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Comprehensive Odor Measurement with AI-Supported Chemical Analytics and a Transition to Sensor Systems

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Summary:
A reliable description of an odor includes both the overall impression of the odor-active volatile compounds and their chemical identity. Efficient methods for the chemical and sensory analysis of the aroma properties of a product or raw material enable a high sample throughput with maximum efficiency. For the evaluation and correlation of the extensive datasets, an AI-supported evaluation procedure was developed, which outputs the maximum information content from the available data in the shortest possible time. Based on the information obtained in this way, instrumental odor measurement systems can be developed to enable efficient odor measurement for specific applications.

Keywords: odor, aroma, odor analysis, sensor system, data analysis

Introduction

The evaluation and decoding of odor characteristics of products and raw materials contributes significantly to the development of new foods, packaging solutions and beverages. Ultimately, it is the sensory perception, especially the aroma, but also the appearance, that determines whether a product appeals or repels to consumers.

Unlike most other human senses, such as hearing and sight, smell is still difficult or impossible to translate into a universally applicable standard unit. On the one hand, this is due to the fact that the sense of smell exhibits strong inter-individual differences, which can be attributed to the genetic predisposition of certain receptors. On the other hand, the human correlation between an olfactory impression and the verbal expression of the impression can be understood as a linguistics of its own, which is learned depending on cultural background and habitat for the most part.

This dramatically complicates the validation of sensors that are intended to supplement or even completely replicate the human sense of smell. However, if this task is approached from the human sensory side, accompanied by instrumental analysis, a number of methods and techniques are already available that make it possible to validate technical odor sensors using established standard units and methods. This also requires the processing of comprehensive datasets from various corresponding measurement methods, for which we present an approach that is as holistic as it is efficient.

Odor Analysis by Comprehensive Measurement Technologies

The volatilome contains numerous volatile compounds, only a fraction of which can be detected by the human nose. Accordingly, the analysis of odor-active volatile organic compounds is based on two detection principles: The overall impression of a product or raw material, in particular direct differences to similar products and raw materials, is analyzed using the human nose as a detector in human sensory tests. The most potent odor-active compounds can then be worked out via sophisticated analytical methods. The previously determined odor-active substances are identified and, if necessary, quantified using gas chromatography (GC) in conjunction with suitable detectors (e.g., mass spectrometer; MS). Coupled systems, such as GC-MS fitted with an odorant detection port (GC-MS/O) enable a comprehensive analysis of odor mixtures and have established themselves as the gold standard in aroma analysis.

Smart Odor Analysis – KI-Assisted Data Analysis for Odor Assessment

The described gold standard enables a comprehensive, but also time-consuming and cost-

intensive analysis of the odor-active compounds in a sample. In many applications, however, the time factor is clearly in the foreground - a high sample throughput must lead to meaningful information in the shortest possible time.

In an attempt to solve this shortcoming, an assessment for AI-assisted odor analysis was developed. Based on efficient methods for human sensory investigations and complementary chemical analyses, a pipeline that supports efficient data analysis using statistical methods for data correlation and automated data processing is being continuously developed and expanded [1] [2]. The correlation of odor impressions and identities of single compounds opens the path to a variety of compiled information on odor characteristics in order to gain maximum information content with minimum effort. The concept is by- and inline-capable and allows the comparison of large sample sets. Following the successful proof of principle, as well as the testing and validation of different approaches and methods, e.g., using whiskey as an example, the transferability of the smart odor assessment approach to other product groups, such as new foods and plastic regrinds, is now under investigation [3].

Miniaturizing Gas Chromatography – a Toolbox for Instrumental Odor Measurement Systems

Instrumental gas analysis as laboratory analysis is ideal for obtaining comprehensive information on all volatile compounds present in a sample. For many applications, however, only specific information is required for a small selection of odor-active compounds, for example, to observe the formation of certain volatile markers for spoilage or fruit ripening [4].

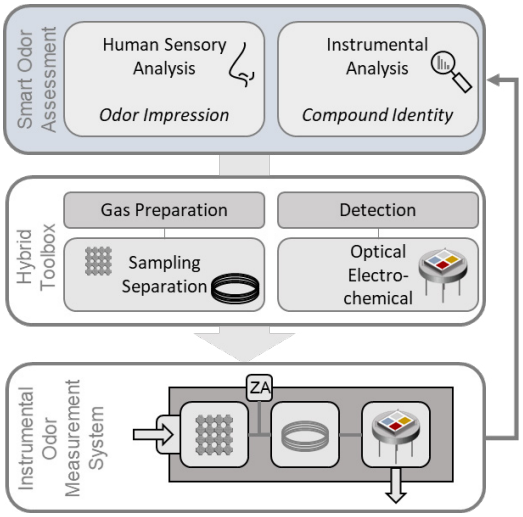

Figure 1: Workflow towards smart odor assessment supported by instrumental odor measurement systems.

Since these systems should be suitable for continuous monitoring in the production process or storage, a structural miniaturization of gas chromatography is an obvious choice. Many of the components required for this are already manufactured in series and are available in large quantities at low cost. This applies in particular to small, cost-effective broadband detectors, such as those found in the field of infrared sensors and metal oxide semiconductor gas sensors. For the latter it has been shown that they can have remarkably low detection limits of below 100 fg [5]. In order to increase selectivity, the volatile compounds are separated into their individual components on a short separation column prior to detection and detected individually on the sensor. Equipped with suitable software for calibration, such smart sensing systems can be used for continuous monitoring of odorants. Implemented in or in addition to the smart odor assessment approach, this has high potential for efficient low-cost odor evaluation.

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