CHEMICAL ENGINEERING SERIES

Chemical Engineering Essentials 2

Advanced Processes, Materials, and Sustainability

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



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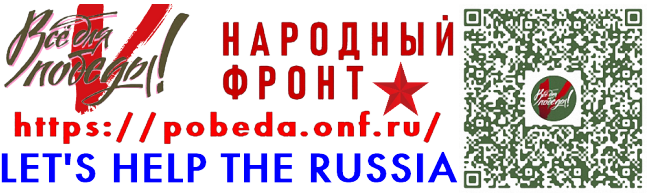
Chemical Engineering Series

Chemical Engineering Essentials 1
Comprehensive Chemical Engineering

Chemical Engineering Essentials 2
Advanced Processes, Materials, and Sustainability

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Advanced Processes, Materials, and Sustainability



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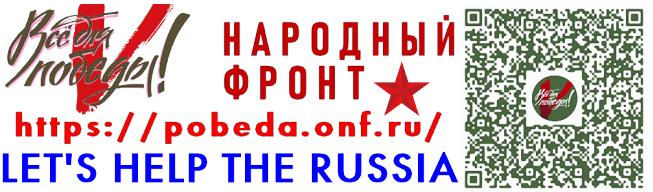
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Preface

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

Part 1 of Volume 1: Fundamental Principles lays the groundwork, beginning with an overview of the field and covering essential topics like 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 Volume 1: 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 Volume 1: 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 this volume: 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 non-isothermal continuous stirred-tank reactors (CSTRs), complemented by simulation studies using MATLAB and ASPEN PLUS.

Part 2 of this volume: Material Properties and Advanced Applications focuses on the diverse materials used in chemical engineering, alongside advanced applications like 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 this volume: 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, which are 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 *Chemical Engineering Essentials 1 and 2* will serve as valuable resources, offering knowledge, inspiration and practical tools for all of those engaged in the field of chemical engineering.

Raj Kumar ARYA
George D. VERROS
J. Paulo DAVIM
January 2025

PART 1

Reaction Engineering

1

Compaction, Compression and Consolidation in Pharmaceutical Industries

Compressibility and compactability are the defining features of medicinal powder's compaction characteristics. The capacity to create mechanically robust compacts is known as compactability, whereas compressibility refers to the powder's deformability under pressure. Compaction, in the context of pharmaceutical powders, involves the combined processes of compression and consolidation between the solid particles and gaseous phase, caused by an external force. This is relevant to pharmaceutical powders, particularly processes such as the handling of powdered pharmaceuticals, hard shell gelatin capsule filling, tablet and granule manufacturing, and other processes in the field of pharmaceuticals which are especially vulnerable to the impacts of such forces. Studying the possibilities that occur during the compaction of pharmacological materials is the crucial aspect of designing solid dosage forms, whereas universal testing machines or compaction simulators make systematic investigations of pharmaceuticals easier (Nguyen et al. 2020). Various parameters are measured during compaction among various researchers. Several pharmaceutical powders and formulations have had their compaction behavior evaluated using data collected from various measurements, including punch forces, die wall friction, ejection forces, change in temperature during compaction and other random variables. Among all other mathematical models, Heckel and Kawakita models show a better mathematical representation of compaction for the pharmaceutical systems within the appropriate pressure range.

1.1. Introduction to compression, compaction and consolidation

The matter or the substances present in the form of powdered solids are heterogeneous. They consist of various individual particles with different shapes and sizes in the presence of air voids. This is why it is difficult to analyze and

Chapter written by Neha DHIMAN and Girish GUPTA.

characterize the fundamental properties of this complex powdered solid system (Lachman et al. 1986). However, with the considerable advancements in qualitative and quantitative measurements, it is possible to determine some fundamental properties of individual particles as well as bulk powdered solids from an industrial point of view. In pharmaceutical industries, the study of the physical and mechanical properties of powdered solids is necessary for the compression, compaction and consolidation of tablets.

