

NANOTECHNOLOGY

Basic Calculations for Engineers and Scientists

Louis Theodore, Eng. Sc. D.

Consultant, Theodore Tutorials
East Williston, New York

 **WILEY-
INTERSCIENCE**
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Nature is neutral. Man has wrestled from nature the power to make the world a desert or to make the deserts bloom. There is no evil in the atom; only in men's souls.

—Adlai Stevenson, 1952

Ill can he rule the great, that cannot reach the small.

—Edmund Spenser, 1596

The small and tiny shall become all-powerful

—L. Theodore, 2006

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Preface

It is not a secret that the teaching of a nanotechnology course will soon be required in most engineering and science curricula. It is also generally accepted as one of the key state-of-the-art courses in applied science. The need to develop an understanding of this general subject matter for the practicing engineer and scientist of the future cannot be questioned.

One of the problems with nanotechnology is that its range of subject matter is so broad that nearly every engineering and science discipline falls under the nano umbrella; in effect, it is interdisciplinary. Adding to the confusion is that no clear-cut definition of nanotechnology has emerged since its infancy nearly a half century ago. The reader will soon note that the author has not laid claim to an end-all definition, but rather refers to nanotechnology simply as nanotechnology.

This project was a unique undertaking. Rather than prepare a textbook on nanotechnology, the author considered writing a problem-oriented book because of the dynamic nature of this emerging field. Ultimately, it was decided to prepare an overview of this subject through illustrative examples rather than to provide a comprehensive treatise. One of the key features of this book is that it could serve both academia (students) and industry. Thus, it offers material not only to individuals with limited technical background, but also to those with extensive industrial experience. As such, it can be used as a text in either a general engineering or science course and (perhaps primarily) as a training tool for industry.

As is usually the case in preparing a manuscript, the question of what to include and what to omit has been particularly difficult. However, the problems and solutions in this work attempt to address principles and basic calculations common to nanotechnology.

This basic calculations workbook is an outgrowth of the 2005 John Wiley & Sons book “Nanotechnology: Environmental Implications and Solutions”. The desirability of publishing a workbook that focuses almost exclusively on nanotechnology calculations was obvious following the completion of that book.

This book contains nearly 300 problems related to a variety of topics of relevance to the nanotechnology field. These problems are organized into the following four Parts or Categories:

- Chemistry Fundamentals and Principles
- Particle Technology
- Applications
- Environmental Concerns

Each Part is divided into a number of problem Sections (or Chapters), with each set containing anywhere from 8 to 12 problems and solutions. The interrelationship between the problems is emphasized in all Parts.

The general approach employed involved the use of solved illustrative examples. However, introductory paragraphs are included in each Part and each Section. The remainder of the text consists of solved examples. In each Part, these have been chosen to emphasize the most important basic concepts, issues, and applications that arise in the topic covered by that Part.

Another feature of this work is that the solutions to the problems are presented in a stand-alone manner. Throughout the book, the problems are laid out in such a way as to develop the reader's technical understanding of the subject in question. Each problem contains a title, problem statement, data, and solution, with the more difficult problems located at or near the end of each problem set (Section). Although some of the topics are somewhat segmented and compartmentalized (relative to each other), every attempt was made to present and arrange each subject in a logical order.

The author cannot claim sole authorship to all the problems and material in this book. The main sources that were employed in preparing the problems included numerous Theodore Tutorials (plus those concerned with the professional engineering exam) and the Reynolds, Jeris and Theodore 2004 Wiley-Interscience text, "Handbook of Chemical and Environmental Engineering Calculations". Finally, the author wishes to acknowledge the National Science Foundation for supporting several faculty workshops that produced a number of problems appearing in this work.

The author also wishes to thank Dr. Albert Swertka, Professor Emeritus of Physics, U.S. Merchant Marine Academy, for contributing an outstanding write-up in layman terms on "Quantum Mechanics". It can be found in the Appendix. This material was included for those readers interested in obtaining a (better) understanding of how quantum mechanics is related to nanotechnology.

Somehow, the editor usually escapes acknowledgement. I was particularly fortunate to have Bob Esposito ("Espo" to us) of John Wiley & Sons serve as my editor. His advice, support, and encouragement is appreciated.

It is the hope of the editor and author that this basic calculations text provides support in developing an understanding of nanotechnology, and that it will become a useful resource for the training of engineers and scientists in mastering this critical topic area.

Louis Theodore
January 2006

Introduction

Technical individuals have traditionally conducted calculation-related studies using one of a combination of the following approaches (see Figure A):

1. Macroscopic level
2. Microscopic level
3. Molecular level

These studies generally involve the application of a conservation law, e.g., mass, energy, and momentum. For example, if one were interested in determining changes occurring at the inlet and outlet of a system under study, the conservation law is applied on a “macroscopic” level to the entire system. The resultant equation describes the overall changes occurring to the system without regard for internal variations *within* the system. This approach is usually employed in a Unit Operations (for chemical engineers) course. The microscopic approach is employed when detailed information concerning the behavior *within* the system is required, and this is often requested of and by technical personnel. The conservation law is then applied to a differential element within the system, which is large compared to an individual molecule, but small compared to the entire system. The resultant equation is then expanded, via an integration, to describe the behavior of the entire system. This has come to be defined by some as the *transport phenomena approach*. The molecular approach involves the application of the conservation law to individual molecules. This leads to a study of statistical and quantum mechanics – both of which are beyond the scope of this text.

