

The Handbook of Environmental Chemistry

Founded by Otto Hutzinger

Editors-in-Chief: Damià Barceló • Andrey G. Kostianoy

Volume 57

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Modelling the Fate of Chemicals in the Environment and the Human Body

Volume Editors: Philippe Ciffroy · Alice Tediosi ·
Ettore Capri

With contributions by

A. Altenpohl · Z. Banjac · D. Barceló · P. Bataillard · R. Bonnard ·
C. Brochot · E. Capri · P. Ciffroy · C. Couégnas · A. Critto ·
T. De Wilde · N. Duhanyan · J. Garatt · A. Ginebreda ·
E. Giubilato · V. Guérin · P. Isigonis · M. Krimissa · V. Loizeau ·
L. Musson-Genon · A. Paini · S. Panizzi · P. Quindroit ·
A. Radomyski · A. Radovnikovic · Y. Roustan · N.A. Suciu ·
T. Tanaka · A. Tediosi · F. Verdonck · A. Zabeo

Editors

Philippe Ciffroy
National Hydraulics and
Environment Laboratory
EDF R&D
Chatou, France

Alice Tediosi
Aeiforia srl
Gariga di Podenzano, Piacenza
Italy

Ettore Capri
OPERA Research Center
Università Cattolica del Sacro Cuore
Piacenza, Italy

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Editors-in-Chief

Prof. Dr. Damià Barceló

Department of Environmental Chemistry
IDAEA-CSIC

C/Jordi Girona 18–26
08034 Barcelona, Spain
and

Catalan Institute for Water Research (ICRA)
H2O Building
Scientific and Technological Park of the
University of Girona

Emili Grahit, 101
17003 Girona, Spain
dbcqam@cid.csic.es

Prof. Dr. Andrey G. Kostianoy

P.P. Shirshov Institute of Oceanology
Russian Academy of Sciences

36, Nakhimovsky Pr.
117997 Moscow, Russia
kostianoy@gmail.com

Advisory Board

Prof. Dr. Jacob de Boer

IVM, Vrije Universiteit Amsterdam, The Netherlands

Prof. Dr. Philippe Garrigues

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Prof. Dr. Alice Newton

University of Algarve, Faro, Portugal

Prof. Dr. Donald L. Sparks

Plant and Soil Sciences, University of Delaware, USA

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- Aims and Scope
- Instructions for Authors
- Sample Contribution

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Aims and Scope

Since 1980, *The Handbook of Environmental Chemistry* has provided sound and solid knowledge about environmental topics from a chemical perspective. Presenting a wide spectrum of viewpoints and approaches, the series now covers topics such as local and global changes of natural environment and climate; anthropogenic impact on the environment; water, air and soil pollution; remediation and waste characterization; environmental contaminants; biogeochemistry; geoecology; chemical reactions and processes; chemical and biological transformations as well as physical transport of chemicals in the environment; or environmental modeling. A particular focus of the series lies on methodological advances in environmental analytical chemistry.

Series Preface

With remarkable vision, Prof. Otto Hutzinger initiated *The Handbook of Environmental Chemistry* in 1980 and became the founding Editor-in-Chief. At that time, environmental chemistry was an emerging field, aiming at a complete description of the Earth's environment, encompassing the physical, chemical, biological, and geological transformations of chemical substances occurring on a local as well as a global scale. Environmental chemistry was intended to provide an account of the impact of man's activities on the natural environment by describing observed changes.

While a considerable amount of knowledge has been accumulated over the last three decades, as reflected in the more than 70 volumes of *The Handbook of Environmental Chemistry*, there are still many scientific and policy challenges ahead due to the complexity and interdisciplinary nature of the field. The series will therefore continue to provide compilations of current knowledge. Contributions are written by leading experts with practical experience in their fields. *The Handbook of Environmental Chemistry* grows with the increases in our scientific understanding, and provides a valuable source not only for scientists but also for environmental managers and decision-makers. Today, the series covers a broad range of environmental topics from a chemical perspective, including methodological advances in environmental analytical chemistry.

