

NANOTECHNOLOGY

BASIC CALCULATIONS FOR ENGINEERS AND SCIENTISTS

LOUIS THEODORE

Contents

Preface	xvii
Introduction	xix
PART 1: CHEMISTRY FUNDAMENTALS AND PRINCIPLES	1
1 Units, Conversion Constants, and Dimensional Analysis	3
1.1 Background on the Metric System	4
1.2 Describe the SI System of Units	6
1.2.1 Seven Base Units	7
1.2.2 Two Supplementary Units	8
1.2.3 SI Multiples and Prefixes	8
1.3 The Conversion Constant g_c	9
1.4 Unit Conversion Factors: General Approach	10
1.5 Temperature Conversions	11
1.6 Pressure Calculations	11
1.7 Density and Thermal Conductivity	13
1.8 Viscosity Conversions	14
1.9 Air Quality Standard	14
1.10 Conversion Factors for Particulate Measurements	15
1.11 Significant Figures and Scientific Notation	15
1.12 Uncertainty in Measurement	17
2 Atoms, Elements, and the Periodic Table	19
2.1 Atomic Theory	21
2.2 The Avogadro Number	21
2.3 Mass and Size of Atoms	22
2.4 Atomic Conversions	23
2.5 Atomic Number, Atomic Weight, and Mass Number	24
2.6 Bismuth Application	24
2.7 Elements	24
2.8 Symbols for Elements	27
2.9 Periodic Table Application	28
2.10 Isotopes	29

3	Molecular Rearrangements	31
3.1	License Plate Sets	31
3.2	Chemical Permutations and Combinations	32
3.3	Formula Weight and Molecular Weight	34
3.4	Mole/Molecule Relationship	34
3.5	Pollutant Chemical Formulas	35
3.6	Stoichiometry	36
3.7	Limiting and Excess Reactants	36
3.8	Combustion of Chlorobenzene	37
3.9	Metal Alloy Calculation	39
3.10	Chemical Production	40
4	Concentration Terms	43
4.1	Density, Specific Gravity, and Bulk Density	43
4.2	Classes of Solution	45
4.3	Molality versus Molarity	45
4.4	Molar Relationships	46
4.5	Concentration Conversion	47
4.6	Chlorine Concentration	48
4.7	Trace Concentration	49
4.8	Ash Emission	50
4.9	Dilution Factor	51
4.10	Nano Exhaust to Atmosphere	52
4.11	Flue Gas Analysis	52
4.12	pH	53
5	Particle Size, Surface Area, and Volume	55
5.1	Sphere, Cube, Rectangular Parallelepiped, and Cylinder	56
5.2	Parallelogram, Triangle, and Trapezoid	57
5.3	Polygons	57
5.4	Ellipse and Ellipsoid	58
5.5	Cones	58
5.6	Torus	59
5.7	Area to Volume Ratios	59
5.8	Area to Volume Calculation	60
5.9	Increase in Sphere Surface Area	60
5.10	Increase in Cube Surface Area	61
6	Materials Science Principles	63
6.1	Metals, Polymers, and Ceramics	63
6.2	Composites, Semiconductors, and Biomaterials	64
6.3	Crystal Coordination Numbers	64
6.4	Geometry of Metallic Unit Cells	70
6.5	Geometry of Ionic Unit Cells	75
6.6	Packing Factor	78

- 6.7 Density Calculation 80
- 6.8 Directions and Planes 83
- 6.9 Linear Density 88
- 6.10 Planar Density 90

7 Physical and Chemical Property Estimation 95

- 7.1 Property Differences 96
- 7.2 Material Selection 97
- 7.3 Vapor Pressure 97
- 7.4 Vapor Pressure Calculation 98
- 7.5 Heat of Vaporization From Vapor Pressure Data 99
- 7.6 Critical and Reduced Properties 100
- 7.7 Estimating Enthalpy of Vaporization 101
- 7.8 Viscosity 104
- 7.9 Thermal Conductivity 106
- 7.10 Thermal Conductivity Application 108
- 7.11 Nokay Equation and Lydersen's Method 109
- 7.12 The Rihani and Doraiswamy Procedure, and the Lee-Kesler Equation 113