Approaches (1) and (2) are normally in the domain of the engineer, while (2) and (3) are employed by the scientist, particularly the physicist. In a very real sense, this

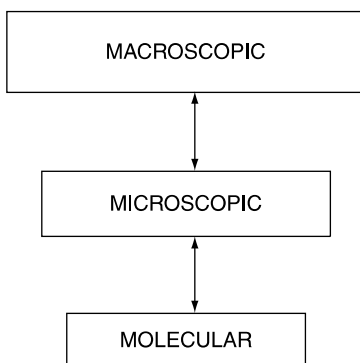


Figure A Engineering and Science Approaches

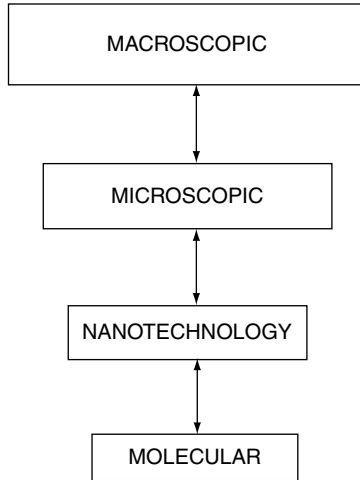


Figure B Nanotechnology Approach

text emphasizes (1), since it has been written for the practicing engineer and scientist, and attempts to provide solutions to real-world nanotechnology applications. Notwithstanding this, material in Part 1 delves into some science principles and fundamentals, and an abbreviated introduction to quantum mechanics can be found in the Appendix.

However, nanotechnology has disrupted the above classical approach to the describing behavior of systems. The nanotechnology field today belongs somewhere between (2) and (3), i.e., between the microscopic and molecular approaches (Figure B).

Nanoparticles cannot be correctly described by applying either the microscopic or molecular method of analysis. This new, so-called, in-between field gives rise to some very unusual physics.

This unusual behavior results because the (physical, chemical, and so on) properties are a strong function of the size of the substance. At microscopic or macroscopic sizes, one chunk of iron (an element) has the exact same properties of another chunk of iron. At the molecular level, an atom of iron has the exact same properties of another atom of iron. However, something happened on the way to the forum . . . when the size of the iron particle is in the nano range. The chemical, physical, mechanical, electrical, etc., properties of these bulk materials are different in the nanometer range. Further, a 10 nanometer particle has different properties than a particle of different size, e.g., 20 nanometers. (Note: A nanometer is one billionth of a meter; thus, one nanometer equals 10^{-9} meters.) The same phenomena is experienced with iron oxide or any other solid particle. What does all of this mean? It permits a new way to vary and control the properties of materials. In effect, one need only change the size of the particle rather than its composition.

PART 1

Chemistry Fundamentals and Principles

One of the most used definitions of chemistry is that it is concerned with the study of the properties of materials and the changes that materials undergo. It has also been said that chemistry deals with the combination of atoms, and physics with the forces between atoms. One of the objects of physical chemistry is to interpret the relationship between atoms and molecules by examining the forces that exist at the atomic level.

As indicated above, chemistry involves studying the properties and behavior of matter. *Matter* is the physical material that composes the universe; it represents anything that has mass and occupies space. It can take any and many forms. Over the years, the chemist learned that the tremendous variety of matter is due to special combinations of 112 very “elementary” substances, called *elements*. The properties of matter can be related to *atoms*, the special or infinitesimally small building blocks of matter. The atoms can be combined to form molecules. Molecular properties are a function of the number of different atoms and how their component atoms connect to each other. For example, consider the two molecules methane and methanol. Methane molecules contain one atom of carbon and four atoms of hydrogen. Methane is also referred to as natural gas, since the principle component in natural gas is methane. The addition of one oxygen atom to a molecule of methane converts it to methanol. Methanol is a liquid alcohol. This demonstrates how simple changes in the atomic structure of matter can cause significant changes in its properties.

One of the future challenges facing nanotechnology is to change molecules in a controlled way, creating new substances with very special properties. These changes can lead to improvement of healthcare, conservation of natural resources, protection of the environment, and provision of everyday needs for food, clothing, and protective armaments.

When familiar materials such as metals, metal oxides, ceramics, and polymers, and novel forms of carbon are converted into infinitesimally small particle sizes, the resulting particles have orders of magnitude increases in available surface

area. It is this remarkable surface of particles in the nanometer range (1.0 nanometer = 10^{-9} meter) that confers upon them unique properties, especially when compared to macroscopic particles of the same material [1].

This first Part of the book is specifically devoted to chemistry principles and fundamentals. An understanding of this subject is a prerequisite for understanding the basics of nanotechnology. Atoms, the modern theory of atomic structure, elements, the periodic table, molecules, conversion constants and dimensional analysis, concentration terms, surface area determination, crystal structure, and physical/chemical property estimation all can be factored into the mix when studying nanotechnology.

The objective of Part 1 is to introduce the reader to some simple science principles and fundamentals. Most of this material can be directly or indirectly related to the nanotechnology field. A more basic analysis of subatomic particles can be found in the Appendix (see Quantum Mechanics).

The first Part contains a host of solved problems that concentrate on seven important areas, arranged in Chapters:

1. Units, Conversion Constants, and Dimensional Analysis
2. Atoms, Elements, and the Periodic Table
3. Molecular Rearrangements
4. Concentration Terms
5. Particle Size, Surface Area, and Volume
6. Crystal Structure
7. Physical and Chemical Property Estimation

1 Units, Conversion Constants, and Dimensional Analysis

This first Chapter is primarily concerned with units, conversion constants, and dimensional analysis. Each of these receives treatment in the problems that follow; emphasis is placed on the conversion of units using a dimensional analysis approach. The Chapter concludes with two problems on significant figures.