In recent years, there has been a growing tendency to include subject matter of societal relevance in the broad view of environmental chemistry. Topics include life cycle analysis, environmental management, sustainable development, and socio-economic, legal and even political problems, among others. While these topics are of great importance for the development and acceptance of *The Handbook of Environmental Chemistry*, the publisher and Editors-in-Chief have decided to keep the handbook essentially a source of information on "hard sciences" with a particular emphasis on chemistry, but also covering biology, geology, hydrology and engineering as applied to environmental sciences.

The volumes of the series are written at an advanced level, addressing the needs of both researchers and graduate students, as well as of people outside the field of

“pure” chemistry, including those in industry, business, government, research establishments, and public interest groups. It would be very satisfying to see these volumes used as a basis for graduate courses in environmental chemistry. With its high standards of scientific quality and clarity, *The Handbook of Environmental Chemistry* provides a solid basis from which scientists can share their knowledge on the different aspects of environmental problems, presenting a wide spectrum of viewpoints and approaches.

The Handbook of Environmental Chemistry is available both in print and online via www.springerlink.com/content/110354/. Articles are published online as soon as they have been approved for publication. Authors, Volume Editors and Editors-in-Chief are rewarded by the broad acceptance of *The Handbook of Environmental Chemistry* by the scientific community, from whom suggestions for new topics to the Editors-in-Chief are always very welcome.

Damià Barceló
Andrey G. Kostianoy
Editors-in-Chief

Preface

When studying the environment and the impact of human activities on it, we soon realise that we are dealing with a unique system, where the different compartments are strictly interconnected. On the one hand, we are to make simplifications and to fragment reality; on the other one, we see that the environment is a continuum. Exposure assessment of chemicals, as the majority of the branches of applied sciences, draws together several different disciplines. A number of works describe exposure assessment and chemical fate modelling, either in the environment or in the human body. Nevertheless, in our opinion, there is a lack of tools and information enabling investigators to understand and model the complexity of reality and therefore to obtain solutions to practical problems. The fate of chemicals in both the environment and in the human body is a very complex matter, but despite this, models have to be coupled, if we want to assess the behaviour over the whole chain and to hypothesise the possible impacts not only on the environment but also on human health. Only in this way, modelling the fate of chemicals becomes an actual and useful tool to manage the problems connected to the use of chemicals and to take actions to solve or at least to limit them. We strongly believe that the future will necessarily guide policy makers, researchers and all stakeholders to the full integration of exposure assessment.

It is with this challenge in mind that we decided to write a book about modelling the fate of chemicals in the environment *and* the human body. This work is the outcome of many years of experience and of different research activities that have led to the development of MERLIN-Expo, a software for simulating the fate of chemicals in the main environmental systems and in the human body in an integrated way (<http://merlin-expo.eu/>).

The book is composed of ten chapters. The first chapter considers the challenges of exposure assessment for the future and the evolution of human health and environmental risk assessment. The second chapter is concerned with the SWOT analysis performed to evaluate the potential of MERLIN-Expo and its relevance in legislative frameworks. In the third chapter, the standard documentation of exposure models that was developed in collaboration with CEN (European Committee

for Standardization) is described. Fourth to ninth chapters describe the modelling of different environmental compartments (i.e. surface waters, atmosphere, soil, groundwater, plants, aquatic organisms and mammals). The tenth chapter focuses on the fate of contaminants in humans using a lifetime physiologically based pharmacokinetic model.

