CHEMICAL ENGINEERING SERIES

Chemical Engineering Essentials 1

Comprehensive Chemical Engineering

Edited by
Raj Kumar Arya
George D. Verros and J. Paulo Davim

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Preface

The field of chemical engineering has evolved significantly over the decades, expanding its horizons to encompass a range of interdisciplinary applications and cutting-edge advancements. *Chemical Engineering Essentials 1* is designed as a comprehensive resource for both students and professionals, providing fundamental insights along with in-depth discussions on advanced topics. With the rapid advancements in technology and growing concerns over sustainability and safety, chemical engineering is at a transformative juncture, poised to offer sustainable and innovative solutions across industries. This handbook seeks to serve as a definitive guide for the current generation of engineers, providing both foundational knowledge and modern approaches required to navigate and excel in this dynamic field.

Volume 1 is organized into three sections, as is Volume 2, each addressing critical aspects of chemical engineering.

Part 1 of this volume: Fundamental Principles lays the groundwork, beginning with an overview of the field and covering essential topics such as material and energy balances, thermodynamics and phase equilibrium. These fundamental principles form the bedrock upon which more specialized knowledge is built, equipping readers with a strong theoretical base.

Part 2 of this volume: Fluid Mechanics and Transport Phenomena delves into the physics and behavior of fluid systems and heat transfer. Chapters on fluid flow, heat conduction, convection, radiation and mass transfer provide essential understanding for designing and analyzing chemical processes.

Part 3 of this volume: Separation Processes covers the vital area of chemical separations, with discussions on extraction, distillation, filtration and emerging membrane processes such as pervaporation. Mathematical modeling techniques for binary and multicomponent distillation are also covered to provide a deeper insight into process design and optimization.

Part 1 of Volume 2: Reaction Engineering introduces readers to various reaction mechanisms and reactor designs, with a special focus on applications within the pharmaceutical industry and the concept of reactive chromatography. The section concludes with the mathematical modeling of batch reactors and nonisothermal continuous stirred-tank reactors (CSTRs), complemented by simulation studies using MATLAB and ASPEN PLUS.

Part 2 of Volume 2: Material Properties and Advanced Applications focuses on the diverse materials used in chemical engineering, alongside advanced applications such as hydrogen production, vinyl chloride production, process intensification and the integration of nanotechnology in the field. These topics underscore the importance of selecting the right materials and processes to achieve efficiency and innovation in chemical engineering applications.

Part 3 of Volume 2: Sustainability and Safety highlights the importance of green chemistry and sustainable practices in chemical engineering. This section also covers waste minimization, resource recovery and safety management, including hazard identification and risk assessment – critical components of responsible engineering practice in today's world.

This handbook represents the collective effort of numerous contributors, whose expertise and dedication have shaped this comprehensive guide. We extend our deepest gratitude to each author who has contributed invaluable insights and research to make this work possible. Our heartfelt thanks also go to our families, whose unwavering support, love and encouragement made this journey possible.

Special acknowledgment goes to the team at ISTE. Their efforts and guidance were instrumental in bringing this book to completion.

It is our sincere hope that the two volumes of *Chemical Engineering Essentials* will serve as a valuable resource, offering knowledge, inspiration and practical tools for all of those engaged in the field of chemical engineering.

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PART 1

Fundamental Principles

1

Overview of Chemical Engineering

1.1. Introduction

Chemical engineers have been enhancing our overall welfare for over a century. Chemical engineers have contributed to several advancements that impact our daily lives, ranging from the creation of more efficient computer chips to improvements in recycling, illness treatment, water purification and energy generation.

Chemical engineering (CE), also referred to as process engineering, is a branch of engineering that uses mathematics, economics, physical sciences and biological sciences to create and modify chemicals, energy and materials. Chemical Engineering was originally developed as a combination of mechanical engineering and applied chemistry, with a specific focus on its application in the petrochemical and heavy chemical industries.

Chemical engineers convert laboratory-developed procedures into practical applications for the commercial manufacturing of products, and then strive to uphold and enhance such processes. They depend on the fundamental principles of engineering, namely mathematics, physics and chemistry. Biology is assuming a progressively significant role.