Many engineering and scientific terms are *quantitative*; i.e., they are associated with numbers. When a number represents quantity, the units (unless dimensionless) of that quantity should be specified, i.e., both a number and unit need to be provided. To say that the diameter of an atom is 1.5 is meaningless. To say that it is 1.5 nanometers (nm) correctly specifies the length. The units used for scientific applications, particularly in nanotechnology, are those of the *metric* and *SI systems*. These two systems are reviewed in the first two Problems.

Converting a measurement from one unit to another can conveniently be accomplished by using *unit conversion factors*; these factors are obtained from the simple equation that relates the two units numerically. For example, from

$$1 \text{ foot(ft)} = 12 \text{ inches(in)}$$

the following conversion factor can be obtained

$$12 \text{ in/1 ft} = 1$$

Since this factor is equal to unity, multiplying some quantity (e.g., 18 ft) by the factor cannot alter its value. Hence

$$18 \text{ ft}(12 \text{ in/1 ft}) = 216 \text{ in}$$

Note that the old units of *feet* on the left-hand side cancel out leaving only the desired units of *inches*.

Similarly

$$1 \text{ meter (m)} = 10^9 \text{ nanometer (nm)}$$

and the corresponding conversion constant or factor is

$$10^9 \text{ nm}/1 \text{ m} = 1$$

Physical equations must be dimensionally consistent. For the equality to hold, each term in the equation must have the same dimensions. This condition can be and should be checked when solving engineering problems. Throughout the text, and in particular in this Chapter, great care is exercised in maintaining the dimensional formulas of all terms and dimensional homogeneity of each equation. Note that equations are generally provided or developed in term of specific units rather than general dimensions (e.g., nanometers, rather than length). This approach should help the reader to more easily attach physical significance to the terms and equations presented in this text.

Since conversion constants are equal to unity with no units, more than one conversion factor can be employed in the solution of a problem. Further modification of an equation can be accomplished if the units for one or more of the terms of the equation are altered through the use of conversion factors. This is discussed in the next paragraph.

One of the properties of equations that has a rational basis and is deduced from general relations is that they must be dimensionally homogeneous, or consistent. This can be demonstrated theoretically. If two sides of an equation should have different dimensions, the equation is in error. Thus, one test for the consistency of an equation is whether all the terms in the equation contain the same units. If this condition is satisfied, the equation is said to be dimensionally consistent (correct); if not, it is incorrect. However, this aforementioned property of dimensional homogeneity does not apply to empirical (not based on theoretical or physical principles) equations. Also note that the application of the principle of consistency not only must be applied to the magnitude of the terms in an equation, i.e., one term cannot be finite in magnitude while another term is a differential or is differentially small, but also to significant figures.

1.1 BACKGROUND ON THE METRIC SYSTEM

Provide background information on the metric system.

SOLUTION

The need for a single worldwide coordinated measurement system was recognized over 300 years ago. Gabriel Mouton, Vicar of St. Paul in Lyons, proposed a comprehensive decimal measurement system in 1670 based on the length of one minute of arc of a great circle of the earth. In 1671, Jean Picard, a French astronomer, proposed the length of a pendulum beating seconds as the unit of length. (Such a pendulum would have been fairly easily reproducible, thus facilitating the widespread

distribution of uniform standard.) Other proposals were made, but over a century elapsed before any action was taken.

In 1790, in the midst of the French Revolution, the National Assembly of France requested the French Academy of Sciences to “deduce an invariable standard for all the measures and weights.” The commission appointed by the Academy created a system that was, at once, simple and scientific. The unit of length was to be a portion of the Earth’s circumference. Measures for capacity (volume) and mass (weight) were to be derived from the unit of length, thus relating the basic units of the system to each other and to nature. Furthermore, the larger and smaller versions of each unit were to be created by multiplying or dividing the basic units by 10 and its multiples. This feature provided a great convenience to users of the system by eliminating the need for calculating and dividing by 16 (to convert ounces to pounds) or by 12 (to convert inches to feet). Similar calculations in the metric system could be performed simply by shifting the decimal point. Thus, the metric system is a *base-10* or *decimal* system.

The commission assigned the name *metre* (or *meter*) to the unit of length. This name was derived from the Greek word *metron*, meaning “a measure.” The physical standard representing the meter was to be constructed so that it would equal one ten-millionth of the distance from the North Pole to the equator along the meridian of the Earth running near Dunkirk in France and Barcelona in Spain.

The metric unit of mass, called the *gram*, was defined as the mass of one cubic centimeter (a cube that is 1/100 of a meter on each side) of water as its temperature of maximum density. The cubic decimeter (a cube 1/10 of a meter on each side) was chosen as the unit of fluid capacity. This measure was given the name *litre* (*liter*).

Although the metric system was not accepted with enthusiasm at first, adoption by other nations occurred steadily after France made its use compulsory in 1840. The standardized character and decimal features of the metric system made it well suited to scientific and engineering work. Consequently, it is not surprising that the rapid spread of the system coincided with an age of rapid technological development. In the United States, by Act of congress in 1866, it was made “lawful throughout the United States of America to employ the weights and measures of the metric system in all contracts, dealings, or court proceedings.”

By the late 1860s, even better metric standards were needed to keep pace with scientific advances. In 1875, an international treaty, the “Treaty of the Meter,” set up well-defined metric standards for length and mass, and established permanent machinery to recommend and adopt further refinements in the metric system. This treaty, known as the *Metric Convention*, was signed by 17 countries, including the United States.