References: Part 1 117

PART 2: PARTICLE TECHNOLOGY 119

8 Nature of Particulates 121

- 8.1 Definition of Particulates 121
- 8.2 Dust, Smoke, and Fumes 122
- 8.3 Mist and Drizzle 123
- 8.4 Changing Properties 123
- 8.5 Dust Explosions 123
- 8.6 Adsorption and Catalytic Activity in the Atmosphere 125
- 8.7 Particle Size 125
- 8.8 Particle Volume and Surface Area 126
- 8.9 Volume/Surface Area Ratios 127
- 8.10 Particle Formation 128

9 Particle Size Distribution 131

- 9.1 Representative Sampling 131
- 9.2 Typical Particle Size Ranges 132
- 9.3 Particle Size Distribution and Concentration for Industrial Particulates 132
- 9.4 Particle Size Distribution 133
- 9.5 Median and Mean Particle Size 133

- 9.6 Standard Deviation 136
- 9.7 The Frequency Distribution Curve 137
- 9.8 The Cumulative Distribution Curve 138
- 9.9 The Normal Distribution 139
- 9.10 The Log Normal Distribution 141
- 9.11 Effect of Size Distribution on Cumulative Distribution Plots 143
- 9.12 Nanoparticle Size Variation With Time 145

10 Particle Sizing and Measurement Methods 151

- 10.1 Tyler and U.S. Standard Screens 152
- 10.2 Equivalent Diameter Terms 154
- 10.3 Aerodynamic Diameter 155
- 10.4 Sizing Devices 157
 - 10.4.1 Microscopy 157
 - 10.4.2 Optical Counters 158
 - 10.4.3 Electrical Aerosol Analyzer 158
 - 10.4.4 Bahco Microparticle Classifier 158
 - 10.4.5 Impactors 158
 - 10.4.6 Photon Correlation Spectroscopy (PCS) 159
- 10.5 Rectangular Conduit Sampling 159
- 10.6 Volumetric Flow Rate Calculation 160
- 10.7 Particle Mass Flow Rate Calculation 162
- 10.8 Average Particle Concentration 163
- 10.9 Equal Annular Areas for Circular Ducts 164
- 10.10 Traverse Point Location in Circular Ducts 165
- 10.11 Duct Flow Equation Derivation 166
- 10.12 Source Characteristics and Variations 168

11 Fluid Particle Dynamics 171

- 11.1 The Gravitational Force 172
- 11.2 The Buoyant Force 172
- 11.3 The Drag Force 174
- 11.4 The Drag Coefficient 174
- 11.5 Equation of Particle Motion/Balance of Forces on a Particle 176
- 11.6 Particle Settling Velocity Equations 177
- 11.7 Determination of the Flow Regime 178
- 11.8 Settling Velocity Application 179
- 11.9 The Cunningham Correction Factor 180
- 11.10 Cunningham Correction Factor Values for Air at Atmospheric Pressure 181
- 11.11 Particle Settling Velocity – Different Regimes 182
- 11.12 Brownian Motion/Molecular Diffusion 186

12 Particle Collection Mechanisms	187
12.1 Gravity	188
12.2 Centrifugal Force	188
12.3 Inertial Impaction and Interception	190
12.4 Electrostatic Effects	192
12.5 Thermophoresis and Diffusiophoresis	193
12.6 Acceleration Effects	194
12.7 Brownian Motion/Molecular Diffusion Effects	194
12.8 Nonspherical Particles	196
12.9 Wall Effects	197
12.10 Multiparticle Effects	198
12.11 Multidimensional Flow	198
12.12 Collection Efficiency for Nanosized/Submicron Particles	199
13 Particle Collection Efficiency	201
13.1 Collection Efficiency: Loading Data	202
13.2 Collection Efficiency: Mass Rate	202
13.3 Efficiency of Multiple Collectors	204
13.4 Penetration	204
13.5 Collection Efficiency: Numbers Basis	205
13.6 Particle Size–Collection Efficiency Relationships	206
13.7 Collection Efficiency: Surface Area Basis	207
13.8 Particle Size Distribution/Size–Efficiency Calculation	208
13.9 Check for Emission Standards Compliance: Numbers Basis	210
13.10 Anderson 2000 Sampler	211
References: Part 2	215

