CHEMISTRY and the CHEMICAL INDUSTRY

A Practical Guide for Non-Chemists

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Preface

The chemical industry affects virtually all aspects of our lives. Were it to disappear suddenly, we would find ourselves living again in the early nineteenth century without cars, airplanes, television, electric lights, most of our colorful clothing, most perishable food, most drugs and medicine, plastics, and all the rest of the modern conveniences that most of us take for granted.

Consider how the chemical industry contributes to your daily life. For example, when you get up in the morning, you brush your teeth using toothpaste, which is a mixture of chemicals squeezed from a plastic tube onto plastic bristles mounted in a plastic handle. You may take a shower using soap and shampoo, each made by the chemical industry, and finally dry, brush, or comb your hair with other articles made of plastic. While doing this, you will likely be looking into a mirror over a porcelain or cultured marble sink while standing on vinyl plastic floorcovering, tile, or carpeting, all of which are products of the chemical industry. The varnish coating the wooden floors of your house and the paint or wallpaper covering the walls are products of the chemical industry. At breakfast, it is likely that the kitchen counters and table are topped with plastic, as are the chairs. The refrigerator would not work without chemicals either for the refrigeration unit or the insulation in its walls. The interior is plastic lined and the exterior has a durable coating made possible by the chemical industry. Your breakfast food is probably fresh because it was treated with chemical preservatives and/or shipped in a box with a plastic lining. The car or bus that you go to work in is totally chemical dependent, from the anti-corrosion treatment of the metal, the protective paint and the plastic parts and tires to the chemical battery that starts the vehicle, the oil that lubricates it, and the gasoline that fuels it. And so it goes.

The fact that our daily lives are so dependent on the chemical industry does not appear to be widely recognized, even by those working in the chemical industry. And so, as companies are forced in a world economy to become more productive and more quality conscious, as well as having a greater concern for the environment, it becomes essential that their present and future employees understand the basic concepts upon which the chemical industry (indeed, our modern existence) is based. This book is designed to aid in that understanding by reviewing the important aspects of industrial chemistry in a way that can be understood even by those who have not taken any formal chemistry courses.

No mathematics is used and basic physical science is minimized. Why chemicals behave as they do is not explained. It is assumed that the end result of the manufacturing processes presented is the information wanted by the reader and not the science or engineering involved. If needed, the latter information can be obtained from listed sources.

The first chapter begins with a description of the chemical industry and its unique features and branches. The most common terms used in chemistry are defined, using nonscientific analogies where possible. In the following chapters, some basic organic chemistry is presented so that later descriptive explanations of the largest and most important products of the chemical industry can be better understood. The product descriptions include the raw material sources, manufacturing processes, and, of most importance, their commercial uses. Finally, there is a short compilation of general information sources.

The style of the book is to present only a small amount of information on each page with a slide-like illustration using short descriptions and easily understood chemical equations and structures. Under each illustration is additional information or comments with room for the reader to make notes if desired. Although there is obvious continuity, an attempt has been made to make each page subject somewhat independent so that readers can study the contents of the book one page at a time at their own pace. Of necessity, because of this format, there is considerable repetition. We do not consider this bad.

Robert A. Smiley
Harold L. Jackson

Authors

Robert A. Smiley, Ph.D. retired from the DuPont Company in 1990, after which he became an independent consultant in general industrial chemistry. Clients have included ICI, Westinghouse, Clorox, Arco, and many smaller chemical companies. Currently he consults for Dixie Chemical Company where he holds the title of corporate research fellow. He is also the president of Falcon Lab LLC, a company engaged in patent licensing. His fields of expertise include nitrile chemistry, diisocyanate and polyurethane chemistry, nitric acid oxidation, and nitration chemistry and explosives. For many years he gave sponsored seminars on industrial chemistry and polyurethane chemistry both in Europe and the U.S. He received a B.S. degree in industrial chemistry from Case Institute of Technology and a Ph.D. in organic chemistry from Purdue University and joined DuPont as a research chemist in 1954. After a number of successful assignments in the process development of polymer intermediates, he became a research supervisor and then moved on to other positions in technology licensing, business analysis and back to research as research associate and research fellow. He holds 26 U.S. patents and is the author or co-author of 13 publications.

