
Contents

Foreword by Jean-Luc Fugit.	xvii
Jean-Luc FUGIT	
Foreword by Ignasi Palou-Rivera	xxi
Ignasi PALOU-RIVERA	
Foreword by Magali Smets.	xxiii
Magali SMETS	
Acknowledgments	xxv
Jean-Pierre DAL PONT	
General Introduction	xxix
Jean-Pierre DAL PONT	
Part 1. Eco-Chemistry for Sustainable Products®: Solutions for a Chemical Transition	1
Introduction to Part 1.	3
Philippe GIRARDON and Valérie LUCAS	

Chapter 1. Our Home: The Earth	7
Philippe GIRARDON	
1.1. Current situation	7
1.2. Climate change.	7
1.3. Greenhouse gas emissions	8
1.4. Finite resources	8
1.5. Consumption of raw materials (excluding water and energy)	9
1.6. Energy resources.	11
1.7. Strategic minerals and materials	12
1.8. Water: the most precious commodity; a source of strategic challenges	14
1.9. References	15
 Chapter 2. Toward a Holistic Approach to the Chemical Industry Cycle	17
Ismahane REMONNAY	
2.1. Transparency, traceability, sustainability, a new collaboration for sustainable and responsible chemistry.	18
2.2. A new European strategy to support the “zero pollution” ambition of the European Green Deal	19
2.3. New concepts to support the creation of sustainable products: safe and sustainable by design	20
2.3.1. Toward progressive phasing out of harmful substances	20
2.3.2. Toward an approach to “convenience” chemistry versus essential and sustainable chemistry: the concept of essential and nonessential use	22
2.4. Toward a better understanding of harmful pollutants through the acquisition of robust scientific data	22
2.4.1. Pollutants of concern: a constantly evolving list and increasingly precise criteria.	22
2.4.2. Reaffirming the chemical iceberg concept	23
2.4.3. Mixtures and cocktail effects	24
2.4.4. A substance, an assessment and the grouping approach	24
2.4.5. An ambitious roadmap.	26
2.5. The new international framework.	28
2.6. Conclusion and prospects	30
2.7. References	31

Chapter 3. How Can Action Be Managed? The Fundamentals: Ecodesign, Life Cycle Assessment and Circular Economy 33

Guy-Noël SAUVION

3.1. Taking stock of existing technologies	34
3.2. Shifting from a linear to a circular economy	38
3.3. Ecodesign	45
3.3.1. Ecodesign or ecoinnovation?	49
3.3.2. Creating environmental value.	51
3.3.3. Sustainability in the broadest sense	52
3.4. Lifecycle assessment	53
3.4.1. Principle and general information	54
3.4.2. Applications for the chemical industry	60
3.4.3. Points to consider when implementing LCA.	62
3.4.4. Applying the LCA results	63
3.5. Tools more specific to the chemical industry	65
3.6. Carbon footprint and carbon content of products.	70
3.6.1. Connection with the company's GHG balance sheet	76
3.7. Conclusion	77
3.8. References	77

Chapter 4. Greenhouse Gases and Climate Change 79

Quentin TIZON

4.1. Greenhouse gases?	79
4.2. What effects do greenhouse gases have on the climate?	80
4.2.1. Pros and cons of the greenhouse effect	81
4.3. Measuring and assessing greenhouse gases	83
4.4. The <i>bilan carbone</i> [®] : principle and method	84
4.5. What the <i>bilan carbone</i> [®] could mean for the chemical industry.	86
4.6. Sector transition strategy: the example of ammonia	87
4.6.1. The example of ammonia	87
4.7. References	90

Chapter 5. Ecodesigned Products: Issues and Solutions 93

Valérie LUCAS

5.1. Plant-based chemistry: a source of biobased raw materials.	93
5.1.1. Plant-based chemistry	93
5.1.2. Biobased chemical synthons and intermediates	94
5.1.3. Bioprocesses and biotechnologies	94
5.1.4. Biorefineries.	95
5.1.5. Biofuels.	96