PART 3: APPLICATIONS **217**

14 Legal Considerations	219
14.1 Intellectual Property Law	219
14.2 Patents	220
14.3 Contract Law	220
14.4 Tort Law	221
14.5 Recent Patent Activity	222
14.6 Conservation Law For Mass	222
14.7 Conservation Law for Energy	224
14.8 The Second Law of Thermodynamics	226
14.9 Allowable Patent Application Claims	228
14.10 Practicing One's Own Invention	229

15	Size Reduction	231
15.1	Size Reduction Objectives	231
15.2	Plasma-Based and Flame-Hydrolysis Methods	232
15.3	Chemical Vapor Deposition and Electrodeposition	233
15.4	Sol-Gel Processing	233
15.5	Mechanical Crushing	235
15.6	Promising Technologies	235
15.7	Energy and Power Requirements	236
15.8	Potential Dust Explosions With Size Reduction	238
15.9	Material Balance Size Reduction	238
15.10	Size Reduction Surface Area Increase	239
15.11	Fines Eductor Application	241
15.12	Fines Eductor Size Reduction	242
16	Prime Materials	245
16.1	Metals	246
16.2	Iron	246
16.3	Aluminum	247
16.4	Nickel	247
16.5	Silver	248
16.6	Gold	248
16.7	Iron Oxides	248
16.8	Aluminum Oxide	249
16.9	Zirconium Dioxide	249
16.10	Titanium Dioxide	250
16.11	Zinc Oxide	251
16.12	Silica Products	251
17	Production Manufacturing Routes	253
17.1	Carbon Nanotubes and Buckyballs	254
17.2	Semiconductor Manufacturing	255
17.3	Advanced Composites	256
17.4	Advanced Ceramics	258
17.5	Catalytic and Photocatalytic Applications	260
17.6	Gas Sensors and Other Analytical Devices	261
17.7	Consumer Products	262
17.8	Drug Delivery Mechanisms and Medical Therapeutics	262
17.9	Microelectronics Applications	264
17.10	Future Activities	264
18	Ventilation	267
18.1	Indoor Air Quality	268
18.2	Indoor Air/Ambient Air Comparison	269
18.3	Sources of Contaminants in Indoor Air	269
18.4	Industrial Ventilation System	271

- 18.5 Dilution Ventilation vs. Local Exhaust Systems 271
- 18.6 Ventilation Definitions 273
- 18.7 Air Exchange Rate 276
- 18.8 Accidental Emission 278
- 18.9 Dilution Ventilation Application 279
- 18.10 Vinyl Chloride Application 280
- 18.11 Ventilation Models 282
- 18.12 Minimum Ventilation Flowrate 286

19 Dispersion Considerations 289

- 19.1 Atmospheric Deposition Calculation 290
- 19.2 Ground Deposition of Particles 291
- 19.3 Plume Rise 293
- 19.4 Pasquill-Gifford Model 294
- 19.5 Ground-Level Particle Deposition 298
- 19.6 Line and Area Sources 300
- 19.7 Instantaneous "Puff" Model 303
- 19.8 Instantaneous "Puff" Sources 306
- 19.9 U.S. EPA Dispersion Models 307
- 19.10 Dispersion in Water Systems and Soils 308
- 19.11 Canal Concentration Profile 309
- 19.12 Accidental/Emergency Discharge into a Lake/Reservoir 311

20 Ethics 315

- 20.1 Determination of Ethical Values 315
- 20.2 Do's and Don'ts 316
- 20.3 Codes of Ethics 316
- 20.4 The Heavy Metal Dilemma 317
 - Fact Pattern 317
- 20.5 Let Them Worry About It 319
 - Fact Pattern 319
- 20.6 It's In the Air 321
 - Fact Pattern 321
- 20.7 Cheap at What Price 322
 - Fact Pattern 322
- 20.8 Safety Comes First 323
 - Fact Pattern 323
- 20.9 Intellectual Property 324
 - Fact Pattern 324
- 20.10 There's No Such Thing as a Free Seminar 325
 - Fact Pattern 325