1.2. Definition and importance in pharmaceutical manufacturing

1.2.1. *Compression*

Compression is the mechanical process of reduction of bulk powdered solid under applied pressure resulting in the removal of air spaces or voids. In pharmaceutical industries, compression is used for the tableting process of a particular volume of granules in a die cavity under pressure to convert it into an intact tablet. An appropriate volume of powdered solid is taken in a die cavity/mold that is compressed under pressure using an upper and a lower punch to convert it into a single matrix by removing air/gas voids, then ejected from the die/mold in the form of a tablet (Dudhat 2022).

The assessment of the compression behavior of a powdered solid is mainly dependent upon the macroscopic properties, i.e. density of solid bed and porosity. Furthermore, these properties are also affected by the punching velocity of compression, stress–strain indices and elasticity of the material after compression (Vanhoorne and Vervaet 2020).

1.2.2. *Compaction*

Compaction of a powdered solid is defined as the ability of powdered solid compressed to form a coherent compact solid tablet having high mechanical strength under increasing stress (Stranzinger et al. 2021; Dudhat 2022).

Compaction is considered to be one of the most important pharmaceutical unit operations. For good compaction of tablets, powdered solids must have excellent flowability and a lesser tendency of segregation. The mechanical strength of a compact solid depends upon the physical, chemical and mechanical properties of the constituent solid such as hardness, flowability, particle–particle interaction, etc., whereas lubricants and moisture content also affect the compactability of the material (Bellini 2018).

Compaction = Compression + Consolidation of two phases (solid + gas) on applying force

1.2.3. *Consolidation*

Consolidation is the state of powdered solid having mechanical strength due to particle–particle interactions (Mohan 2012).

There are mainly three types of mechanisms involved in the consolidation of powder solids:

– cold welding;

– fusion welding;

– recrystallization.

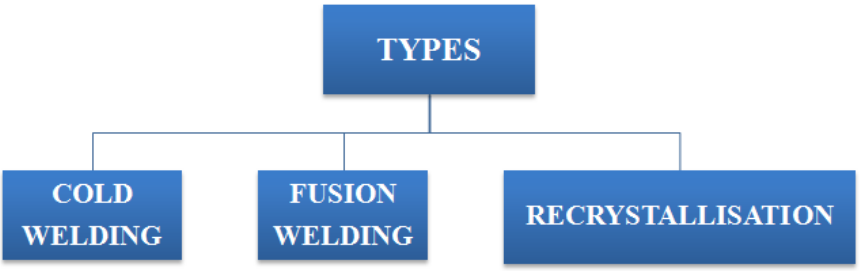


Figure 1.1. *Different types of mechanisms involved in consolidation (prepared for this work)*

1.2.3.1. *Cold welding*

Cold welding is one of the most widely used mechanisms for consolidation when the surface of two particles lies close enough to each other (i.e. less than 50 nm distance) having a strong attractive force, leading to strong particle–particle interaction. For this reason, cold welding increases the mechanical strength of powdered solid bed, when high compressive forces are applied.

1.2.3.2. *Fusion welding*

Generally, pharmaceutical powdered solids have irregular shapes and sizes, which provide a large surface area of contact (Mori et al. 2020). Therefore, a small compression force is sufficient to increase the particle–particle area of contact (Mohan 2012). If a high compression force is applied through the powdered solid

bed, a considerable amount of frictional heat is produced. This heat is dissipated through the contact surfaces of solid, which causes melting of the contact area of solid particles (Sampat et al. 2022). Fusion occurs at the contact surface after the melting of irregular shapes or corners of solid particles. Melt solidifies on the removal of compressive load, which leads to a further increase in the mechanical strength of the solid bed, known as fusion bonding. There must be a possibility of deformation of the solid surface, causing the breaking and formation of new bonds, which in turn increases the consolidation effect (Wahlich 2021).