Harold L. Jackson, Ph.D. has 51 years of experience in the chemical industry. After receiving a Ph.D. in organic chemistry from the University of Illinois in 1949, he joined DuPont's central research department where he made significant contributions in the areas of inorganic, organic, and polymer chemistry. He later moved to other research responsibilities in DuPont's chemicals and petrochemicals departments where he studied polymer synthesis and characterization, polymer intermediate development, and solvent chemistry. He has been involved in and assisted with marketing efforts on commercial products resulting from his research work. He retired in 1992 as a research fellow. Dr. Jackson holds 32 U.S. patents and is the author of numerous technical articles. In addition to his industrial activities, Dr. Jackson served as visiting professor of organic chemistry at the University of Kansas.

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1 Introduction

The objective of this chapter is to provide a basis for some understanding of chemistry and the chemical industry. Segments and characteristics of the industry together with important events in chemical history are briefly presented. The “language” of chemistry is introduced and important chemical terms are defined.

CHEMICAL AND ALLIED PRODUCTS INDUSTRIES

IMPORTANT SEGMENTS

Inorganic chemicals
Petrochemicals
Synthetic resins and plastics
Textile fibers
Synthetic rubber
Pharmaceuticals and drugs
Soap, detergents, and cosmetics
Paint, varnishes, and printing inks
Fertilizers and other agricultural chemicals
Adhesives and sealants
Dyes and pigments
Paper
Glass

In terms of total product value, the worldwide shipments of the chemical and allied products industries were almost 1600 billion dollars in 1999. In the U.S. alone, the value was 435 billion dollars (source: *Chemical & Engineering News*, June 26, 2000). The U.S. has the largest chemical economy by far of any country in the world, followed by Japan and Germany as distant second and third.

CHEMICAL INDUSTRY

CHARACTERISTICS

Large, diverse, and complex
Global
Strong technology base
Many segments, highly fragmented
Subject to business cycles
Highly competitive
Capital intensive
Committed to research and development
Advanced in use of computers and computer controls
Over 50% of the products are based on petroleum
Best employee safety record among all major industries
Criticized for many environmental problems

Because of the absolute necessity for chemicals in almost every manufacturing industry, it is difficult to define exactly what the chemical industry is. A good definition, however, is that the chemical industry consists of all companies engaged in converting raw materials obtained from the environment (air, ore, petroleum, trees, crops, etc.) into chemical intermediates plus the companies that convert these intermediates into consumer end products. Chemicals derived from petroleum or natural gas, known as *petrochemicals*, comprise about 55% of the total chemicals produced. Some of the globalization of the chemical industry now taking place is due to the shifting of production by petrochemical producers to energy-rich regions of the world such as Indonesia, Mexico, and the Middle East.

CHEMICAL INDUSTRY

The Beginnings

Pre-1600	Alchemists sought to turn base metals (iron, zinc, lead) into gold using the four "elements"— earth, fire, air, and water.
About 1600	The idea of the four "elements" was challenged and the chemical era began.
1600s	Robert Boyle worked out scientific experimental methods and published his findings (the scientific method).
1700s	Joseph Priestly discovered oxygen.
	Antoine Lavoisier distinguished between chemical and physical changes and enumerated and verified the fundamental law of the conservation of mass.
1800s	Dmitri Mendeleev published the Periodic Table of the Elements.

Ancient man (prehistoric–600 BC) practiced certain chemical arts such as extraction and working of metals, manufacture of leather, production of alcoholic beverages, and the use of vegetable oils, alkaloids, and narcotics. The Greek philosophers (600–200 BC) speculated on problems in the realm of what we now call chemistry, but they did little or no experimentation. In the Dark and Middle Ages, alchemy flourished and gradually evolved into an experimental science as the result of the thinking of men such as Roger Bacon (1214–1294), Paracelsus (1493–1541), and Francis Bacon (1561–1626). The birth of modern chemistry as an exact science, based on the law of the conservation of mass and on the quantitative study of chemical reactions, is dated from the work of Lavoisier.

