PTR-MS monitoring of VOCs and BVOCs in food science and technology

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Volatile organic compounds (VOCs) and biogenic VOCs (BVOCs), in particular, are a major topic in food science and technology. They play an important role in the perception of odor and flavor and, thus, in food appreciation. Their fast, non-invasive detection helps to control product quality and to monitor fundamental and industrial processes. Furthermore, there is increasing concern about the impact of VOCs and BVOCs from food production on our environment and health.

In this contribution, we discuss food-related applications of proton transfer reaction mass spectrometry (PTR-MS), an emerging technique that allows direct, fast, sensitive monitoring of VOCs. After introducing the principles of PTR-MS, we review its applications in food science and technology, highlighting its capabilities from using complete mass spectra as characteristic fingerprints all the way to identifying and quantifying single compounds in a complex food matrix. We end with a description of fundamental studies from food sciences and outline new opportunities offered by recent technological advances.

Keywords: Aroma; Biogenic volatile organic compound; BVOC; Direct-injection mass spectrometry; Fingerprinting mass spectrometry; Flavor; Proton transfer reaction mass spectrometry; PTR-MS; VOC; Volatile organic compound

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1. Introduction

In environmental studies and atmospheric chemistry, the origin of VOCs (volatile organic compounds) is typically characterized as either ''biogenic'' or, the opposite, ''anthropogenic''. So the term ''biogenic VOC'' (BVOC) is one of the typical trademarks of these fields and is less used in other contexts. However, VOCs in general and BVOCs, in particular, play a most relevant role in agro-industrial processes, and food science and technology.

The principal reason is that they are at the origin of both the aroma and flavor of food and hence control human sensory perception of food. For example, the smell, also called orthonasal stimulation, is caused by the appealing scent of fresh fruit, while the flavor released during eating or drinking, is part of the long-lasting pleasure (e.g., of a glass of wine that is modified by the changes of the VOCs released in our mouth and reaching our nose, this being a vivid example of retronasal stimulation). Thus, improvement in food quality must also consider its complex flavor profile, the origin of this profile, its evolution in time and the interaction with people [1,2]. It is worth noting that, among the human senses, olfaction (also termed a chemical sense) is probably the most complex and least understood. In contrast to the physical senses, hearing and sight, or taste, the olfactory system comprises a large number of receptors, more than 900, and it has only relatively recently been deciphered [3]. It is clear that the success of future research in this field will also depend on the available methods to identify, to quantify and to monitor the olfactory stimuli (i.e. VOCs).

A second reason for the relevance of VOCs in food science is that they are produced and released in most stages of the food-production chain ''from farm to fork'' (i.e. from plants and crops, during fruit ripening and maturation, in food processing and storage and, eventually, during food consumption). They also create an interesting link to atmospheric studies because, in several regions, BVOC emissions are, at least for certain species, dominated by emissions from crops [4]. Direct BOVC monitoring is therefore an

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important non-invasive tool for product characterization and process monitoring in agro-industrial applications. With regards to the latter, there is also increasing awareness about BVOC emission from food industries, farms or composting plants because of public health and environmental issues [5]. Moreover, food-related BVOCs were recently investigated in connection with emerging themes {e.g., their possible link with health [2,6] or ecological issues also in view of organic pest management [7]}.

Given this, it does not come as a surprise that there is a huge literature on VOCs in food, mostly of biogenic origin. A general reference for technical aspects, not limited to foods, is the book edited by Berger [8], which also includes interesting chapters on biogenic precursors of flavor compounds and bioprocessing. Two additional references in this context are a recently edited book by Taylor and Linforth [9], and the review of Ross on studies related to sensory analysis and instrumental characterization of food [10].

From a technical point of view, gas chromatography (GC) [11] is the reference method for the analysis of food VOCs. But there is also a growing need to develop rapid, simpler methods [12] to overcome its main limitations, as GC is still a time-consuming procedure. There is therefore genuine interest in the development of methods for rapid, non-invasive and very sensitive monitoring of volatile compounds emitted from food samples. On the one hand, a rapid procedure is necessary to go in the direction of high-throughput analysis that can be of benefit for analytical laboratories, quality control and, in view of possible connections of BVOC profiles, genomics and metabolomics [13]. On the other hand, high time resolution will allow real-time monitoring of fast processes in agro-industry [14,15], oral processing during food consumption and model mouth experiments in connection with textural changes [16].

Among the various possibilities proposed and investigated for rapid identification and quantification of VOCs in food [9] is proton transfer reaction mass spectrometry (PTR-MS) [17,18], which allows rapid, direct and highly sensitive on-line monitoring of VOCs.

In this contribution, we review the work of the various groups that have addressed the above-mentioned issues in food science and technology by PTR-MS. In Section 2, we briefly describe the technique and give a methodological perspective, in order to provide a rationale for its use in food science and technology. In Section 3, we review several practical applications, and, in Section 4, we describe recent developments. Section 5 is dedicated to conclusions and future trends.

2. The PTR-MS technique

PTR-MS has been described in detail in several reviews: the first by Lindinger and co-workers [17]; a more recent, general review by Blake et al. [18]; and, the very thorough one by de Gouw and Warnecke, focusing on environmental applications [19]. Here, we briefly describe its main characteristics and highlight the benefits of applying PTR-MS in food science and technology. In the most common version of PTR-MS apparatus (Fig. 1), a hollow cathode ion source produces an intense, pure H_3O^+ ion beam that is driven by a homogeneous, relatively high, electrical field through a drift-tube reactor

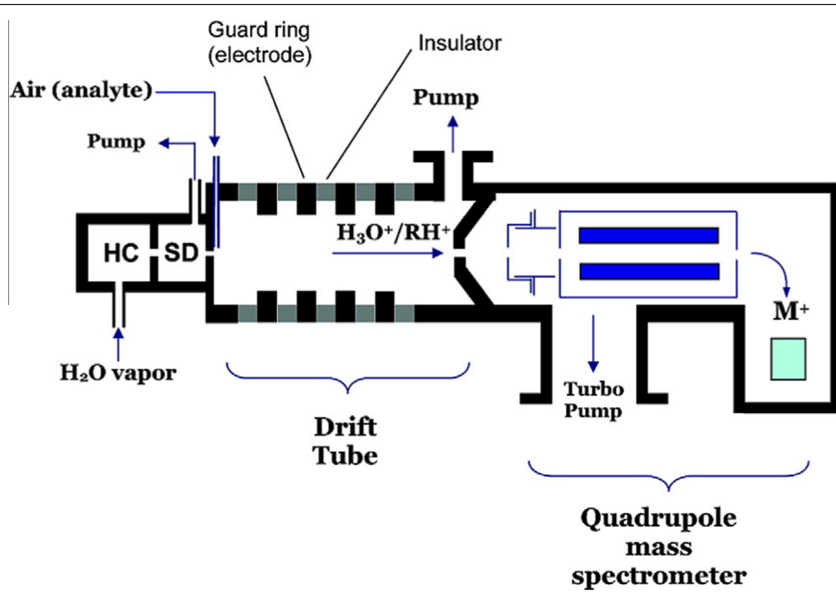

Figure 1. Simplified representation of a proton-transfer reaction mass spectrometer utilizing a quadrupole mass filter (HC = hollow-cathode discharge source, SD = source drift region) (Reprinted with permission from [18]; © 2009 American Chemical Society).