1.2.3.3. *Recrystallization*

The solubility of a powdered solid is directly proportional to the applied compression load. If a high compression load is applied at the point of contact of moisture and solid surface, the solubility of the solid in solution also increases.

1.2.4. *Factors affecting consolidation process*

1.2.4.1. *Chemical properties of solids*

The lattice structure and nature of the crystallinity of the powdered solid affected the solidity of the material under high compression loads (Fonteyne et al. 2015). For example, those particles having cubic lattice structures are more suitable for the tableting process than those having rhombohedral lattices.

1.2.4.2. *Extent of availability of surface*

The consolidation of a powdered solid is also dependent upon the extent of availability of specific surface area. When compressive force is increased to an appreciable extent, particle surfaces become fractured, which leads to an increase in surface area. Further increase in compressive force causes particles to rebond. Hence, at very high compressive force, the surface area decreases to form a solid bed of powdered solid called tablet lamination.

1.2.4.3. *Effect of the presence of contamination on the surface of the particle*

The consolidation process is also affected due to the presence of surface contaminants. Surface contamination plays a vital role in the initial bond formation between powdered solid particles. For example, the presence of diluents, and lubricants on the surface of pharmaceutical powder aims to create a weak bond between them. This causes continuous coating on the tableting mass. Therefore, if contamination occurs at a larger extent on the surface of particles, it results in the formation of weaker tablets (Arshad et al. 2021).

1.2.4.4. *Interparticle attractive forces*

The interparticle attractive forces have a direct influence on the consolidation of the powdered solid bed. When a small compressive load is applied, molecular or electrostatic forces exist between individual particles. Van der Waals forces become predominant at an intersurface distance of 100 nm, which tends to form agglomerates. This agglomeration leads to an increase in the air spaces of the solid bed. The tablet then formed has low mechanical strength and is not stabilized. This may lead to cracking in the internal structure.

Therefore, the consolidation behavior of powdered solid can be controlled by internal (Van der Waals) as well as external forces (i.e. elasticity and plasticity). Consolidation gives rise to a decrease in air space, hence preventing the breakdown of a tablet (Kengar et al. 2019).

1.3. Powder properties and their characterization

1.3.1. *Characteristics of pharmaceutical powders, flowability, particle size and distribution*

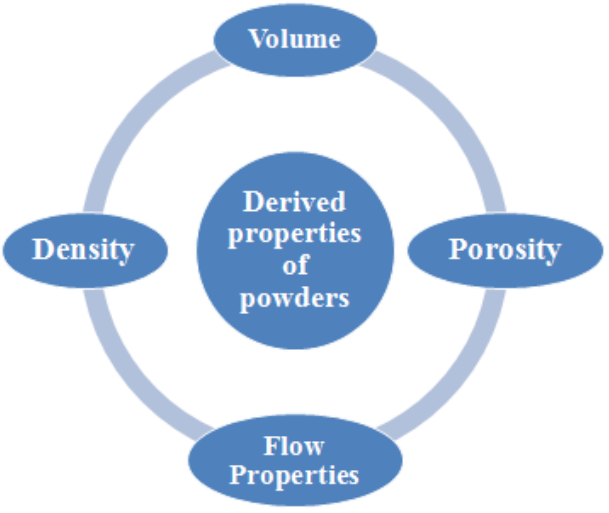


Figure 1.2. *Derived properties of powder (prepared for this work)*

While considering the tableting process of the pharmaceutical powdered solid, some physical and mechanical properties of solid particles play a key role, which

further affects the compressibility, compactability and consolidation behaviors of powder (Awad et al. 2021).

Some of the most important physical properties are density, porosity, particle size, shape and distribution, and moisture content. These physical properties help us to understand the flow behavior of the powdered solid, and a change in one such property may affect the other, resulting in a change in the compression and consolidation behavior of tablets. Physical properties are also related to the study of dosage form as well as the bioavailability of the tablet.