5.1.6. Bioproducts: biosolvents, biosurfactants, biolubricants and bioplasticizers	96
5.1.7. Biopolymers and plant-based plastics	96
5.2. Biomimicry	97
5.3. Impact on health and the environment	98
5.4. An example case study: biobased paints	98
5.5. References	100
 Chapter 6. Paints and Durability	101
Bernard CHAPUIS	
6.1. Components of paint	102
6.2. Paint production	104
6.3. Industrial hygiene	104
6.4. Norms and regulations	104
6.5. Certification	106
6.6. References	107
 Chapter 7. A Few Case Studies	109
Philippe GIRARDON	
7.1. Fashion and apparel	109
7.2. Cosmetics	110
7.3. Packaging materials: recycling challenges	111
7.4. Waste: recycling plastics and other materials	111
7.5. References	114
 Chapter 8. Packaging and Tracers for the Industry of the Future	115
Claude LAMBERT	
8.1. Purpose of packaging? Product protection and traceability	116
8.2. Why trace packages?	116
8.3. Principle and definitions: the marker/tracer procedure	117
8.4. Strategy and selection, ecodesign	118
8.4.1. Surface marking	118
8.4.2. Mass marking	119
8.4.3. Compatibility of different markers used simultaneously	119
8.5. Applications	119
8.5.1. Plastics	119
8.5.2. Packages	120
8.5.3. Recycling: new materials	120

8.6. Tracers and 3D printers	120
8.7. Health: harmless – food safety	121
8.8. Tracers and society	121
8.9. References	122

Conclusion to Part 1. Between Contradictions, Challenges and Opportunities	123
Jean-Pierre DAL PONT	

Part 2. Toxicology and Ecotoxicology: A Contribution to the Design of New Chemical Substances.	127
---	------------

Introduction to Part 2. Aim of the Technical Guide	129
Alain LOMBARD	

Chapter 9. Methodology at the Research Stage of New Molecules, New Substances and New Ingredients	131
Alain LOMBARD, Philippe LEMAIRE, Jacques L'HARIDON, Michel ROYER and Paule VASSEUR	

9.1. Process for defining the target chemical structure	134
9.1.1. Defining alerts based on potential hazards: using in silico models	134
9.1.2. Detection of CMR (carcinogenic, mutagenic or reprotoxic) potential using in silico methods	135
9.2. Physical–chemical properties of substances.	137
9.3. Modeling strategy and acceptability of health, environment and safety alert levels.	142
9.4. Persistence and bioaccumulation (P–B) properties.	143
9.4.1. Persistence (P).	144
9.4.2. Bioaccumulation (B).	145
9.5. Ecotoxicology and environmental toxicity	145
9.5.1. Rapid screening tests in ecotoxicology	145
9.5.2. Screening tests for potential endocrine disrupting effects for the environment	148
9.6. Human toxicology.	149
9.6.1. Strategy for local tolerance tests on cell cultures	149
9.6.2. Acute, subchronic and chronic systemic toxicity studies.	151

9.6.3. Identification of CMR properties: carcinogenic, mutagenic and reprotoxic	152
9.6.4. Detection of endocrine disrupting properties.	156
9.7. Conclusion to the technical guide.	158
9.7.1. Drawing up a summary table	158
9.7.2. How to use the summary table	159
9.7.3. Practical uses of the guide.	159
9.8. References	160

Chapter 10. Detailed Test Explanations: Decision Support for Hazard Assessment of New Substances. 163