As a result of the Treaty, metric standards were constructed and distributed to each nation that ratified the convention. Since 1893, the internationally agreed metric standards have served as the fundamental weights and measures standards of the United States.

By 1900 a total of 35 nations – including the major nations of continental Europe and most of South America – had officially accepted the metric system. Today, with the exception of the United States and a few small countries, the entire world is

predominantly using the metric system or is committed to such use. In 1971 the Secretary of Commerce, in transmitting to Congress the results of a three-year study authorized by the Metric Study Act of 1968, recommended that the United States change to predominant use of the metric system through a coordinated national program.

The International Bureau of Weights and Measures located at Sevres, France, serves as a permanent secretariat for the Metric Convention, coordinating the exchange of information about the use and refinement of the metric system. As measurement science develops more precise and easily reproducible ways of defining the measurement units, the General Conference of Weights and Measures – the diplomatic organization made up of adherents to the Convention – meets periodically to ratify improvements in the system and the standards.

1.2 THE SI SYSTEM OF UNITS

Describe the SI system of units.

SOLUTION

In 1960, the General Conference adopted an extensive revision and simplification of the system. The name *Le Systeme International d'Unites* (International System of Units), with the International abbreviation *SI*, was adopted for this modernized metric system. Further improvements in and additions to SI were made by the General Conference in 1964, 1968, and 1971.

The basic units in the SI system are the *kilogram* (mass), *meter* (length), *second* (time), *Kelvin* (temperature), *ampere* (electric current), *candela* (the unit of luminous intensity), and *radian* (angular measure). All are commonly used by the scientist engineer. The Celsius scale of temperature (0°C – 273.15 K) is commonly used with the absolute Kelvin scale. The important derived units are the *newton* (SI unit of force), the *joule* (SI unit of energy), the *watt* (SI unit of power), the *pascal* (SI unit of pressure), and the *hertz* (unit of frequency). There are a number of electrical units: *coulomb* (charge), *farad* (capacitance), *henry* (inductance), *volt* (potential), and *weber* (magnetic flux). One of the major advantages of the metric system is that larger and smaller units are given in powers of ten. In the SI system, a further simplification is introduced by recommending only those units with multipliers of 10^3 be employed, e.g., there are 10^9 nanometers in a meter. Thus, for lengths in engineering, the nanometer *micrometer* (previously *micron*), *millimeter*, and *kilometer* are recommended, and the *centimeter* is generally avoided. A further simplification is that the decimal point may be substituted by a comma (as in France, Germany, and South Africa), while the other number, before and after the comma, will be separated by spaces between groups of three, i.e., one million dollars will be \$1 000 000,00. More details are provided below.

1.2.1 Seven Base Units

Length, Meter (*m*) The meter (common international spelling, *metre*) is defined as 1 650 763.00 wavelengths in vacuum of the orange-red line of the spectrum of krypton-86. The SI unit of area is the *square meter* (m^2). The SI unit of volume is the *cubic meter* (m^3). The *liter* (0.001 cubic meter), although not an SI unit, is commonly used to measure fluid volume.

Mass, Kilogram (*kg*) The standard for the unit of mass, the *kilogram*, is a cylinder of platinum–iridium alloy kept by the International Bureau of Weights and Measures at Paris. A duplicate in the custody of the National Bureau of Standards serves as the mass standard for the United States. This is the only base unit still defined by an artifact. The SI unit of force is the *newton* (N). It is the force which, when applied to a 1 kilogram mass, will give the kilogram mass an acceleration of 1 (meter per second) per second: $1 \text{ N} = 1 \text{ kg}\cdot\text{m}/\text{s}^2$. The SI unit for pressure is the *pascal* (Pa), where $1 \text{ Pa} = 1 \text{ N}/\text{m}^2$. The SI unit for work and energy of any kind is the *joule* (J): $1 \text{ J} = 1 \text{ N}\cdot\text{m}$. The SI unit for power of any kind is the *watt* (W), where $1 \text{ W} = 1 \text{ J}/\text{s}$.

Time, Second (*s*) The *second* is defined as the duration of 9 192 632 770 cycles of the radiation associated with a specified transition of the cesium-133 atom. It is realized by tuning an oscillator to the resonance frequency of cesium-133 atoms as they pass through a system of magnets and a resonant cavity into a detector. The number of periods or cycles per second is called *frequency*. The SI unit for frequency is the *hertz* (Hz). One hertz equals one cycle per second. The SI unit for speed is the *meter per second* (m/s). The SI unit for acceleration is the (*meter per second*) per second (m/s^2).

Electric Current, Ampere (*A*) The *ampere* is defined as that current which, if maintained in each of two long parallel wires separated by one meter in free space, would produce a force between the two wires (due to their magnetic fields) of 2×10^{-7} newtons for each meter of length. The SI unit of voltage is the *volt* (V), where $1 \text{ V} = 1 \text{ W}/\text{A}$. The SI unit of electrical resistance is the *ohm* (Ω), where $1 \Omega = 1 \text{ V}/\text{A}$.

Temperature, Kelvin (*K*) The *Kelvin* is defined as the fraction $1/273.16$ of the thermodynamic temperature of the triple point of water. The temperature 0 K is *absolute zero*. Water freezes at about 0°C and boils at about 100°C . The $^\circ\text{C}$ is defined as an interval of 1 K, and the Celsius temperature 0°C is defined as 273.15 K. 1.8 Fahrenheit scale degrees are equal to 1.0°C or 1.0 K; the Fahrenheit scale uses 32°F as a temperature corresponding to 0°C .