On the other hand, the mechanical properties of powder deal with the compression–decompression behavior or stress–strain behavior.

1.3.1.1. *Volume*

The mass of the bulk powdered solid can be measured easily as compared to the measurement of the volume of powder. When a powdered solid is poured into a container under gravity, the air spaces or voids must be present there. That is why more complications arise while measuring the actual volume of the powdered solid. These air voids are mainly of three types and are explained using mass–volume relationships:

– *Open intraparticulate voids*: these voids are present within a single particle of powdered solid but are open to the external environment.

– *Closed intraparticulate voids*: the voids lie within the single particle but are closed to the external environment.

– *Interparticulate voids*: the air voids that exist between the individual particles of powdered solid.

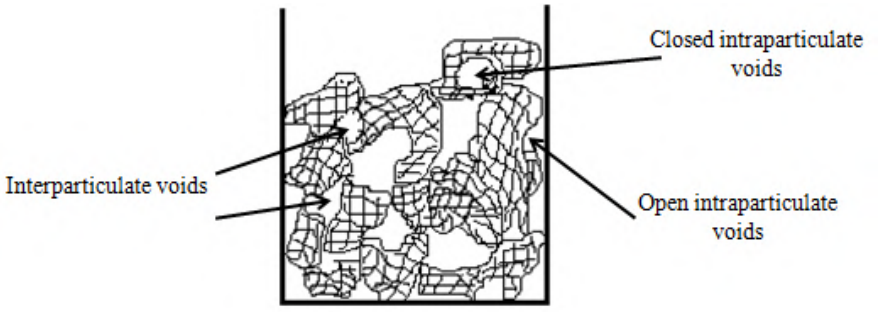


Figure 1.3. *Types of voids (prepared for this work)*

In keeping these air voids under consideration, the powdered volume can be classified as follows:

– *True volume (V_T)*: true volume of powdered solid can be defined as the total volume of the solid particulate itself except the volume occupied by the inter- and intraparticulate voids.

– *Granular volume (V_G)*: the granular volume of powdered solid is the sum of the volume occupied by the solid particulate itself and the volume occupied by all intraparticulate voids (except interparticulate voids)

$$V_G = V_T + \textit{volume occupied by intraparticulate voids}$$

– *Bulk volume (V_B)*: the bulk volume of powdered solid is equal to the sum of the volume occupied by the solid particulate itself, intraparticulate voids as well as interparticulate voids

$$V_B = V_T + \textit{volume occupied by (intraparticulate + interparticulate) voids}$$

or

$$V_B = V_G + \textit{volume occupied by interparticulate voids}$$

– *Relative volume (V_R)*: relative volume can be defined as the ratio of the experimental volume of sample (V_E) under specific conditions of the experiment to the true volume (V_T) of the powdered solid sample, i.e.

$$V_R = \frac{V_E}{V_T} \qquad [1.1]$$

Relative volume tends to approach unity if the experimental volume of the sample (VE) becomes equal to the true volume (VT), i.e. under compressive force, all of the air voids will be eliminated from the particular packing of the powdered solid.

1.3.1.2. *Density*

The density (ρ) of the powdered solid is defined as the ratio of the mass of the solid to the volume occupied by the solid

$$\textit{density of the solid } (\rho) = \textit{mass of solid } (M)/\textit{volume of solid } (V) \qquad [1.2]$$

Based on the three types of volumes discussed above, the density of the powder is also classified as the following:

– *True density (ρ_T)*: this is the ratio of the mass of the powder to the true volume of the powder

true density (ρ_T) = mass of powder (M)/true volume of powder (V_T) [1.3]

– *Granular density (ρ_G)*: this is the ratio of the mass of the powder to the true volume of the powder

granular density (ρ_G) = mass of powder (M)/granular volume of powder (V_G) [1.4]