CHEMICAL INDUSTRY

Research and Development/Engineering Technology

Important base for chemical industry:
- R&D spending for 2000 was over $250 billion.
- Most of the R&D in the U.S. is funded and carried out by the chemical industry.
- High investment facilities required with modern (state-of-the-art) scientific equipment.

R&D activities:
- Basic chemical research (by trained chemists); much of this is done in universities
- Improve existing products (e.g., better quality)
- Improve existing processes (by chemists and engineers), including cost reductions
- By-product disposal and utilization
- Solution of environmental problems

The size of today's chemical industry is a result of research and development (R&D) activities that generated new products and processes resulting in rapid industry growth. Over the years, R&D emphasis shifted from basic research aimed at new chemicals and their uses to improvement of existing products and processes. Today, substantial R&D is directed toward solving problems related to the environment and to satisfying governmental regulations.

CHEMICAL INDUSTRY

History

Pre-1900	Cement, lye, soap, explosives, dyes, paint, fertilizer, chemicals based on coal
1920s–30s	Cellophane and rayon (based on wood), medicinals, photographic chemicals, nylon, plastics
1940s	Synthetic rubber, pesticides, plastic films, chemicals based on petroleum
1950s	Engineering plastics, preservatives, new catalysts
1960s	Foreign investment, lower prices, performance improvements, pollution awareness
1970s	Energy and feedstock problems, higher raw materials costs
1980s	Imports, environment, and health concerns
1990s	Global industry, governmental regulations

Industrial chemistry is barely 100 years old, but tremendous developments were made during that time because of advances in basic chemical and engineering science. These advances resulted from research efforts conducted within chemical industry laboratories as well as in university laboratories. During the 1950s, the nature of the industry changed from emphasis on development of totally new products to refinement of existing types of products. In recent years, product refinements have been guided by concerns about human health and protection of the environment.

LANGUAGE OF CHEMISTRY

Chemical naming (nomenclature)
- Systematic
- *Chemical Abstracts* (American Chemical Society)
- Common (historical)
- "Nickname" (acronyms and trade names)

Relationship of names to chemical structure
Properties (chemical, physical)
Chemical formulae (chemical shorthand)
Pronunciation

To be knowledgeable in chemistry, one must be familiar with its language. This language includes the naming of chemicals, both systematic and common names, and the names and definitions of significant chemical and physical properties. The relationship of chemical names to chemical structures and formulae is also important. And, just as with any language, if one is to talk chemistry, it helps to be able to pronounce the names and other terms. Many of the terms and names needed to understand chemical "language" are introduced and defined throughout this book.

A major part in the language of chemistry is in learning the names of the chemicals (nomenclature). Many chemicals, particularly the more common ones, are known by several different names. For example, the chemical CH_3CH_2OH has the systematic name "ethanol." The publication *Chemical Abstracts* (American Chemical Society) also uses the name "ethanol." The historical or common name is "ethyl alcohol" or "grain alcohol." A "nickname" for it is just "alcohol," and there are various tradenames, depending on the manufacturer. For example, the Eastman Company sells it under the name of Tecsol®. Even trained chemists have trouble with nomenclature, which makes the use of and need for written chemical formulae common among chemists.

CHEMISTRY

PROPERTIES AND CHANGES

Properties	Characteristics of a substance
Physical properties	Observable characteristics such as density, color, smell, hardness, solubility, etc.
Chemical properties	Properties of a substance that cause specific behavior during chemical reactions
Chemical reaction	Any change that alters the chemical properties of a substance or forms a new substance
Reactants	The substances present at the beginning of a chemical reaction
Products	The substances formed in a chemical reaction

One of the important tasks of chemistry is to study how substances can be identified or distinguished from each other, that is, a study of properties. Such studies are also essential in determining how substances can be used in human endeavors.

There are two types of physical properties: *qualitative* properties and *quantitative* properties. Qualitative properties are those that cannot be measured, such as smell or taste. Quantitative properties, on the other hand, can be given precise mathematical values, for example, the weight of a certain volume of a substance (density), the temperature at which the substance boils (boiling point), or electrical conductivity.

