

# Contaminant Levels and Ecological Effects

Understanding and Predicting with Chemometric Methods



### **Emerging Contaminants and Associated Treatment Technologies**

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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,

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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.

Štip, Republic of North Macedonia Skopje, Republic of North Macedonia Biljana Balabanova Trajče Stafilov

### **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

viii List of Abbreviations

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

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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

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## Chapter 1 General Aspects of Environmental Degradation vs. Technological Development Progression



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Biljana Balabanova

Abstract A look at natural resources in terms of life cycle reveals several environmental problems related to production and consumption and combines resource use and waste generation. The use of resources and the generation of waste are special impacts on the environment, but the two issues share many of the same driving forces – largely related to how and where we produce and consume goods and how we use natural capital for economic sustainability development and consumption. More recently, life cycle thinking has been introduced as the guiding principle of resource management. Environmental impacts are considered throughout the life cycle of products and services to avoid or minimize the transfer of environmental stress between different stages of the life cycle and from one country to another. With the passage of time and the long-term activities of the human factor, the contents of certain metals have been completely and permanently changed in relation to their natural existence in the environment. These changes can have a significant influence on the physiology and ecology of the organisms adapted to survive in thus created conditions of higher metal contents. The anthropogenic activities for exploitation of natural resources and their processing through adequate technological processes and management of the waste produced by the same represent a global problem of pollution of the environment. The distribution of the different chemical elements, including the potentially toxic metals, creates characteristic conditions for the living organisms. Considering that their contents in the environment are variable, it is important to identify the regions with changed contents, differing from the natural distribution of the elements in the different segments of the biosphere.

**Keywords** Bio-toxic hazards  $\cdot$  Environmental pollution  $\cdot$  Mass spectroscopy  $\cdot$  Toxicity

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