Chemical engineers primarily conceptualize and develop procedures related to chemical production on a large scale. Chemical engineers primarily focus on designing and resolving issues related to the manufacturing of various substances such as chemicals, fuels, foods, pharmaceuticals and biologicals. They are primarily hired by industrial facilities of significant size to optimize efficiency and enhance the quality of products, while minimizing expenses.

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Chemical engineering encompasses the synthesis and fabrication of goods using chemical reactions and procedures. This includes the creation of machinery, systems and procedures for the purification of basic substances and the blending, combining and treatment of chemical compounds.

Chemical engineers enhance food processing processes and develop more efficient methods for fertilizer production, with the aim of augmenting both the amount and quality of food resources. In addition, they fabricate artificial fibers that enhance the comfort and water resistance of our garments; they devise techniques for the large-scale production of pharmaceuticals, thereby reducing their cost; and they invent safer and more efficient processes for refining petroleum products, thereby increasing the productivity and cost-effectiveness of energy and chemical resources.

Additionally, chemical engineers devise strategies to address environmental issues, such as pollution control and remediation. Indeed, they engage in the manipulation of chemicals, which are employed in the production or enhancement of virtually all the objects within your surroundings.

1.2. History of chemical engineering

Chemical engineering is a field that emerged from the practice of "industrial chemistry" in the late 19th century, as stated by Wikipedia (2024a, 2024b). Prior to the Industrial Revolution in the 18th century, the production of industrial chemicals and consumer items such as soap primarily relied on batch processing methods. Batch processing involves manual labor, when workers combine predetermined quantities of materials in a container and then subject the mixture to heating, cooling or pressurization for a specific duration. Subsequently, the product can be separated, refined and examined in order to obtain a marketable product.

Currently, batch processes are still used for more valuable products, such as pharmaceutical intermediates, specialty and formulated products such as perfumes and paints, or in food production such as pure maple syrups. Despite being slower and less efficient in terms of labor and equipment usage, batch methods are still profitable in these cases.

Chemical engineering approaches have enabled the production of higher volumes of chemicals through continuous "assembly line" chemical processes in industrial process development. The Industrial Revolution marked the transition from batch processing to a more continuous processing approach. The Industrial Revolution resulted in an unparalleled increase in demand, in terms of both quantity and quality, for large quantities of chemicals such as soda ash. This entailed two objectives: firstly, expanding the scale of the activity and enhancing operational efficiency, and secondly, exploring viable alternatives to batch processing, such as continuous operation. The practice of industrial chemistry dates back to the 1800s, and its academic study in British universities commenced with the publishing of the influential book "Chemical Technology" in 1848 by Friedrich Ludwig Knapp, Edmund Ronalds and Thomas Richardson.

According to Wikipedia (2024a, 2024b), James F. Donnelly is credited with referencing an 1839 mention of chemical engineering in the context of sulfuric acid manufacturing. However, it was noted in the same piece that George E. Davis, an English consultant, was attributed with originating the word. In addition, Davis made an attempt to establish a Society of Chemical Engineering. However, it ended up being called the Society of Chemical Industry in 1881, with Davis serving as its inaugural secretary.

The term "chemical engineering", which refers to the application of mechanical equipment in the chemical industry, gained widespread usage in England after 1850. The inaugural effort to establish a Society of Chemical Engineers in London took place in 1880. Consequently, the Society of Chemical Industry was established in 1881. The American Institute of Chemical Engineers (AIChE) was established in 1908, while the U.K. Institution of Chemical Engineers (IChemE) was established in 1922. The term "chemical engineer" was widely used in Great Britain and the United States by 1910.

1.3. Chemical engineering profession

Commonly known as process engineering, chemical engineering is a discipline of engineering that uses physical and biological sciences, mathematics and economics to produce and modify chemicals, energy and materials, as stated by AIChE (2024).

Traditionally, it encompasses the fields of heat transfer, mass transfer, momentum transfer, kinetics and reaction engineering, chemical thermodynamics, control systems and dynamic simulation, separation processes and unit operations.

Chemical engineering, traditionally used in the petrochemical and heavy chemical sectors, has experienced significant advancements and expanded its applications to many domains such as climate change, environmental systems, biomedical science, novel materials and complex systems. Chemical engineers have a significant impact on the manufacturing of nearly every item produced on a large scale in industry.