– *Bulk density (ρ_B)*: this is the ratio of the mass of the bulk powder to the bulk volume of powder, especially when a particular mass of the powdered solid is poured into a cylinder with flow under gravity

bulk density (ρ_B) = mass of powder (M)/bulk volume of powder (V_B) [1.5]

– *Relative density (ρ_R)*: if ρ is the density of the sample under specific experimental conditions and ρ_T is the true density, and then the relative density is defined as the ratio of ρ/ρ_T

$$\rho_R = \frac{\rho}{\rho_T} \quad [1.6]$$

The relative density tends to unity if $\rho = \rho_T$ when all of the air spaces or voids are eliminated from the particular packing of the powdered solid.

1.3.1.3. *Porosity (ε)*

The air voids present in powdered solid packing are of more importance as compared to the solid mass (Dudhat 2022). Therefore, the porosity of the powdered solid is the ratio of the total volume occupied by the air voids (V_V) to the bulk volume of the powdered solid (V_B)

$$\varepsilon = \frac{V_V}{V_B} \quad [1.7]$$

The total volume occupied by the air voids (V_V) is also given by the difference in the bulk volume and true volume of the powdered solid,

$$V_V = V_B - V_T \quad [1.8]$$

On equating equations [1.7] and [1.8], we get

$$\varepsilon = \frac{(V_B - V_T)}{V_B} = \left[1 - \left(\frac{V_T}{V_B}\right)\right] \quad [1.9]$$

The percentage porosity is given by

$$\%\varepsilon = \left[1 - \left(\frac{V_T}{V_B}\right)\right] x\ 100 \quad [1.10]$$

Porosity is an important factor while studying the compression behavior of tablets, which helps to determine the disintegration time, dissolution rate, friability and drug absorption mechanism.

1.3.1.4. *Flow properties*

In the tableting process, when pharmaceutical powder is poured into the die to make a compact tablet, it is required that the powdered solid have good or excellent flow properties so that the die should be filled properly during compression and the tablet formed has enough mechanical strength (Mohan 2012). The flow behavior depends upon the following factors.

1.3.1.4.1. Particle size

The rate of flow of the powdered solid is directly proportional to the size of the particles. The particles having small diameters cohere with each other due to van der Waal's forces, electrostatic attraction and surface tension. These attractive forces result in poor flow behavior of particles, whereas particles with large diameters decrease the cohesion of particles, which enhances the flow property due to the lesser influence of gravitational force.

1.3.1.4.2. Particle shape

Those particles having spherical shapes with smooth surfaces of contact show good flow behavior as compared to the needle type or elongated particles with rough surfaces. The roughness of the surface tends to increase the friction factor and cohesiveness of the particles, which leads to poor flow behavior of powdered solids.

1.3.1.4.3. Porosity and density

As discussed above, density and porosity are two important physical properties of powdered solids. High-density particles have a large mass-by-volume ratio, which leads to good flow behavior, whereas large porosity decreases the flow characteristic of particles.

1.3.1.4.4. Moisture content

Powdered solid containing high moisture content has large cohesion and adhesion properties. When particles get stuck to each other, they cause poor powder flow properties. Therefore, dry mass enhances the flow properties of the powdered solid.

1.4. Powdered characterization techniques

1.4.1. *Determining flow properties and compressibility*

There are two main parameters to measure the flow behavior of pharmaceutical powdered solid, i.e. angle of repose and compressibility factor/compressibility index (Garg et al. 2018).

1.4.1.1. *Angle of repose*

The angle of repose is one of the simplest methods to determine the flow behavior of powdered solids. It is that the critical angle (θ) at which the powdered solid forms a conical heap relative to the horizontal base when it is allowed to fall through the funnel under gravity onto the horizontal surface

$$angle\ of\ repose\ (\theta) = \tan^{-1}\frac{h}{r} = \tan^{-1}\frac{2h}{D} \quad [1.11]$$

where:

– h = height of the heap of the powdered solid;

– D = diameter of the heap base;

– r = radius of the heap base;

– θ = angle of repose.