Alain LOMBARD, Philippe LEMAIRE, Jacques L'HARIDON
and Paule VASSEUR

10.1. Applying models: in silico testing.	163
10.1.1. Quantitative structural activity/quantitative structural activity relationship (QSAR)	163
10.1.2. Trend analysis, read across	164
10.1.3. Dose–response models	165
10.1.4. Rule-based models	165
10.1.5. The OECD toolbox model.	166
10.2. Ecotoxicology	167
10.2.1. Definitions	167
10.2.2. Ecotoxicological impact assessment	168
10.2.3. Ecotoxicity tests	170
10.3. Toxicology	174
10.3.1. Ocular corrosion.	174
10.3.2. Cutaneous irritation	174
10.3.3. Ocular irritation	175
10.3.4. Cutaneous sensitization	176
10.4. Assessing toxic potential	178
10.4.1. Cytotoxicity studies.	178
10.4.2. Software for chemical molecule design from the Swiss Institute of Bioinformatics (SIB).	178
10.5. Risk models based on uncertainty factors (UF models)	179
10.6. Rapid tests for the detection of mutagenicity	179
10.6.1. First option: two regulatory micromethod tests	180
10.6.2. Second option: high-throughput biomarker method	183
10.6.3. Add-and-read test strategy.	186
10.7. Detection of in vitro carcinogenic potential	189
10.7.1. Tests on human organoids	189

10.8. Tests to determine the reprotoxic potential of substances	190
10.8.1. Reproductive toxicity.	190
10.8.2. Embryonic development toxicity	191
10.9. Detection of in silico and in vitro endocrine disruptors	196
10.9.1. Endocrine disruptors (EDs): a general overview	196
10.9.2. Nuclear and membrane receptors and cytochrome P450	197
10.9.3. Detection of ED potential via in silico testing	201
10.9.4. Detection of ED potential via in vitro tests	202
10.9.5. Testing for effects not mediated by nuclear receptors.	205
10.9.6. In vitro cellular methods and bioluminescent lines	206
10.9.7. In vitro tests under development	206
10.10. List of acronyms	207
10.11. Contributor backgrounds	209
10.12. References	210
 Chapter 11. Contributions from Guest Experts.	 217
Alain LOMBARD with contributions by guest experts	
Stéphane PIRNAY, Patrick BALAGUER and Philippe HUBERT	
11.1. The expert toxicologist... expertise in service to the safety of all!	217
11.1.1. Further reading	221
11.2. Study of interactions between environmental compounds and nuclear receptors	222
11.2.1. EDC action on hormones	223
11.2.2. Nuclear receptors	223
11.2.3. Nuclear receptor detection methods	225
11.2.4. Examples	226
11.2.5. MELN (luciferase-transfected human breast cancer cell line gene-reporter assay)	227
11.2.6. Automation of the luciferase method	228
11.2.7. Interactions with environmental compounds	230
11.2.8. In conclusion.	232
11.3. PEPPER, accelerating the fight against endocrine disruptors.	233
11.3.1. PEPPER: accelerating the fight against endocrine disruptors through validation of tests	234
11.3.2. Endocrine disruptors	236
11.3.3. The need to escape the world of doubt.	239
11.3.4. PEPPER's works and governance	242
11.3.5. The future of PEPPER in Europe: achievements and challenges.	248
11.4. References.	249

Part 3. Product Industrialization	251
 Introduction to Part 3.	253
Jean-Pierre DAL PONT, Patrick DUCOURET, Michel ROYER and Mongi SAKLY	
 Chapter 12. The Company and Its Manufacturing Facilities	255
Michel ROYER and Patrick DUCOURET	
12.1. The founding fathers.	256
12.2. The four pillars of a company	258
12.3. Anatomy of a company: functions	258
12.4. Manufacturing facilities.	260
12.4.1. Anatomy of a factory: its functions	260
12.4.2. Typology of the means of production: VAT analysis	261
12.4.3. The company and industrial production as seen through flows	262
12.5. The company's industrial strategy.	263
12.6. References.	267
 Chapter 13. From Research to the Factory: The Industrialization Process	269
Jean-Pierre DAL PONT	
13.1. Basic concepts	269
13.2. Organization of a project, from the laboratory to completion.	271
13.3. Organization of a project in the execution phase	272
13.4. Project management	273
13.5. The pitfalls of project management	273
13.6. References.	274
 Chapter 14. Working by Project	275
Jean-Pierre DAL PONT, Patrick DUCOURET and Michel ROYER	
14.1. Industrialization: steps for the process engineer	275
14.2. Simulation and modeling in the age of artificial intelligence (AI)	277
14.3. Project engineering	280
14.3.1. A series of stages	280
14.3.2. Project engineering: basic concepts and engineering companies	281