Amount of Substance, Mole (*mol*) The *mole* is the amount of substance of a system that contains as many elementary entities as there are atoms in 0.012 kilograms of carbon-12. When the mole is used, the elementary entities must be

specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles. The SI unit of concentration (of amount of substance) is the *mole per cubic meter* (mol/m^3).

Luminous Intensity, Candela (*cd*) The *candela* is defined as the luminous intensity of $1/600\,000$ of a square meter of a blackbody at the temperature of freezing platinum (2045 K). The SI unit of light flux is the *lumen* (lm). A source having an intensity of 1 candela in all directions radiates a light flux of 4π lumens.

1.2.2 Two Supplementary Units

Phase Angle, Radian (*rad*) The *radian* is the plane angle with its vertex at the center of a circle that is subtended by an arc equal in length to the radius.

Solid Angle, Steradian (*sr*) The *steradian* is the solid angle with its vertex at the center of a sphere that is subtended by an area of the spherical surface equal to that of a square with sides equal in length to the radius.

1.2.3 SI Multiples and Prefixes

These are provided in Table 1.1

TABLE 1.1 SI Multiples and Prefixes

| Multiples and Submultiples | | Prefixes | Symbols |
|----------------------------|------------|----------------|---------|
| 100 000 000 000 | 10^{12} | tera (ter'a) | T |
| 100 000 000 | 10^9 | giga (ji'ga) | G |
| 100 000 | 10^6 | mega (meg'a) | M |
| 1 000 | 10^3 | kilo (kil'o) | K |
| 100 | 10^2 | hecto (hek'to) | h |
| 10 | 10^1 | deka (dek'a) | da |
| Base unit 1 | 10^0 | | |
| 0.1 | 10^{-1} | deci (des'i) | d |
| 0.01 | 10^{-2} | centi (sen'ti) | c |
| 0.001 | 10^{-3} | milli (mil'i) | m |
| 0.000 001 | 10^{-6} | micro (mi'kro) | μ |
| 0.000 000 001 | 10^{-9} | nano (nan'o) | n |
| 0.000 000 000 001 | 10^{-12} | pico (pe'ko) | p |
| 0.000 000 000 000 001 | 10^{-15} | femto (fem'to) | f |
| 0.000 000 000 000 000 001 | 10^{-18} | atto (at'to) | a |

1.3 THE CONVERSION CONSTANT g_c

Define the “gravitation” conversion constant g_c .

SOLUTION

The momentum of a system is defined as the product of the mass and velocity of the system.

$$\text{Momentum} = (\text{mass} \times \text{velocity})$$

One set of units for momentum are, therefore, (lb)(ft)/s. The units of the time rate of change of momentum (hereafter referred to as rate of momentum) are simply the units of momentum divided by time, that is

$$\text{Rate of momentum} \equiv \frac{\text{lb} - \text{ft}}{\text{s}^2}$$

The above units can be converted to lb_f if multiplied by an appropriate constant. A defining equation from Newton’s Law is

$$\text{Force} = 1 \text{ lb}_f = 32.2 \frac{(\text{lb})(\text{ft})}{(\text{s}^2)}$$

If this equation is divided by lb_f , one obtains

$$1.0 = 32.2 \frac{(\text{lb})(\text{ft})}{(\text{lb}_f)(\text{s}^2)}$$

This serves to define conversion constant g_c . If the rate of momentum is divided by g_c as $32.2 (\text{lb})(\text{ft})/(\text{lb}_f)(\text{s}^2)$ – this operation being equivalent to dividing by 1.0 – the following units result:

$$\begin{aligned} \text{Rate of momentum} &\equiv \left(\frac{\text{lb} - \text{ft}}{\text{s}^2} \right) \left(\frac{\text{lb}_f - \text{s}^2}{\text{lb} - \text{ft}} \right) \\ &\equiv \text{lb}_f \end{aligned}$$

Thus a force is equivalent to a rate of momentum from the above dimensional analysis.

10 UNITS, CONVERSION CONSTANTS, AND DIMENSIONAL ANALYSIS

Similarly, in the SI system in which the unit of force is defined to be the newton (N), then when 1 kg is accelerated at 1 m/s^2 , it will experience a force of 1 N.

$$\text{Force} = 1 \text{ N} = (1 \text{ kg}) \left(\frac{1 \text{ m}}{\text{s}^2} \right)$$

$$g_c = \frac{1 \text{ N}}{\text{kg} - \text{m/s}^2} = 1$$

Thus, this form of the conversion constant in SI units is unity with no units (dimensionless).

