Emerging Contaminants and Associated Treatment Technologies

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Contaminant Levels and Ecological Effects

Understanding and Predicting with Chemometric Methods

Springer

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Preface

The biosphere is the medium that is naturally optimized for the growth and development of a huge number of biological organisms. Nature itself creates natural disasters that degrade the ecosystems and organisms that live in it. Humans, in spite of their existential question in nature, still continuously degrade nature and its living environment. This anthropogenic factor affects all segments of the environment, the lower parts of the atmosphere, the upper parts of the lithosphere, as well as the hydrosphere. Intensive technological development as well as the availability of natural raw materials for their utilization have significantly enabled the progress of these degradation processes in nature. On the other hand, the chemical and pharmaceutical industry, with their intensive development, have generated substances that are not only unnatural but also highly risky for the human population and the environment. Pollutants and potentially toxic substances are continuously introduced into all segments of the biosphere, shifting the natural balance of natural normal distributions. The environmental pollutants create abnormal media for living organisms. These days, we are increasingly faced with the fact of the ecological risk for the survival of many species. In recent decades, researchers have paid great attention to environmental risk, determining the pollution index and identifying polluted sites where it is necessary to prevent further degradation. Therefore, several critical aspects should be involved when we initiate and launch environmental research or monitoring. One of the aims of the modern environmental investigations is to obtain more objective data for the complex but silent environmental markers, which will be identified as typical pollutants in various parts of the environment. The modern analytical approaches involve sophisticated and sensitive instrumental technique, but the main question is how to create a corresponding data matrix and proper data analysis. Chemometrics is a routine chemical sub-discipline, which involves several mathematical methods for extracting more realistic and proper environmental information. The implementation of modern and novel chemometric methods becomes a critical point in the environmental studies these days. Therefore, this book summarizes the latest investigations of the concerning parts of the biosphere, affected with hazards substances. Moreover, selected case studies investigation with spacious applicability will create general framework of the opportunities, advantages, weaknesses, and anomalies of the mathematical approaches of the analysts. Furthermore, a properly defined chemometric model of each environmental investigation will provide long-term applicability potential.

This book consists of 13 chapters contributed by relevant experts in various fields correlated with environmental issues. All the chapters are logically selected and arranged to provide comprehensive state-of-the-art information about the practical aspects of environmental chemometric approaches. In this volume, the introductory chapter gives an overview of the critical environmental issues, such as degradation, ecological risks, and silent hazards. The next five chapters are on air pollution aspects: pollutants, hazardous emissions, monitoring, indication, as well as spatial indication of emission sources. This chapters give attention to air pollution, air deposition, and distribution models. Certain emphasis is given to the moss effectiveness for bioindication of the potential ecological risk. Another chapter is dedicated to the application of lichens as the main indicator in biological monitoring of air quality. Water pollutants and their determination issues are the main topics in the next two chapters, covering key issues in spatial distribution of various metals in different parts of the environment. These chapters deals with improving effective analytical methodologies of GC–MS and ICP-MS for tracking potential contaminants. This is followed by research into the effective removal of toxic hazard from aquatic systems. The next group of chapters is dedicated to the state of chemical characterization of the plant food and endemic plant species as characteristic media that involves the potential ecological risks. The presented are multidisciplinary approaches which enable detailed and precise elaboration of the set research subject.

All the chapters and their contents are supported by extensive citation of available literature; calculation and assumptions are based on realistic facts and figures of the present status of research and development in this field. This book will provide a wealth of information based on a realistic evaluation of contemporary development in environmental investigations with special emphasis on the latest research studies. Furthermore, this book also highlights the potential and perspective use of the multidisciplinary aspect for enchasing environmental pollution and potential ecological risks.

Most of the chapters cover advanced research as well as the use of more sophisticated methodologies. Therefore, we believe that the usefulness of this book will be primarily directed to experienced researchers. But of course we also encourage young researchers to use the book, because in many of the chapters, the methodologies used by the authors are explained very basically. We also believe that certain institutions and state regulatory bodies can use this book as an initiator for critical issues related to environmental degradation, environmental risks and their determination, and future prevention.

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List of Abbreviations

AAS	Atomic absorption spectrometry
AED	Atomic emission detector
AES	Atomic emission spectrometry
AF	Attenuation factor
AFR	Revised attenuation factor
AFT	Log-transformed attenuation factor
ALA	Alpha linolenicacid
ANN	Artificial neural networks
ANOVA	Analysis of variance
APCI	Atmospheric pressure chemical ionization
ATP	Adenosine triphosphate
BAF	Biological accumulation factor
BTF	Biotransfer factor
CA	Cluster analysis
CART	Classification and regression trees
CDI	Chronic daily intake dose
CEC	Cation exchange capacity
CHCA	A-cyano-4-hydroxycinnamic acid
CR	Carcinogenic risk
CVAAS	Cold vapor atomic absorption spectrometry
DBCP	Dibromochloropropane
DCM	Dichloromethane
DHA	Docosahexaenoic
DMT	Digital terrain models
DRC	Dynamic reaction cell
DTPA	Diethylenetriamine pentaacetic acid
DW	Dry weight
EC	Elemental carbon
ECD	Electron capture
EDB	Ethylene dibromide
EDS	Energy dispersive X-ray spectrometry