Common tasks include:

– ensuring adherence to health, safety and environmental regulations;

– engaging in research to enhance manufacturing processes;

– creating and strategizing the arrangement of equipment implementing safety protocols for handling hazardous compounds;

– supervising and enhancing the efficiency of manufacturing procedures. Calculating the expenses associated with production.

Chemical engineers employed in corporate and managerial settings frequently make visits to research and production sites. Engaging with individuals and fostering teamwork are essential for the achievement of chemical engineering projects.

Chemical engineers commonly operate in manufacturing plants, research laboratories or pilot plant facilities. They operate in the vicinity of expansive manufacturing machinery that is located both indoors and outdoors. Hence, it is frequently necessary for them to don personal protective gear such as hard hats, goggles and steel-toe shoes. Chemical engineering is used in several industries and sectors, and is primarily employed in industrial facilities that focus on large-scale production, aiming to optimize efficiency and the excellence of the final product, while minimizing expenses. Chemical engineering is used by several industries including aerospace, automotive, biomedical, electronic, environmental, medical and military sectors to enhance and advance their technical goods. These products encompass a wide range of applications.

Advanced materials have exceptional strength, durability and bonding properties for use in automobiles. Materials that are compatible with living organisms can be used for implants and prosthesis. Optoelectronic devices are designed to use light for various purposes. One important aspect of these devices is the use of films, which play a crucial role in their functionality. These films are specifically engineered to enhance the performance and efficiency of optoelectronic devices.

1.4. Features and challenges in chemical engineering

According to Garnier (2014) and Hipple (2017), numerous captivating and productive difficulties in the field of chemical engineering arise from the amalgamation of chemical engineering with chemistry, physics and biology, which necessitates a redefining of the control volume. This list does not encompass all of the forthcoming difficulties in the field of chemical engineering and the areas where chemical engineering abilities will be applicable:

– Energy resources and use: in this context, it is necessary to disregard any “agendas” that may be primarily driven by political constituents, such as corn-based ethanol. Energy is necessary for the provision of food, shelter and transportation. In order to accommodate the growing global population and the increasing demand for Western standards of living in what are currently referred to as "Third World" countries, it is imperative that we adopt more efficient sources of energy, unless we choose to revert to a completely agrarian society and lower our current standard of living. A recent breakthrough has occurred in the understanding of underground fluid flow and mechanics, commonly known as "fracking". This breakthrough enables the recovery of hydrocarbons that were previously trapped in underground rock formations. It involves injecting high-pressure fluids to break apart the rock formations. Enhanced oil recovery incorporates advanced surface chemical techniques into the conventional process of drilling wells into liquid reservoirs underground. Energy conservation will hold equal significance. It is impractical to believe that inhabitants in developing countries will not aspire to the same luxuries that are commonly enjoyed by those in more developed nations. If this is to occur, there will be a need for greater energy resources and improved energy efficiency. In recent decades, there has been a significant improvement in energy efficiency in various industries and goods, which can be attributed, at least in part, to the increase in energy prices. While there has been a recent shift in this trend, once these energy saving measures are implemented, it is improbable that they will be reversed. As a component of this endeavor, there will be a gradual advancement in the conversion of solar energy. While solar energy is abundant worldwide, its energy density is far lower than that of petroleum fuels. Efforts to enhance the efficiency of solar power conversion, for both thermal and electrical energies, have made consistent advancements. However, these improvements are still insufficient to sustain a solar-based economy. Chemical engineers will have a crucial role in the progress of this technology, particularly in terms of improving catalysts, enhancing collection material efficiency and advancing energy distribution technologies. Affordable energy is crucial for enhancing the quality of life for the majority of individuals in underdeveloped countries. Given the well-established fact of anthropogenic greenhouse gasses leading to gradual global warming, a major task is to generate energy that has a minimal impact on the environment. Chemical engineers are tasked with the job of verifying and ensuring that energy balances and thermodynamics are optimized in the most economically feasible manner. The utilization of renewable sources and the application of green chemistry in chemical production is an expansion of the task. It is the duty of chemical engineers to identify processes and reactions with favorable thermodynamics and energy balances, and subsequently enhance these processes through collaboration with economists, environmental scientists and society as a whole. The efficient storage of solar energy, which includes energy derived from wind and ocean currents, in order to facilitate its distribution during periods of high human demand, continues to be a significant challenge. Hence, it is crucial to prioritize the advancement of reversible processes that enable efficient energy storage and usage, while also exhibiting prompt initiation and termination properties. Efficiently releasing significant amounts of electrical energy is crucial for meeting societal demands. However, it is equally important to recognize the immense advantages of capturing and storing solar energy in a manner that imitates natural photosynthesis. This involves storing solar energy in chemical bonds, rather than as heat or electronic charge separation. If the artificial photosynthetic reaction, which harnesses solar energy, uses carbon dioxide, then two significant goals would be accomplished with a single technological advancement. It is important to note that although the reaction between carbon monoxide and oxygen releases a large amount of heat, the opposite reaction, which is the breaking apart of carbon dioxide into carbon monoxide and oxygen due to heat, can occur at the temperatures achievable in a solar furnace. The outstanding technological challenges involve the creation of sophisticated refractory materials capable of enduring the necessary temperatures to facilitate the reaction, effective heat exchange and the efficient separation of the resulting products. The process of dissolving carbon monoxide in a solution of alkali metal in water to produce alkali metal forms appears to be a highly favorable method.