14.4. Credit application: investment file	285
14.5. References.	286
Chapter 15. Understanding Margins	287
Jean-Pierre DAL PONT	
15.1. Notions of product cost price.	287
15.2. Profit and loss accounting as a decision-making tool, limited to gross margin.	289
15.2.1. Sales figures	289
15.2.2. The contribution margin	289
15.2.3. The gross profit margin	290
15.2.4. Depreciation and amortization	291
15.3. Other margins.	292
15.3.1. The workshop	292
15.3.2. Cash flow.	293
15.4. A few aphorisms	294
15.5. References.	294
Chapter 16. Technology Management	295
Jean-Pierre DAL PONT and Patrick DUCOURET	
16.1. Nature and the importance of technology	295
16.2. Technology, know-how and knowledge management	296
16.3. Enterprise and ecosystem, technology and industrial enterprise	298
16.4. Strategic analysis and framework for progress	300
16.5. Existing and incremental improvements	301
16.6. Breakthrough research	302
16.7. Serendipity and innovation: the barriers to change, the research and development function (innovation)	303
16.8. Technological readiness.	305
16.9. Japanese methods	305
16.10. Intellectual property	306
16.11. References	307
Chapter 17. Choosing Industrial Sites	309
Jean-Pierre DAL PONT	
17.1. Building “new” on a new site	310
17.1.1. Site.	310

17.1.2. Resources	310
17.1.3. Regulations	311
17.1.4. Financial aspects	311
17.2. Building “new” on an existing site	311
17.2.1. Governance aspects	311
17.2.2. Resource availability and costs	312
17.3. Relationship between existing factory and new workshop	312
17.3.1. Cultural aspects: comparing two modes of industrial operation.	313
17.4. Building abroad	314
17.5. References.	315
 Chapter 18. The Factory of the Future: A New Paradigm	 317
Jean-Pierre DAL PONT, Patrick DUCOURET and Michel ROYER	
18.1. The digital revolution and digital tools	320
18.1.1. Internet of Things (IoT) and Industrial Internet of Things (IIoT).	321
18.1.2. Digital twins	321
18.1.3. 3D printers and additive manufacturing (AM)	322
18.1.4. The augmented operator	323
18.1.5. Cognitive assistance, augmented reality and virtual reality	324
18.1.6. Physical assistance: robots and people.	324
18.1.7. The human/machine interface and human/machine interaction (HMI) in the digital age	326
18.1.8. Corporate IT management and factory IT management	327
18.2. The process at the heart of industrialization	329
18.2.1. Process efficiency and intensification	329
18.2.2. CAPEX-OPEX optimization	331
18.2.3. Sustainability approach.	331
18.3. The fundamentals	332
18.3.1. Operations management	332
18.3.2. The transparent factory, a customer-oriented factory	333
18.3.3. The pursuit of resilience, robustness and dependability.	333
18.3.4. Toward the factory and company of the future.	335
18.4. References.	338

Chapter 19. Generative Intelligence: A Revolution on Our Doorstep	339
Willi MEIER	
19.1. Addressing challenges and seizing opportunities: a snapshot of the global chemical industry in 2024	340
19.2. Transforming the global chemical industry: the role of AI and ChatGPT in 2024	342
19.3. Optimization of reaction conditions for chemical synthesis.	343
19.4. Supply chain and operations	345
19.5. Scenario: compliance with REACH regulations	347
19.6. Scenario: detection and intervention in the event of a toxic gas leak.	349
19.7. Scenario: development of a biodegradable plastic for food packaging	352
19.8. Application of ChatGPT to a liquid/liquid separation problem.	354
19.9. References.	356
 Conclusion to Part 3	357
Jean-Pierre DAL PONT	
 Glossary. For Further Information.	361
Jean-Pierre DAL PONT	
 General Conclusion. What Does the Future Hold?	365
Jean-Pierre DAL PONT, Philippe LEMAIRE, Alain LOMBARD and Valérie LUCAS	
 List of Authors	379
 Index	381