EEA	European Environment Agency
ELISA	Enzyme-linked immunosorbent assay
EPA	Environmental Protection Agency
EPA	Eicosapentaenoic
ESI	Electrospray ionization
ETAAS	Electrothermal atomic absorption spectrometry
FID	Flame ionization detector
FS	Fluorescence spectroscopy
GC	Gas chromatography
GHG	Greenhouse gas
GLI	Global leachability index
GUS	Groundwater ubiquity score
GWCP	Groundwater contamination potential
HI	Hornsby index
HPLC	High-performance liquid chromatography
ICP–AES	Inductively coupled plasma – atomic emission spectrometry
ICP–MS	Inductively coupled plasma – mass spectrometry
IR	Infrared spectroscopy
IRMS	Isotope ratio spectrometry
LA	Linoleic acid
LC	Liquid chromatography
LDA	Linear discriminant analysis
LEACH	Leaching index
LIX	Screening leachability index
LLE	Liquid-liquid extraction
LOD	Limit of detection
LOQ	Limit of quantification
LPI	Leaching potential index
LSD	Least significant differences
MAC	Maximum permissible concentrations
MALDI	Matrix-assisted laser desorption/ionization
MS	Mass spectrometry
MSA	Multivariate statistical analysis
NMR	Nuclear magnetic resonance
ORS	Octopole reaction system
PC	Principal components
PCA	Principal component analysis
PDA	Photodiode array
PDO	Protected designation of origin
PGI	Protected geographical indication
PLP	Pesticide leaching potential index
PTFE	Polytetrafluoroethylene
PTH	Parathyroid hormone
PTR-MS	Proton transfer reaction mass spectrometry
RAF	Relative accumulation factors

REEs	Rare earth elements
RLP	Relative leaching potential index
SA	Sinapic acid
SEM	Scanning electron microscopy
TDS	Total dissolved solids
TEP	Thermoelectric power plant
TF	Translocation factor
TGA/DTA	Thermogravimetric and differential thermal analysis
TIN	Triangular irregular network
TLC	Thin layer chromatography
TOF	Time-of-flight
TPP	Triphenylphosphate
VI	Volatility index

Contents

Chapter 12
Characterization of Multi-element Profiles and Multi-isotope Ratio Records as a Tool for Determination of the Geographical Origin of Various Plant Species

Liping Fan, Minxiu Yan, Meicong Wang, Yanqiu Liang, Xiaoguang Kong, Chong Li, and Biljana Balabanova

Abstract Determination of food authenticity is an important issue in quality control and food safety. In recent years, many serious diseases appeared related to foodstuffs, so providing the motivation for the scientific community to work more intensively in this area. Authenticity is a quality criterion for food and food ingredients and is required more and more worldwide, as a result of legislative protection for regional foods. Reviews of analytical methods for the determination of geographical origin of food and beverages have been published. However, organic components of a food crop production depend on various conditions (e.g. fertilization, history of the field, climatic conditions in the year of cultivation, geographic location and soil composition), so it is not always possible to determine the origin of a product by analysing the organic components. Additionally, methods based on elemental composition have been reviewed as have methods based on isotope ratios. Over the past decade, with the development of new advanced analytical techniques [e.g. thermal ionization MS (TIMS), inductively coupled plasma MS (ICP-MS) and dynamic reaction cell-ICPMS (DRC-ICPMS)], we can successfully retrieve elemental and isotopic compositions of any given food sample and determine the geographic origin successfully. The growing concern of the consumers stimulated

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scientific research and publications in recent years, including multi-element and isotope ratio methods of analysis in food authentication after statistical evaluation of the results. Several aspects will be described: (a) propose a new technique for evaluating spatially explicit trace element profile in various environmental samples (with organic and inorganic complex matrixes); (b) evaluate whether element composition of the environmental samples can be attributed to large-scale geographic trace element variation associated with underlying geology or fine-scale spatial differences related to foraging habitat; (c) determine whether element profiles along the individual species are autocorrelated (i.e. occurring in a predictable or random pattern); (d) prove spatially resolved multi-element information that could be used for identification of geographical origin of various environmental samples and foodstuffs.

Keywords Isotopic ratio · Trace elements · Foodstuff · Mass spectrometry

12.1 Introduction

Historically, food products have always been linked with a specific geographical origin. Food consumption habits were created by the local natural resources and the social or cultural factors of the community. Such links have disappeared over the time for various reasons, mostly because of the globalization of the food industry, following the extensive growth in technological means over the past century. Thus, food consumption in a region no longer necessarily reflects food production of that area. However, in recent years, consumers have renewed their interest in food strongly identified with a place of origin (Giovannucci et al. 2009). The reasons for this increasing interest of consumers vary from the global trend for organic and health products to their concern about animal welfare and environmental friendly methods of production (Heaton et al. 2008). Resulting from this trend, local products around the world regained their fame and brought wealth to local producers, so product authenticity and authentication are emerging topics. Consumers in developed countries demand food products of high quality, one of the basic parameters being origin (Giovannucci et al. 2009).

A modern trend is the consumption of food produced locally, in order to reduce energy footprint and pollution through transportation. Determination of food authenticity is an important issue in quality control and food safety. In recent years, many serious diseases appeared related to foodstuffs, so providing the motivation for the scientific community to work more intensively in this area. Authenticity is a quality criterion for food and food ingredients and is required more and more worldwide, as a result of legislative protection for regional foods.

Foodstuff authentication may cover many different aspects, including mislabelling, misleading claims about origin and adulteration, which is defined as a process by which the quality or the nature of a given substance is reduced by adding a