



Food Chemistry, Function and Analysis

Food Contact Materials Analysis

Mass Spectrometry Techniques

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Preface

Evolution of Mass Spectrometry Methods for Food Contact Materials Applications

Food packaging is surely a topic of worldwide relevance and importance. In recent decades, mass spectrometry (MS) has made incredible progress; in parallel, packaging solutions devoted to food have increased their number and varieties in many ways. The handling of issues with food contact materials (FCMs) requires a deep contemporaneous knowledge of both the materials and the food worlds.

Consumers' needs and expectations have been growing for many years in combination with true globalization of the markets; at the same time, the legal requirements and harmonized international regulations for FCMs are still far from being achieved.

Food safety, quality and traceability topics imply more and more continuous analytical improvements and efforts, and these find most of their solutions and effectiveness in the MS technique. In particular, this book, in addition to highlighting the mentioned topics, places special emphasis on the following three aspects:

- *demonstrates how in the last 20 years MS has become more and more available and diffused in many analytical laboratories and industrial facilities;*
- *combines different approaches utilizing MS as a tool for solving many different food packaging problems;*
- *gives concrete and practical MS protocols to stakeholders that testify to the great flexibility of MS.*

The book is therefore aimed at a wide potential audience such as postgraduates, academics and industrialists.

The first two chapters start to set the scene about risk assessment for both paper/board-based and plastic-based FCMs. In fact, the law requires the determination of contaminants or specific substances used for different purposes in the production of FCMs. A combination of analytical protocols with very high sensitivity and resolution allows a thorough description of all the species that must be monitored, and many of the standard methods used to determine these specific substances involve the use of MS.

Chemical substances intentionally added to FCMs to enhance the physico-chemical properties and extend the product shelf life can be released during the various recycling steps and recovery processes. Starting compounds and additives (fillers, absorbers, antioxidants, photoinitiators, ...) are commonly used in the manufacture of FCMs and may remain unreacted in the matrix and consequently migrate into food, leading to a potential health issue: the third chapter illustrates the chemical nature and properties of these additives explored through MS.

Chapter 4 then reviews MS studies devoted to the complex world of adhesives (employed in packaging to manufacture laminates or to build up the final form of a packaging) and their various formulations, which involve a large number of volatile and semivolatile compounds. In this context, headspace solid-phase extraction (HS-SPE), headspace solid-phase micro-extraction (HS-SPME) and gas chromatography–olfactometry (GC-O) are usually combined with MS detection.

Indeed, GC-O is a suitable technique for the determination of off-odours resulting from the presence of odour-active compounds. This aspect is discussed in Chapter 5, where key parameters that have an impact on mass transfer in the migration of volatile substances from/to FCMs are considered, introducing migration and permeation tests in combination with proper sampling methods and analytical solutions, with GC-FID (flame ionization detection) and GC-MS in the foreground. In this chapter, the typical instrumentation applied for tackling different migration analytical scenarios is discussed in detail, by showcasing also the screening potential of ambient desorption and direct injection MS.

Every time migration phenomena occur within food packaging materials, they can potentially lead to sensory changes, playing a key role in how packaged food is received by consumers. Chapter 6 considers the interactions between packaging, food and the environment surrounding food. Sometimes it is necessary to avoid them as much as possible, but on other occasions, such as with so-called “active packaging,” there is an intentional need to favour them. Understanding these interactions implies the application of multidisciplinary knowledge, ranging from molecular chemistry to cognitive psychology, where, again, MS maintains a place of primary importance.

Let us now move on “opening the black box” of non-intentionally added substances (NIASS): these are chemical compounds that can migrate from FCMs but were not added on purpose. Their origin can be related to, for

example, degradation of the material's components, impurities of raw materials used in processing, *etc.* Is MS the right tool also for investigating these “not added originally”/not present in the positive list of authorized starting substances and additives? Chapter 7 says yes!

The identification of unknown migrants from FCMs is a really complicated issue since neither chemical and spectral databases nor analytical standards are available. Here a particularly strategic approach is the implementation of liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS) in combination with proper statistical data treatment. Chapter 8 addresses the most relevant non-target/HRMS data acquisition modes and also the data handling used for the identification/characterization of food packaging contaminants.

The application of engineered nanomaterials in FCMs represents a new direction for interesting new functions, but the toxicological implications are still a partially unknown menace. Chapter 9 comments constructively on how information collected especially by inductively coupled plasma mass spectrometry (ICP-MS) can be combined with that derived from other microscopy/fractionation techniques in order to detect the size and concentration of nanoparticles and better understand the mechanisms of the migration of nanoparticles from FCMs to food.

A final question remains after having considered such an intricate scenario: what are the best analytical solutions that can be efficiently and commonly applied among industries and/or outsourced to expert laboratories? Chapter 10 gives the answer to this delicate question, illustrating how these analytical solutions are really based on MS with a clear tendency towards HRMS, focusing on multi-methods to cover several analytes in parallel, screening out of simulants and opening the door in the future to the more comprehensive full screening of food itself.

This is the first book to be exclusively dedicated to the topic of the interconnections of mass spectrometry and FCMs and its facets. It will provide the interested reader with an excellent overview of the topic and with detailed insights into the rapidly developing field of these analytical approaches.

This book will take the reader to a final overall conclusion: “*The great effectiveness of mass spectrometry in solving food contact materials issues*”. Enjoy!

Michele Suman

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