– Water: the issue of providing drinking water to a growing worldwide population is compounded by the fact that only a tiny percentage of water resources are readily available for consumption. Therefore, it is necessary to explore alternative sources of non-fresh water for drinking purposes, as well as implement effective water recycling and reuse strategies. The provision of safe drinking water, together with food and energy, is sometimes referred to as the "great nexus" of engineering challenges in the 21st century.

– Green chemicals: it is important to fully use renewable feedstock and make the most of all its components. Due to the relatively low energy density of biomass compared to fossil carbon sources, it is necessary to carefully reassess the energy efficiency of biomass processing. This includes the creation of smaller mobile processing units that can be transported to regions where biomass is accessible during specific seasons. It is important to consider potential social and community advantages when doing a re-evaluation. An essential element in optimizing the utilization of biomass will involve the advancement of novel chemical routes that enable more efficient exploitation of the compositions of polysaccharides and lignins. The manipulation of cell differentiation and tissue formation in higher plants by certain insects in the families *Hemiptera* and *Hymenoptera*, resulting in the formation of galls and related protective structures, is a topic that deserves thorough multidisciplinary investigation. Although numerous beneficial enzymes are already manufactured, extracted and used in large-scale commercial applications, their catalytic rates are often constrained by heat instability, denaturation caused by surfactants and deviations in pH from the neutral range. Chemical engineers have conventionally employed heat, pressure and pH to expedite chemical reactions. However, the investigation of extremophile organisms and their enzymes, which have evidently developed to endure extreme temperatures, pressures and pH levels found in deep ocean vents and volcanic pools, seems to be at an early stage.

– Materials: chemical engineering will play a significant role in two long-term elements of this topic. Plastics recycling is the first and most frequently discussed method. The process of segregating polymers into readily recyclable components is highly expensive and inefficient, yielding materials that are seldom as functional as the initial raw ingredients. The economic justification for the separation process of materials such as polyethylene, polystyrene, ABS, nylon, etc., is seldom found, and instead, is supported by taxpayer financing. During this process, the characteristics of the polymer usually deteriorate, mostly due to a decrease in molecular weight, rendering them unsuitable for their original intended use. There are numerous instances of products in the store that bear a label indicating that they include a maximum of 10% recycled materials. Adding more would render the properties that the user is paying for unattainable. Several long-term events will occur, all of which will necessitate substantial involvement from chemical engineering. One possible solution is the implementation of separation technologies that can effectively and cost-efficiently separate different types of discarded plastics. This would enable a greater utilization of these plastics in their original products. The second objective is minimizing plastic consumption by implementing packaging and system modification. For instance, there are situations where a sizable plastic container can be transformed into a "shrink wrap" style packaging, resulting in a significant reduction in the amount of plastic used. It might also be feasible to completely eliminate conventional packaging by using different kinds of coatings. Furthermore, cost-effective pyrolysis methods (heating materials to high temperatures without oxygen, in contrast to combustion) could potentially turn polymers back into their original monomers, such as polystyrene to styrene, polyethylene to ethylene, polypropylene to propylene, etc. By generating conventional hydrocarbon monomers, it becomes simpler to separate them using typical chemical engineering techniques such as distillation. Additionally, these monomers can be used in various applications, not limited to the plastic they were derived from. Efforts are now being made in all of these areas, although the second option is likely to be the most resilient and sustainable in the long run. In addition, we must include "nanomaterials" in this category, as they are increasingly being incorporated into consumer items to offer distinctive features. The possible influence of 10–9 particle size materials and their distribution within the environment is currently being debated and analyzed. Nevertheless, these materials of significant size have a profound and beneficial effect on numerous material characteristics. Chemists and chemical engineers will encounter significant hurdles in the surface chemistry, contact with other materials and affordable manufacture of such materials. The performance of any separation process will vary dramatically when the particles to be separated fall within this particular size range. Within the previously discussed periodic table, there exists a category of substances referred to as "rare earth" metals. Illustrative instances encompass metallic elements such as dysprosium and neodymium. These elements are often used in modest amounts to enhance the characteristics of primary metals. They are infrequent in their incidence and costly to produce. A significant chemical engineering obstacle is the reduction of costs associated with the recovery and manufacturing of rare materials, as well as the exploration of alternative materials and product designs that do not rely on such scarce resources.