Chemical properties depend on the ways in which a substance interacts (reacts) with other substances. Sulfuric acid reacts with iron to form iron sulfate and hydrogen.

$$\text{Iron} + \text{Sulfuric acid} \longrightarrow \text{Iron sulfate} + \text{Hydrogen}$$

This is a chemical reaction. The fact that iron reacts when it comes into contact with sulfuric acid is a chemical property of iron. Conversely, the ability of sulfuric acid to affect iron is a chemical property of sulfuric acid. The sulfuric acid and iron are called *reactants* in the above equation, and the iron sulfate and hydrogen are the *products* of the reaction.

CHEMISTRY

Substance States

Solid state	The state (or phase) in which a substance has a definite volume and shape
Liquid state	The state in which a substance has a definite volume, but can change shape
Gaseous state	A state in which a substance has no definite volume or shape
Melting	The change of state from solid to liquid
Vaporization	A change of state from liquid to gaseous
Condensation	A change of state from gaseous to liquid
Sublimation	The change of state from solid to gaseous without going through the liquid state

A change of state is a physical change that does not alter chemical properties. It usually takes place by increasing or decreasing the temperature of a substance. The ability to change the state of substances is important in the synthesis and purification of chemicals.

Water from a tap is an example of a chemical in the liquid state, whereas ice is water in a solid state. When liquid water boils, it turns to steam, which is water in the gaseous state. A dripping icicle on a warm winter day is an example of melting, whereby the solid phase of water (ice) is converted back to the liquid state. Droplets of water forming on a cool surface is the result of condensation of gaseous water (steam) back to liquid water. Carbon dioxide, the gas in carbonated beverages, is known as dry ice when it is in the solid state. When dry ice is heated, it goes directly to a gas without first becoming liquid. This is sublimation.

CHEMISTRY

Chemical Substances

Matter	All substances
Element	A substance that cannot be split into simpler substances by a chemical reaction
Atom	The smallest particle of an element that retains the chemical properties of that element
Compound	A combination of two or more elements held together in some way. It has different physical and chemical properties from the elements it contains. The proportion of each element in a compound is constant, for example, the compound known as water always contains two atoms of hydrogen and one of oxygen
Molecule	The smallest particle of an element or compound that exists on its own and still retains its properties

All matter is composed of elements. Most matter contains two or more elements and some in the form of compounds contain thousands or even millions of atoms. Water, for example, is a compound that contains two elements: hydrogen and oxygen. The chemical compound we know as sugar contains three elements: carbon, hydrogen, and oxygen. Table salt is composed of the elements sodium and chlorine.

Mixtures are blends of two or more elements and/or compounds that are not chemically bound to each other. Mixtures can usually be separated by physical means.

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Chemical Representation

Chemical symbol	A way of expressing an *element* in written form. It represents one atom and often is the first one or two letters of the name of the element.
Molecular formula	A combination of symbols representing one *molecule* of an element or compound. It shows which elements are in the molecule and the number of atoms of each element.
Reaction equation	A written expression of a chemical reaction where the reacting chemicals are shown to the left of an arrow pointing to the products of the reaction on the right. Either words or formulae can be used.
Balanced equation	An equation using formulae where the number of atoms of each element involved in the reaction is the same on each side of the arrow.

The language of chemistry is understood better when the symbols of the more common elements are known, such as those shown on the following page. Use of these symbols provides a convenient shorthand method for chemists to represent molecular formulae. In these formulae, the subscript number following the atomic symbol denotes how many atoms of that element are in the molecule, for example, the formula for water is H_2O, which means each molecule of water contains two atoms of hydrogen (symbol H) and one atom of oxygen (symbol O).

The process (chemical reaction) by which a chemical product is made, as depicted by an equation, is called *synthesis*. Working in laboratories, chemists devise new ways to synthesize known chemicals or new chemicals never made before and not found in nature. Synthesis chemists working in industrial laboratories also must find or develop uses for the new chemicals that they synthesize while considering the costs of eventual manufacture.