Gariga di Podenzano, Piacenza, Italy
Chatou, France
Piacenza, Italy

Alice Tediosi
Philippe Ciffroy
Ettore Capri

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Contents

Evolution and Future of Human Health and Environmental Risk Assessment	1
Nicoleta Alina Suciu, Silvia Panizzi, Philippe Ciffroy, Antoni Ginebreda, Alice Tediosi, Damià Barceló, and Ettore Capri	
SWOT Analysis of the MERLIN-Expo Tool and Its Relevance in Legislative Frameworks	23
Tineke De Wilde, Frederik Verdonck, Alice Tediosi, Taku Tanaka, Roseline Bonnard, Zoran Banjac, Panagiotis Isigonis, Elisa Giubilato, Andrea Critto, Alex Zabeo, Nicoleta Alina Suciu, James Garratt, and Philippe Ciffroy	
Standard Documentation of Exposure Models: MERLIN-Expo Case Study	59
Annette Altenpohl, Philippe Ciffroy, Alicia Paini, Anita Radovnikovic, Nicoleta Alina Suciu, Taku Tanaka, Alice Tediosi, and Frederik Verdonck	
Modelling the Fate of Chemicals in Surface Waters	77
Philippe Ciffroy	
Modelling the Fate of Chemicals in the Atmosphere	101
Vincent Loizeau, Yelva Roustan, Nora Duhanyan, Luc Musson-Genon, and Philippe Ciffroy	
Modelling the Fate of Chemicals in Soils	127
Philippe Ciffroy	
Modelling the Fate and Transfer of Substances Discharged into Soil Unsaturated Zones and Water Tables	149
Mohamed Krimissa, Cécile Couégnas, Philippe Bataillard, and Valérie Guérin	

Modelling the Fate of Chemicals in Plants	167
Philippe Ciffroy and Taku Tanaka	
Modelling Bioaccumulation in Aquatic Organisms and in Mammals . . .	191
Artur Radomyski, Elisa Giubilato, Nicoleta Alina Suciu, Andrea Critto, and Philippe Ciffroy	
Modelling the Fate of Chemicals in Humans Using a Lifetime Physiologically Based Pharmacokinetic (PBPK) Model in MERLIN-Expo	215
Céline Brochot and Paul Quindroit	
Index	259

List of Abbreviations

Acronyms

1D	One-Dimensional
3D	Three-Dimensional
ABL	Atmospheric Boundary Layer
ACF	Atom-Centred Fragment
ADME	Absorption, Distribution, Metabolism and Excretion
AE	Assimilation Efficiency
AF	Assimilation Fraction
AGB	Above-Ground Biomass
ATP	Adenosine Triphosphate
BAF	Bioaccumulation Factor
BC	Black Carbon
BCF	Bioconcentration Factor
BDW	Body Weight
BIC	Bank Identifier Code
BMF	Biomagnification Factor
BSAF	Biota Sediment Accumulation Factor
BSE	Bovine Spongiform Encephalopathy
CAC	Codex Alimentarius Commission
CEC	Cation Exchange Capacity
CEMN	Canadian Environmental Modelling Network
CEN	Comité Européen de Normalisation (French; in English: European Committee for Standardization)
CEP	Canadian Environmental Protection
CERCLA	Comprehensive Environmental Response, Compensation and Liability Act
COMMPS	Combined Monitoring-Based and Modelling-Based Priority Setting
CRA	Comparative Risk Assessment

CRR	Critical Root Radius
CWA	CEN Workshop Agreement
DBH	Diameter at Breast Height
DDT	Dichlorodiphenyltrichloroethane
DRPC	Danube River Protection Convention
DYNAMEC	Dynamic Selection and Prioritisation Mechanism for Hazardous Substances
EC	Elemental Carbon
EC	European Commission
ECB	European Chemicals Bureau
ECHA	European Chemicals Agency
EEA	European Environment Agency
EEA	Environmental Exposure Assessment
EEC	European Economic Community
EFSA	European Food Safety Authority
EIONET- SOIL	European Environment Information and Observation Network for Soil
EMEP	European Monitoring and Evaluation Programme
EPA	Environmental Protection Agency
EPER	European Pollutant Emission Register
EQS	Environmental Quality Standards
ERA	Environmental Risk Assessment
ES	Estonia
ET	Evapotranspiration
EU	European Union
EUPRA	EU Pesticide Risk Assessment
EUSES	European Union System for the Evaluation of Substances
EXAFS	Extended X-Ray Absorption Fluorescence Spectrometry
FAO	Food and Agriculture Organization of the United Nations
FOCUS	Forum for Co-ordination of Pesticide Fate Models and Their Use
FP7	Seventh Framework Programme
GIGO	Garbage In, Garbage Out
GIS	Geographical Information System
GIT	Gastrointestinal Tract
GM	Geometric Mean
GM	Genetically Modified
GMO	Genetically Modified Organism
GPG	General Protection Goal
GSD	Geometric Standard Deviation
GSM	Global System for Mobile Communications
HHRA	Human Health Risk Assessment
IARC	International Agency for Research on Cancer
IBAN	International Bank Account Number
ICPR	International Commission for the Protection of the Rhine
ICRP	International Commission on Radiological Protection