PART 4: ENVIRONMENTAL CONCERNS	331
21 Environmental Regulations	333
21.1 The Regulatory System	334
21.2 Air Quality Issues	335
21.3 Particulate Loading	337
21.4 Clean Air Act Acronyms	339
21.5 Water Pollution Control	342
21.5.1 Federal Water Pollution Control Act	342
21.5.2 Safe Drinking Water Act	342
21.5.3 Oil Pollution Control Act	343
21.6 Water Quality Issues	343
21.7 Clean Water Act and PWP's	345
21.8 Wastewater Composition	346
21.9 Solid Waste Management Issues	348
21.10 Hazardous Waste Incinerator	349
21.11 Nanotechnology Environmental Regulations Overview	350
21.12 Nanotechnology Opponents	352
22 Toxicology	353
22.1 The Science of Toxicology	353
22.2 Toxicology Classifications	354
22.3 Routes of Exposure	354
22.4 Threshold Limit Value (TLV)	355
22.5 Toxicology Terminology	356
22.6 TLV vs. PEL	357
22.7 Toxicity Factors	357
22.8 OSHA and NIOSH	358
22.9 Toxicology Determination	359
22.10 IDLH and Lethal Level	359
22.11 Chemical Exposure	361
22.12 Threshold Limit Values	362
23 Noncarcinogens	365
23.1 Hazard Quotient	365
23.2 Reference Dose	366
23.3 Concept of Threshold	367
23.4 Exposure Duration Classification	368
23.5 Risk For Multiple Agents: Chronic Exposure	369
23.6 Risk for Multiple Agents: Subchronic Exposure	370
23.7 Multiple Exposure Pathways	371
23.8 MCL and RfD	372
23.9 Uncertainty and Modifying Factors	372
23.10 Calculating an RfD from NOAEL	373

23.11	Metal Plating Facility Application	374
23.12	Noncarcinogen Calculation Procedure	374
24	Carcinogens	377
24.1	Nonthreshold Concept	377
24.1	Weight of Evidence and Slope Factor	378
24.3	Carcinogenic Toxicity Values	380
24.4	Benzene in Water Application	381
24.5	Excess Lifetime Cancer Cases	382
24.6	Action Level	382
24.7	Accidental Spill	383
24.8	Uncertainties and Limitations	384
24.9	Multiple Chemical Agents and Exposure Pathways	385
24.10	Exponential Risk Model	386
24.11	Risk Algorithm	386
24.12	Risk Algorithm Application for Benzene	388
25	Health Risk Assessment	391
25.1	Risk Definitions	392
25.2	The Health Risk Evaluation Process	392
25.3	Standard Values for Individuals	394
25.4	Qualitative Risk Scenarios	395
25.5	Example of a Health Risk Assessment	396
25.6	Chemical Exposure in a Laboratory	397
25.7	Laboratory Spill	398
25.8	Respirators	399
25.9	Performance of a Carbon Cartridge Respirator	400
25.10	Sampling Program	402
26	Hazard Risk Assessment	407
26.1	Example of a Hazard	408
26.2	Risk Evaluation Process for Accidents	408
26.3	Plant and Process Safety	411
26.4	Series and Parallel Systems	412
26.5	Binomial Distribution	413
26.6	The Poisson Distribution	414
26.7	The Weibull Distribution	415
26.8	The Normal Distribution	416
26.9	Soil Contamination	419
26.10	Event Tree Analysis	420
26.11	Fault Tree Analysis	421
26.12	Upper and Lower Flammability Limits	425
27	Epidemiology	429
27.1	Historical View	429

xvi **CONTENTS**

27.2	Occupational Health	430
27.3	Descriptive Studies	431
27.4	Probability	432
27.5	Prevalence	432
27.6	Incidence Rate	433
27.7	The Mean	434
27.8	The Variance and the Standard Deviation	435

References: Part 4	437
--------------------	-----

Appendix	Quantum Mechanics	439
-----------------	--------------------------	------------

Index	447
--------------	------------