

Contents

Preface *ix*

1	Introduction	1
1.1	Life Sciences – A Definition	1
1.1.1	A Short Definition of Life	1
1.1.2	What Is Life Sciences?	2
1.2	Automation – A Definition	4
1.3	History of Automation	5
1.3.1	Automation from the Beginnings to the Nineteenth Century	5
1.3.2	Automation Since the Nineteenth Century	10
1.3.3	History of Laboratory Automation	12
1.4	Impact of Automation	15
1.4.1	Advantages and Disadvantages of Automation	15
1.4.2	Social Impact of Automation	16
1.4.3	Limitation of Automation	17
	References	18
2	Automation in Life Sciences – A Critical Review	25
2.1	Overview	25
2.2	Definitions and Basics	26
2.3	Automation in Bioscreening	28
2.3.1	Overview	28
2.3.2	Automation Devices in Biological Screening	31
2.3.2.1	Standardization of Sample Formats	31
2.3.2.2	Robots in Bioautomation	33
2.3.2.3	Liquid-Handling Systems	34
2.3.2.4	Additional Components	37
2.3.3	Application Examples	40
2.4	Automation in Chemical Sciences	43
2.4.1	Overview	43
2.4.2	Automation Devices for Combinatorial Chemistry	45
2.4.2.1	Vessel Based Systems	46
2.4.2.2	Microplate-Based Systems	48
2.4.2.3	Robot-Based Synthesis Systems	48
2.4.3	Application Examples	49

2.5	Automation in Analytical Measurement Applications	51
2.5.1	Overview	51
2.5.2	Process Analytical Technology	52
2.5.3	Automation Systems for Analytical Measurement Applications	54
2.6	Requirements for Automating Analytical Processes	56
2.6.1	Bioscreening vs. Analytical Measurement	56
2.6.1.1	Vessels and Vials in Analytical Processes	56
2.6.1.2	Liquids and Reagents in Analytical Measurement	58
2.6.1.3	Process Structure	58
2.6.2	Automation Requirements	58
	References	61
3	Automation Concepts for Life Sciences	73
3.1	Classification of Automation Systems	73
3.2	Classification Concept for Life Science Processes	75
3.3	Robot Based Automation Systems	78
3.3.1	Robot Based Systems in Industrial Automation	78
3.3.2	Robot-Based Automation Systems in Life Sciences	79
3.3.2.1	Concept of the Central Robot as System Integrator	79
3.3.2.2	Concept of the Flexible Robot	80
3.3.3	Summary and Application of Concepts	81
3.4	Degree of Automation	83
3.5	Statistical Evaluations	86
	References	89
4	Automation Systems with Central System Integrator	93
4.1	Centralized Closed Automation System	93
4.1.1	Background and Applicative Scope	93
4.1.2	Automation Goals	98
4.1.3	System Design	99
4.1.4	Process Description	102
4.1.5	Control of the Automation Process	103
4.1.6	Evaluation of the Automation System	104
4.2	Centralized Open Automation System	109
4.2.1	Background and Applicative Scope	109
4.2.1.1	Determination of Mercury in Waste Wood	109
4.2.1.2	Determination of Methacrylates in Dental Materials	111
4.2.2	Automation Goals	114
4.2.2.1	Determination of Mercury in Waste Wood	114
4.2.2.2	Determination of Methacrylates in Dental Materials	115
4.2.3	System Design	116
4.2.4	Process Description	121
4.2.4.1	Process Description for Determination of Mercury in Waste Wood	121
4.2.4.2	Process Description for the Determination of Methacrylates in Dental Materials	122

4.2.5	Control of the Automation Process	124
4.2.6	Evaluation of the Automation System	126
4.3	Decentralized Closed Automation System	130
4.3.1	Background and Applicative Scope	131
4.3.2	Automation Goals	132
4.3.3	System Design	134
4.3.4	Process Description	135
4.3.5	Control of the Automation Process	136
4.3.6	Evaluation of the Automation System	136
4.4	Decentralized Open Automation System	143
4.4.1	System Design	144
4.4.2	Process Description	144
4.4.3	Control of the Automation System	145
	References	148
5	Automation Systems with Flexible Robots	167
5.1	Centralized Closed Automation System	167
5.1.1	System Design	167
5.1.2	Process Description	174
5.1.3	Control of the Automation System	174
5.1.4	Results	179
5.2	Centralized Open Automation System	180
5.2.1	Background and Applicative Scope	180
5.2.2	Automation Goals	183
5.2.3	System Design	184
5.2.4	Process Description	186
5.2.5	Control of the Automation System	187
5.2.6	Results	189
5.3	Decentralized Automation System	191
5.3.1	System Design	192
5.3.2	Process Description	193
5.3.3	Control of the Automation System	193
5.4	Automation Systems with Integrated Robotics	194
5.4.1	System Design	196
5.4.2	Process Description	198
5.4.3	Process Control	198
	References	200
6	Automated Data Evaluation in Life Sciences	205
6.1	Specific Tasks in Data Evaluation in Analytical Measurements	205
6.2	Automation Goals	207
6.3	System Design	208
6.4	System Realization	211
6.4.1	Software Structure	211
6.4.2	Software Operation	214
6.5	Process Description	220
6.6	Application Examples	222

6.6.1	Automated Data Analysis in the Elemental Analysis	222
6.6.2	Automated Data Analysis in the Structural Analysis	224
6.6.3	Automated Data Analysis in Special Applications	225
	References	226
7	Management of Automated Processes	231
7.1	Laboratory Information Systems	231
7.2	Laboratory Execution Systems	231
7.3	Process and Workflow Management Systems	232
7.3.1	Overview	232
7.3.2	Intelligent Scheduling	234
7.3.3	Human Machine Interaction	236
7.4	Business Process Management Systems	239
7.4.1	Initial BPM Activities	239
7.4.2	Relationship to Scientific Workflow Management	241
7.4.3	Life Science Automation Industry Application of BPM	241
7.4.4	Status of Life Science Automation	242
7.4.5	Laboratory IT Integration Status	245
7.4.6	Innovation in End-to-End Process Automation	245
7.4.7	Workflow Automation as a New Top-Level Process Automation Approach	246
7.4.8	Outstanding Position of LIMS as an Established Process Documentation System	248
	References	249
	Index	255