IPCS	International Programme on Chemical Safety
IRA	Integrated Risk Assessment
IRSN	French Institute for Radiological Protection and Nuclear Safety
ISO	International Organization for Standardization
ITS	Integrated Testing Strategy
IVIV	In Vitro In Vivo
JRC	Joint Research Centre
LAI	Leaf Area Index
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
LHWA	Little Hocking Water Association
LRAT	Long-Range Atmospheric Transport
LUC	Land Use Coverage
LWC	Liquid Water Content
MCDA	Multi-criteria Decision Analysis
MEA	Millennium Ecosystem Assessment
MSCE	Meteorological Synthesizing Centre – East
MTC	Mass Transfer Coefficient
NGO	Non-governmental Organisation
NHANES	National Health and Nutrition Examination Survey
NRC	National Research Council
NSB	National Standardisation Body
OC	Organic Carbon
ODD	Overview, Design Concepts and Details
OECD	Organisation for Economic Co-operation and Development
OM	Organic Matter
OSPAR	International Convention for the Protection of Marine Systems
PAH	Polycyclic Aromatic Hydrocarbon
PBCDD	Polychlorinated Dibenzodioxins
PBPK	Physiologically Based Pharmacokinetic
PBT	Persistent, Bioaccumulative and Toxic
PBTK	Physiologically Based Toxicokinetic
PCB	Polychlorinated Biphenyls
PDF	Pedotransfer Function
PEC	Predicted Environmental Concentration
PFC	Perfluorinated Compound
PFOA	Perfluorooctanoic Acid
PFOS	Perfluorooctane Sulphonate
PHS	Priority Hazardous Substance
PNEC	Predicted No-Effect Concentration
POC	Particulate Organic Carbon
POP	Persistent Organic Pollutant
ppLFER	Polyparameter Linear Free Energy Relationship
PPP	Plant Protection Product

PRZM	Pesticide Root Zone Model
PS	Priority Substance
PSR	Priority Substances Under Review
QSAR	Quantitative Structure-Activity Relationship
RA	Risk Assessment
RANS	Reynolds-Averaged Navier-Stokes
REACH	Registration, Evaluation, Authorization and Restriction of Chemical Substances
REV	Representative Elementary Volume
RH	Relative Humidity
SCCS	Scientific Committee on Consumer Safety
SCENIHR	Scientific Committee on Emerging and Newly Identified Health Risks
SCHER	Scientific Committee on Health and Environmental Risks
SCS	Soil Conservation Service
SEA	Single European Act
SME	Small and Medium Enterprise
SPG	Specific Protection Goal
SPM	Suspended Particulate Matter
STOA	Science and Technology Options Assessment
SVOC	Semi-volatile Organic Compound
SWOT	Strengths, Weaknesses, Opportunities and Threats
TCDD	2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin
TG	Test Guideline
TNO	Netherlands Organisation for Applied Scientific Research
TSCA	Toxic Substance Control Act
TSP	Total Concentration of Suspended Particles
TWA	Time-Weighted Average
UK	United Kingdom
UNECE	United Nations Economic Commission for Europe
US	United States
USDA	US Department of Agriculture
UZ	Unsaturated Zone
vPvB	Very Persistent and Very Bioaccumulative
WFD	Water Framework Directive
WHO	World Health Organization

Symbols

Symbols are defined where they appear in the text.