– Medical, biomedical and biochemical applications: artificial organs, which are now commonly used, are familiar to all of us. Artificial hearts and kidney dialysis machines can be understood as pumps and filters that serve as chemical engineering substitutes for the original organs in the human body. The principles we have covered, such as fluid dynamics, fluid characteristics, polymers and filtration, form the foundation for the development of these synthetic organs. As our comprehension of human body functionality advances, it is probable that we will witness the development of more artificial and replacement organs and body parts, with chemical engineering fundamentals playing a crucial role in their design. Examples may encompass artificial lungs, prosthetic joints and bodily fluid filtration. Chemical engineering principles, such as fluid flow, friction, filtration fundamentals, porosity, pressure drop and others, are essential components of these products. Currently, numerous educational institutions have integrated the chemical engineering department with this particular field of study, resulting in its rebranding as either biochemical engineering or biomedical engineering. An artificial heart is a man-made reproduction of the natural human heart. However, from a chemical engineering perspective, it can be described as a pump. All the factors involved in pump design, such as friction, energy requirements, flow rates, valve restriction and control, are equally applicable to these devices as they are to traditional pumps. However, it is important to note that the limitations on available energy, friction and pressure drop are significantly more restrictive in these devices. The materials used in the production of these devices must possess compatibility with human tissue to prevent rejection. This issue of incompatibility is significantly more complex than the previously described concerns of corrosion. It involves not only the degradation of materials, but also the potential risk of human fatalities. There are numerous prescription medications that are preferable to be taken in modest, continuous doses, rather than large doses once or twice a day. The practice of enclosing and gradually releasing various categories of medications using a dermal patch is increasingly prevalent. The process of encapsulating a drug and gradually releasing it is achieved by comprehending the rates at which molecules pass through the skin and aligning this absorption rate with an encapsulation method that releases the drug at an equivalent rate. Creation of a systematic methodology involves modeling and governing the behavior and functionality of the human body and brain processes using engineering principles. Use of simulation and control techniques to address several levels of biological systems, including DNA, RNA, cells, tissues, organs and the human body, in order to enhance the quality of life for those with genetic and related illnesses. Use of minimally intrusive sensors for the purpose of monitoring and regulating blood pressure, blood lipid content and heart rate. Nanotechnology enables precise targeting in the field of oncology and medicine delivery. Advancements in biotechnologies and enhanced biomaterials have the purpose of regenerating organs.