1.4 UNIT CONVERSION FACTORS: GENERAL APPROACH

Convert the following:

1. 8.03 yr to seconds (s)
2. 150 mile/h to yard/h
3. 100.0 m/s^2 to ft/min^2

SOLUTION

The following conversion factors are needed:

365 day/yr
24 hr/day
60 min/hr
60 s/min
5280 ft/mile
30.48 cm/ft
3 ft/yd

1. Arranging the conversion factors so that units cancel to leave only the desired units, the following is obtained:

$$(8.03 \text{ yr}) \left(\frac{365 \text{ day}}{\text{yr}} \right) \left(\frac{24 \text{ h}}{\text{day}} \right) \left(\frac{60 \text{ min}}{\text{h}} \right) \left(\frac{60 \text{ s}}{\text{min}} \right) = 2.53 \times 10^8 \text{ s}$$

2. In similar fashion, $\left(\frac{150 \text{ mile}}{\text{h}} \right) \left(\frac{5280 \text{ ft}}{\text{mile}} \right) \left(\frac{\text{yd}}{3\text{ft}} \right) = 2.6 \times 10^5 \text{ yd/h}$

3. $(100.0 \text{ m/s}^2) \left(\frac{100 \text{ cm}}{\text{m}} \right) \left(\frac{\text{ft}}{30.48 \text{ cm}} \right) \left(\frac{60 \text{ s}}{\text{min}} \right)^2 = 1.181 \times 10^6 \text{ ft/min}^2$

1.5 TEMPERATURE CONVERSIONS

Convert the following temperatures:

1. 20°C to $^{\circ}\text{F}$, K, and $^{\circ}\text{R}$
2. 20°F to $^{\circ}\text{C}$, K, and $^{\circ}\text{R}$

SOLUTION

The following key equations are employed:

$$T(^{\circ}\text{F}) = 1.8T(^{\circ}\text{C}) + 32$$

$$T(\text{K}) = T(^{\circ}\text{C}) + 273$$

$$T(^{\circ}\text{R}) = T(^{\circ}\text{F}) + 460$$

$$T(^{\circ}\text{R}) = 1.8T(\text{K})$$

1. $T(^{\circ}\text{F}) = 1.8(20^{\circ}\text{C}) + 32 = 68^{\circ}\text{F}$
 $T(\text{K}) = (20^{\circ}\text{C}) + 273 = 293 \text{ K}$
 $T(^{\circ}\text{R}) = 1.8(293 \text{ K}) = 527^{\circ}\text{R}$
2. $T(^{\circ}\text{C}) = (20^{\circ}\text{F} - 32)/1.8 = -6.7^{\circ}\text{C}$
 $T(\text{K}) = -6.7^{\circ}\text{C} + 273 = 266 \text{ K}$
 $T(^{\circ}\text{R}) = 20^{\circ}\text{F} + 460 = 480^{\circ}\text{R}$

1.6 PRESSURE CALCULATIONS

The height of a liquid column of mercury is 2.493 ft. Assume the density of mercury is $848.7 \text{ lb}/\text{ft}^3$ and atmospheric pressure is $2116 \text{ lb}_f/\text{ft}^2$ absolute. Calculate the gage pressure in lb_f/ft^2 and the absolute pressure in lb_f/ft^2 , psia, mm Hg, and in. H_2O [2].

SOLUTION

Expressed in various units, the standard atmosphere is equal to:

| | |
|---------------------|--|
| 1.0 | Atmospheres (atm) |
| 33.91 | Feet of water (ft H_2O) |
| 14.7 | Pounds-force per square inch absolute (psia) |
| 2116 | Pounds-force per square foot absolute (psfa) |
| 29.92 | Inches of mercury (in. Hg) |
| 760.0 | Millimeters of mercury (mm Hg) |
| 1.013×10^5 | Newtons per square meter (N/m^2) |

The equation describing the gage pressure in terms of the column height and liquid density is

$$P_g = \rho gh/g_c$$

where P_g = gage pressure, ρ = liquid density, h = height of column, g = acceleration of gravity, and g_c = conversion constant.

Thus,

$$\begin{aligned} P_g &= (848.7 \text{ lb/ft}^3) \left(1 \frac{\text{lb}_f}{\text{lb}} \right) (2.493 \text{ ft}) \\ &= 2116 \text{ lb}_f/\text{ft}^2 \text{ gauge} \end{aligned}$$

The pressure in lb_f/ft^2 absolute is

$$\begin{aligned} P_{\text{absolute}} &= P_g + P_{\text{atmospheric}} \\ &= 2116 \text{ lb}_f/\text{ft}^2 + 2116 \text{ lb}_f/\text{ft}^2 \\ &= 4232 \text{ lb}_f/\text{ft}^2 \text{ absolute} \end{aligned}$$

The pressure in psia is

$$P(\text{psia}) = (4232 \text{ psfa}) \left(\frac{1 \text{ ft}^2}{144 \text{ in.}^2} \right) = 29.4 \text{ psia}$$

The corresponding gage pressure in psig is

$$P(\text{psig}) = 29.4 - 14.7 = 14.7 \text{ psig}$$

The pressure in mm Hg is

$$P(\text{mmHg}) = (29.4 \text{ psia}) \left(\frac{760 \text{ mm Hg}}{14.7 \text{ psia}} \right) = 1520 \text{ mm Hg}$$

Note that 760 mm Hg is equal to 14.7 psia, which in turn is equal to 1.0 atm.

Finally, the pressure in in. H_2O is

$$\begin{aligned} P_{(\text{in. H}_2\text{O})} &= \left(\frac{29.4 \text{ psia}}{14.7 \text{ psia/atm}} \right) \left(\frac{33.91 \text{ ft H}_2\text{O}}{\text{atm}} \right) \left(\frac{12 \text{ in}}{\text{ft}} \right) \\ &= 813.8 \text{ in. H}_2\text{O} \end{aligned}$$

The reader should note that absolute and gage pressures are usually expressed with units of atm, psi, or mm Hg. This statement also applies to partial pressures. One of the most common units employed in industry to describe pressure drop is inches of H₂O, with the notation in. H₂O or IWC (inches of water column).