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Symbols of Common Elements

O	Oxygen	A gaseous element essential to human life; comprises about 20% of the air
H	Hydrogen	The most abundant element in the universe
N	Nitrogen	Necessary element in protein; air is 80% N
C	Carbon	All living matter contains carbon compounds
Cl	Chlorine	Abundant element, always combined in nature with other elements
S	Sulfur	Occurs free in nature
Na	Sodium	Combined with other elements in nature
P	Phosphorous	Combined with other elements in nature; another element essential to life

Chemists know how much by weight of an element or a compound will react exactly with another element or compound because the atoms of each element have an assigned weight called the atomic weight. By scientific agreement, each element's atomic weight is proportional to that of carbon with an assigned weight of 12. In all chemical weight calculations, hydrogen has an atomic weight of 1 (the lightest element), while nitrogen is 14 and oxygen is 16. The molecular weight of a compound is the sum of the weights of all of the atoms in the compound as shown by its chemical formula; for example, the molecular weight of water with the formula H_2O is 2×1 (2 hydrogens) $+ 1 \times 16$ (1 oxygen), which totals 18.

It is desirable for chemical calculations to deal with weighable amounts of various substances that we know contain equal numbers of molecules. For example, the molecular weight of hydrogen is 2 and that of oxygen is 32. This means that 2 g of hydrogen contains the same number of molecules as 32 g of oxygen. These actual weights are called *gram-molecular weights* or *moles*, for short. Thus, a gram-molecular weight (or mole) of any chemical is the quantity of that chemical whose weight is numerically equal to its molecular weight. It has been determined that one gram-molecular weight of a chemical contains 6.023×10^{23} molecules (this is called Avogadro's number).

CHEMISTRY

DIVISIONS

Inorganic	The chemistry of all elements and their compounds except those containing carbon
Organic	The chemistry of all compounds containing carbon
Physical	Applies concepts of physics to chemical phenomena
Analytical	Chemical characterization and identification
Biochemistry	Chemistry of living organisms
Chemical engineering	Design and operation of equipment for the production of chemical products by the use of chemical reactions

No branch of science is broader than chemistry because it deals with all matter in all forms. For convenience, chemistry is usually divided into the above divisions, but there is a great overlap. For example, there are chemicals known that contain inorganic elements and large carbon compound fragments that can be classified as either inorganic or organic. Thus, trained chemists must have a background in all the divisions of chemistry although their work may be in a specialized area such as organic chemistry or analytical chemistry. In the chemical industry, chemical engineers are concerned with the production of bulk materials from basic raw materials by large-scale application of chemical reactions worked out in laboratories. In doing this, they make use of so-called *unit operations* of chemical engineering such as fluid flow, heat transfer, filtration, evaporation, distillation, drying, mixing, adsorption, solvent extraction, and gas absorption.

CHEMISTRY

General Definitions

Ion	An atom or group of atoms (molecule) with an electrical charge. Positively charged ions are called *cations* while negatively charged ions are called *anions*.
Acid	A compound containing hydrogen that dissolves in water to produce hydrogen ions. Hydrogen ions are positively charged.
Base	A compound that will react with (*neutralize*) hydrogen ions to produce water. It is the opposite of an acid. A water-soluble base is an *alkali*.
Salt	Substance in addition to water that is produced from the reaction of an acid with a base.
pH	A measurement of hydrogen ion concentration (*acidity*) in water. Pure water has a pH of 7. Acids have a pH less than 7 while the pH of bases is above 7.

All chemicals, whether inorganic or organic, are either acidic, basic, or neutral. An example of an inorganic acid is sulfuric acid used in automobile batteries, while the acetic acid found in vinegar is an organic acid. Ammonia found in many household cleaners is a base, as are sodium carbonate and sodium hydroxide (lye). Sodium chloride (common salt) is an example of a salt because it is produced by the *neutralization* of hydrochloric acid with sodium hydroxide. A solution of table sugar in water is neutral (pH 7) because it does not contain hydrogen ions nor does it react with bases to produce water.

Control of pH is of critical importance in many industrial operations such as water purification, food and drug preservation, and agriculture.