 2013). Similarly, technologies such as proton transfer reaction-mass spectrometer (PTR-MS), nuclear magnetic resonance (NMR), and liquid chromatography-mass spectrometry (LC/MS) are capable of providing more comprehensive chemical information (the semi-volatiles and higher molecular weight plant metabolites) but are limited to laboratory settings (Alexander et al., 2013). In comparison to MS and other methods discussed above, electronic nose (e-nose) is faster, less expensive, and can be used in field conditions without the requirement of sample preparation. Yet, some of the limitations include: 1) poor reproducibility, 2) lower resolution signal drift, 3) difficulty in correlating e-nose responses with other analytical sensor outputs, and 4) challenges in identifying and quantifying specific compounds (Zhang and Li, 2010; Sankaran et al., 2012; Alexander et al., 2013).

Recently, handheld ion mobility spectrometry (IMS) modules have been developed into field portable systems for warfare chemicals and illegal narcotics detection (Cumeras et al., 2015b). The other common IMS applications are towards 1) detection of drugs and explosives in civil airports, 2) detection of chemical weapons in combat areas, and 3) investigation of ion-molecule reaction, ion structure, and conformation of biomolecules such as peptides and proteins and separation of isomers (Arce and Valcarcel, 2013). Review of scientific publications indicate that about 36% of IMS applications are in explosives and chemical warfare detection, 21% in pharmaceutical and drugs, 14% in clinical and biological studies, 9% in environmental studies, 8% in quality control, 5% in food, 5% in forensic, and 2% in industry and other fields (Arce and Valcarcel, 2013). The portability, high sensitivity, accuracy, ease of optimization, and a fast response time (ms) at room temperature and atmospheric pressure makes IMS a prospective sensing system for detecting volatiles in diverse environment (Harden and Shoff, 1997; Pollard et al., 2011). Moreover, IMS technology offers chemical profile data with higher qualitative and quantitative accuracy during measurements, although it is more expensive than photoionization detectors and e-noses (Arce et al., 2008; Mayer and Borsdorf, 2014). IMS based non-contact sensing technologies has not been applied widely in agriculture. Thus, the major focus of this review will be towards agricultural applications that include: soil contamination assessment, toxic chemicals detection, plant stress monitoring, produce quality and safety, and other pertinent applications such as food and beverage, and wood quality (DeBono et al., 2001; Vautz et al., 2004b; Vautz et al., 2006; Borsdorf et al., 2009; Zhang et al., 2011; Owlstone, 2013; Aksenov et al., 2014; Rutolo et al., 2014).

## 2. Advances in ion mobility spectrometry

The working principle of IMS is illustrated in Fig. 1a. An IMS consists of four main components: 1) sample introduction system, 2) molecule ionization source, 3) drift tube for separation and selection of ions, and 4) ion detector (Márquez-Sillero et al., 2011). The drift tube is considered the heart of an IMS where ions are created utilizing the ionization source under the electric field and allowed to migrate (Hill et al., 1990). Normally, Faraday plates are used as the detector and to measure ion current in IMS instruments (Fig. 1a).

Once the sample is introduced through a carrier gas into the ionization chamber, it is ionized to form different ions (positive or negative ions) depending on the ionization source. These ions are transferred to the separation chamber (drift region) via an electronic grid. Drift region/tube contains an electric field and drift gas that separates the ions according to mobility (Márquez-Sillero et al., 2011). Smaller size ions moves faster and reach the detector earlier than larger ions. A collector (Faraday plate) detects the arrived ions and generates a current. The generated current is amplified for producing a mobility spectrum. The ion mobility ($K_0$) is defined as the ratio of the ion velocity to the magnitude of electric field (Hill et al., 1990) and is dependent on characteristic properties of a sample (i.e. size, charge and mass of the ion). At the detector, ions collide and annihilate, and resulting ion current is recorded with respective time stamp (Márquez-Sillero et al., 2011). Thus, a plot of ion current against $K_0$ forms an ion mobility spectrum, with corresponding ion mobility bands to each of the unique ionic species (Fig. 1b). The spectrum is a fingerprint of the parent compounds.

Please cite this article in press as: Kafle, G.K., et al., State of ion mobility spectrometry and applications in agriculture: A review, Engineering in Agriculture, Environment and Food (2016), http://dx.doi.org/10.1016/j.eaef.2016.05.004