1.7 DENSITY AND THERMAL CONDUCTIVITY

Convert a value of density for copper from lb/ft³ to g/cc, and a value of thermal conductivity for methanol from cal/m-s-°C to Btu/ft-h-°F. Data are provided as follows:

$$\text{Density of copper} = 557 \text{ lb/ft}^3$$

$$\text{Thermal conductivity of methanol at } 60^\circ\text{F} = 0.1512 \text{ cal/m-s-}^\circ\text{C}$$

SOLUTION

Density (to be revisited in earnest in Chapter 4) and thermal conductivity are two physical properties of importance in nanotechnology. Density is the ratio of a material's mass to its volume; typical units are g/m³, g/cm³ (or g/cc), and lb/ft³. Thermal conductivity provides a measure of how fast (or how easily) heat flows through a substance; it is defined as the amount of heat that flows in unit time through a unit area of unit thickness as a result of a unit difference in temperature. Typical units are cal/m-s-°C and Btu/ft-h-°F.

The conversion factors for g/lb and cm/in are 454 g/lb and 2.54 cm/in, respectively. Convert the density of copper from lb/ft³ to g/cc.

$$\begin{aligned} \left(\frac{557 \text{ lb}}{\text{ft}^3}\right) \left(\frac{454 \text{ g}}{\text{lb}}\right) \left(\frac{1 \text{ ft}^3}{12^3 \text{ in}^3}\right) \left(\frac{1 \text{ in}^3}{2.54^3 \text{ cm}^3}\right) &= 8.93 \text{ g/cm}^3 \\ &= 8.93 \text{ g/cc} \end{aligned}$$

The conversion factors for Btu/cal and ft/m are 3.974×10^{-3} Btu/cal and 3.281 ft/m, respectively. Convert the thermal conductivity of methanol from cal/m-s-°C to Btu/ft-h-°F.

$$\begin{aligned} \left(\frac{0.1512 \text{ cal}}{\text{m-s-}^\circ\text{C}}\right) \left(\frac{3.974 \times 10^{-3} \text{ Btu}}{\text{cal}}\right) \left(\frac{1 \text{ m}}{3.281 \text{ ft}}\right) \left(\frac{3600 \text{ s}}{\text{h}}\right) \left(\frac{1^\circ\text{C}}{1.8^\circ\text{F}}\right) \\ = 0.366 \text{ Btu/ft-h-}^\circ\text{F} \end{aligned}$$

1.8 VISCOSITY CONVERSION

What is the kinematic viscosity of a gas in ft^2/s ? The specific gravity and absolute viscosity of a gas are 0.84 and 0.019 cP, respectively.

SOLUTION

This problem requires the conversion of cP to lb/ft-s. Therefore, the viscosity μ , is

$$\mu = \left(\frac{0.019 \text{ cP}}{1} \right) \left(\frac{6.720 \times 10^{-4} \text{ lb/ft-s}}{1 \text{ cP}} \right) = 1.277 \times 10^{-5} \text{ lb/ft-s}$$

The density ρ is given as

$$\rho = (\text{SG})(\rho_{\text{ref}}) = (0.84)(62.43 \text{ lb/ft}^3) = 52.44 \text{ lb/ft}^3$$

Since the kinematic viscosity, ν , is given by μ/ρ ,

$$\nu = \mu/\rho = (1.277 \times 10^{-5} \text{ lb/ft-s})/(52.44 \text{ lb/ft}^3) = 2.435 \times 10^{-7} \text{ ft}^2/\text{s}$$

1.9 AIR QUALITY STANDARD

Convert the air quality standard of 9.0 ppmv for carbon monoxide at 25°C and 1 atm to mg/m^3 .

SOLUTION

The parts per million of volume standard for carbon monoxide (CO) may be written as

$$9.0 \text{ ppmv} = 9.0 \frac{\text{mL}(\text{CO})}{\text{m}^3(\text{air})}$$

From the ideal gas law, at 25°C and 1 atm, 1 gmol CO occupies 24.5 L. Since the

molecular weight of CO is 28,

$$\begin{aligned} \text{CO (STD)} &= \left(9.0 \frac{\text{mL}_{\text{CO}}}{\text{m}_{\text{air}}^3}\right) \left(\frac{\text{L}_{\text{CO}}}{10^3 \text{ mL}_{\text{CO}}}\right) \left(\frac{\text{mole}_{\text{CO}}}{24.5 \text{ L}_{\text{CO}}}\right) \left(28 \frac{\text{g}_{\text{CO}}}{\text{mole}_{\text{CO}}}\right) \left(\frac{10^3 \text{ mg}_{\text{CO}}}{\text{g}_{\text{CO}}}\right) \\ &= 10.3 \text{ mg(CO)/m}^3(\text{air}) \end{aligned}$$

1.10 CONVERSION FACTORS FOR PARTICULATE MEASUREMENTS

Provide a list of common conversion factors for particulates.

SOLUTION

Particulate conversion factors are provided in Table 1.2.

1.11 SIGNIFICANT FIGURES AND SCIENTIFIC NOTATION

Discuss significant figures and scientific notations.

SOLUTION

Significant figures provide an indication of the precision with which a quantity is measured or known. The last digit represents in a qualitative sense, some degree of doubt. For example, a measurement of 8.32 nm implies that the actual quantity is somewhere between 8.315 and 8.325 nm. This applies to calculated and measured quantities; quantities that are known exactly (e.g., pure integers) have an infinite number of significant figures.