– Biochemical engineering is the integration of chemical engineering and biology to efficiently manufacture valuable medical products and systems on a larger scale. From a chemical engineering perspective, there are several distinct obstacles involved in this endeavor. Upon revisiting our analysis of membrane materials, it becomes evident that biological molecules, including viruses and proteins, possess particle sizes ranging from 0.01 to 10 μm. These sizes are considerably lower than the typical particle sizes generated in traditional inorganic and organic chemical reactions. This complicates the separation and retrieval of active, desirable molecules, making it necessary to employ more costly and advanced recovery methods. Typically, the processing of biological entities begins with solutions that are very diluted. The confluence of this component and the particle size presents a significant obstacle in achieving liquid–solid separation in this field, particularly in meeting the stringent pharmaceutical and FDA purity standards. The majority of biological materials are able to exist and carry out their functions under normal body and environmental settings. Therefore, it is impractical to carry out the majority of reactions at elevated temperatures, which could potentially enhance reaction speeds. This fact may also impose constraints on other unit operation notions for consideration. The efficacy of numerous biopharmaceuticals and medications is such that the quantity of substance required for a substantial market share may be comparable to that of a small-scale pilot plant in the conventional chemical or petrochemical sector. While certain scale-up guidelines may not be applicable, the importance of efficient production and high yields of highly valued minerals remains significant. The challenges involved in developing the medicine into an acceptable form for human consumption, such as its dissolving rate in the stomach and gastric tract, as well as the necessary inert components, are significant. The concept of stereo specificity is typically not taken into account in traditional chemical engineering and processing. Nevertheless, it holds great significance in the process of designing and producing physiologically active compounds. The carbon atom possesses a distinctive geometric structure, resembling a pyramid, due to its four bond connections, with the “C” molecule positioned at the middle. If the four molecules connected to this carbon are distinct, there is a chance that the carbon will exhibit chirality, indicating that it lacks symmetry in terms of its geometry. One of the peripheral groups will seem to be receding into the paper when drawn, while the other will protrude outward. The differentiation between these molecules is referred to as “left-hand” and “right-hand” rotations (or d-, l-; denoting dextro or levo rotation, respectively). Biologically relevant or active compounds, such as medicines, are crucial because our human body specifically recognizes and interacts with l- (levo) rotated molecules. These two molecules, which have undergone a chiral rotation, are referred to as enantiomers. This means that they cannot be overlapped with each other, regardless of the physical rotation of the molecule. The human body can only identify and metabolize molecules that are in the "levo" or "l-" configuration. Therefore, whenever there is an optical isomer present, it indicates the existence of an identical molecule that needs to be separated before the material can be used. The lack of absorption of the opposing isomer forms the foundation for many artificial sweeteners available in the market that possess a "right-handed" structure. We have the sensation of the molecule's taste (sweetness), but our bodies do not assimilate it and it is excreted as part of regular bodily fluids. The distinction between molecules with left-handed and right-handed orientations is referred to as various "enantiomers". Separating enantiomers may not always be essential, depending on the potential adverse effects of the other optical isomer. However, when separation is required, it significantly influences decisions in chemical engineering processes. The main point is that while having distinct "optical" characteristics, these molecules share the same physical properties, such as boiling or melting points. Conventional and less expensive methods such as distillation cannot be used to separate these enantiomers. Minor variations in solubility properties can be used in crystallization methods, chromatography and specialized ion-exchange resins. Furthermore, apart from the aforementioned fundamental obstacles, we are also confronted with the obstacle of sluggish response rates. Biological processes generally exhibit slower kinetic speeds in comparison to conventional chemical reactions. Consequently, the capacity to increase temperatures during processes such as tissue culture growth is severely restricted due to temperature sensitivity restrictions. Turbulence is typically necessary in biological reactions, just as it is in other chemical reactions. However, the heightened susceptibility to mechanical forces may need the use of specialized configurations. Additionally, it is worth mentioning that chemical engineers, due to their extensive knowledge of safety, can make valuable contributions to safety assessments of biochemical processes and products. The potential dissemination of hazardous, biochemically strong substances with minute particle dimensions, such as viruses, is a constant source of worry, and the specialized knowledge of chemical engineering in gas management and filtration can be employed to address this issue.

– Reaction engineering: the utilization of a blend of organic, inorganic and biochemical catalysis techniques aims to lower the energy required for chemical reactions, enhance the specificity of the reactions, decrease energy consumption, facilitate the separation of by-products and substitute toxic organic solvents and reagents containing scarce elements with reactions conducted in water-based or bio-based solvents, following environmentally friendly chemical principles. Using photosynthesis to transform solar energy and carbon dioxide into glucose, ligno-cellulosic polymers and their intermediates by the use of enzyme catalysts and/or aqueous systems. Comprehend and enhance the movement of substances, the transfer of energy, the degree of reaction and the ability to choose specific reactions