The significant digits of a number are the digits from the first nonzero digit on the left to either (a) the last digit (whether it is nonzero or zero) on the right if there is a decimal point, or (b) the last nonzero digit of the number if there is no decimal point. For example:

| | |
|---------|---------------------------|
| 370 | has 2 significant figures |
| 370. | has 3 significant figures |
| 370.0 | has 4 significant figures |
| 28 070 | has 4 significant figures |
| 0.037 | has 2 significant figures |
| 0.0370 | has 3 significant figures |
| 0.02807 | has 4 significant figures |

TABLE 1.2 Particulate Conversion Factors

| From | To | Multiply By |
|------------------------------------|------------------------|-------------------------|
| mg/m ³ | g/ft ³ | 283.2×10^{-6} |
| | g/m ³ | 0.001 |
| | μg/m ³ | 1.0×10^3 |
| | ng/m ³ | 1.0×10^6 |
| | μg/ft ³ | 28.32 |
| | ng/ft ³ | 28.32×10^3 |
| g/ft ³ | lb/1000ft ³ | 62.43×10^{-6} |
| | mg/m ³ | 35.3145×10^3 |
| | g/m ³ | 35.314 |
| | μg/m ³ | 35.314×10^6 |
| | ng/m ³ | 35.314×10^9 |
| | μg/ft ³ | 1.0×10^6 |
| | ng/ft ³ | 1.0×10^9 |
| g/m ³ | lb/1000ft ³ | 2.2046 |
| | mg/m ³ | 1.0×10^3 |
| | g/ft ³ | 0.02832 |
| | μg/m ³ | 1.0×10^6 |
| | ng/m ³ | 1.0×10^9 |
| | μg/ft ³ | 28.317×10^3 |
| μg/m ³ | lb/1000ft ³ | 0.06243 |
| | mg/m ³ | 0.001 |
| | ng/m ³ | 1.0×10^3 |
| | g/ft ³ | 28.317×10^{-9} |
| | g/m ³ | 1.0×10^{-6} |
| | μg/ft ³ | 0.02832 |
| | ng/m ³ | 28.32 |
| μg/ft ³ | lb/1000ft ³ | 62.43×10^{-9} |
| | mg/m ³ | 35.314×10^{-3} |
| | g/ft ³ | 1.0×10^{-6} |
| | g/m ³ | 35.314×10^{-6} |
| | μg/m ³ | 35.314 |
| | ng/m ³ | 3.531×10^3 |
| lb/10 ³ ft ³ | lb/1000ft ³ | 2.2046×10^{-6} |
| | mg/m ³ | 16.018×10^3 |
| | g/ft ³ | 0.34314 |
| | μg/m ³ | 16.018×10^6 |
| | ng/m ³ | 16×10^9 |
| | g/m ³ | 16.018 |
| No. of Particles/ft ³ | μg/ft ³ | 353.14×10^3 |
| | no./m ³ | 35.314 |
| | no./l | 35.314×10^{-3} |
| | no./cm ³ | 35.314×10^{-6} |
| ton/mi ² | lb/acre | 3.125 |

| | | |
|----|------------------------|------------------------|
| | lb/1000ft ² | 0.07174 |
| | g/m ² | 0.3503 |
| | kg/km ² | 350.3 |
| | mg/m ² | 350.3 |
| | mg/cm ² | 0.03503 |
| | g/ft ² | 0.03254 |
| lb | gr | 7000.0 |
| μm | in | 39.37×10^{-5} |
| | mm | 1.0×10^{-3} |
| | nm | 1.0×10^3 |

Whenever quantities are combined by multiplication and/or division, the number of significant figures in the result should equal the lowest number of significant figures of any of the quantities. In long calculations, the final result should be rounded off to the correct number of significant figures. When quantities are combined by addition and/or subtraction, the final result cannot be more precise than any of the quantities added or subtracted. Therefore, the position (relative to the decimal point) of the last significant digit in the number that has the lowest degree of precision is the position of the last permissible significant digit in the result. For example, the sum of 3702, 370, 0.037, 4, and 37, should be reported as 4110 (without a decimal). The least precise of the five numbers is 370, which has its last significant digit in the *tens* position. The answer should also have its last significant digit in the *tens* position.

Unfortunately, engineers and scientists rarely concern themselves with significant figures in their calculations. However, it is recommended that the reader attempt to follow the calculational procedure set forth in this and the next Problem.

In the process of performing scientific calculations, very large and very small numbers are often encountered. A convenient way to represent these numbers is to use *scientific notation*. Generally, a number represented in scientific notation is the product of a number and 10 raised to an integer power. For example,

$$28\,070\,000\,000 = 2.807 \times 10^{10}$$

$$0.000\,002\,807 = 2.807 \times 10^{-6}$$

A nice feature of using scientific notation is that only the significant figures need appear in the number.

1.12 UNCERTAINTY IN MEASUREMENT

The size of a nanoparticle has been reported in source X as 9.5 Å, while source Y reports its value as 9.523 Å. What is the difference?

SOLUTION:

Two kinds of numbers are employed in engineering and scientific practice: *exact numbers* (those values that are known exactly) and *inexact numbers* (those values that have some uncertainty). Exact numbers are those that have defined values or are integers. Numbers obtained by measurement are always *inexact*, since *uncertainties always exist in measured quantities*.

Regarding the size of the nanoparticle, most lay people would say there is no difference. However, there is a difference, and the difference resides in the number of significant figures employed. Source X has two significant figures, while source Y has four significant figures. This difference indicates that Y is more precise.

As noted in the previous Problem, a size measurement of 9.5 \AA suggests that the “true” measured value is somewhere between 9.45 and 9.55. For source Y, the measurement indicates that the actual value is in the 9.5225–9.5235 range.