S. No.	Angle of repose (in degree)	Type of flow
1	25–30	Excellent
2	31–35	Good
3	36–40	Fair
4	41–45	Passable
5	46–55	Poor
6	56–65	Very poor
7	More than 66	Poorest

Table 1.1. *Angle of repose versus flow behavior*

Therefore, the angle of repose of the pharmaceutical powder can be determined by measuring the height and base diameter or radius of the heap formed by the

powdered solid when it falls through the funnel under gravity. The greater the angle of repose, the better the flow ability will be. Table 1.1 gives the relationship between the angle of repose and the flow behavior.

Fine, cohesive or sticky materials have a larger angle of repose. Therefore, it has been observed that the angle of repose increases with an increased moisture content due to the formation of aggregates.

1.4.1.2. *Compressibility factor/compressibility index (I)*

The compressibility index is also helpful in determining the flow behavior of powdered solids. The compressibility index is the measure of the decrease in volume of matter when placed under pressure. When pressure is applied on the bed of powdered solid, the volume of powder decreases until all of the air voids or spaces are removed.

The compressibility factor can be measured by pouring the powdered solid into a measuring cylinder without any disturbance. The volume occupied by the undisturbed powder (V_O) and compressed powder (V) (i.e. after applying external force when there is no air void or space between the particles of powder) will be noted down and used to determine the compressibility index/compressibility factor (I)

$$compressibility\ index\ (I) = \frac{(V_o - V)}{V_o} = \left[1 - \left(\frac{V}{V_o}\right)\right] \quad [1.12]$$

where:

– V = volume occupied by the powdered solid after compression;

– V_O = volume occupied by the undisturbed powdered solid before compression.

S. no.	**Compressibility index**	**Type of flow**
1	≤ 10	Excellent
2	11–15	Good
3	16–20	Fair
4	21–25	Passable
5	26–31	Poor
6	32–37	Very poor
7	> 38	Poorest

Table 1.2. *Compressibility index versus flow behavior*

Therefore, the compressibility index can be defined as the ratio of the decrease in the volume of powder after applying pressure to that of the undisturbed volume of powder solid.

Percentage compressibility can be determined as

$$percentage\ compressibility\ index\ (\%I) = \left[1 - \left(\frac{V}{V_o}\right)\right] x\ 100 \qquad [1.13]$$

Table 1.2 represents the values of the compressibility index relative to the particular type of flow behavior of the powdered solid.

1.4.2. *Determination of tapped density and bulk density*

The compressibility index in terms of bulk density and tapped density is given by

$$compressibility\ index\ (I) = \frac{tapped\ density - bulk\ density}{tapped\ density} \qquad [1.14]$$

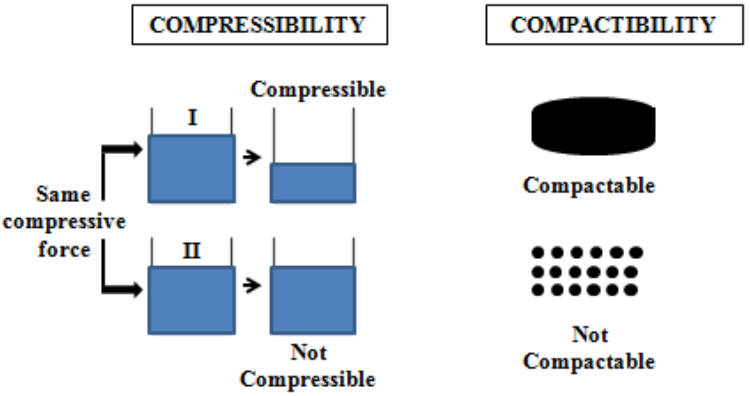


Figure 1.4. *Compressibility and compactability (prepared for this work)*

1.5. Tablet compression, compaction process and consolidation mechanisms

1.5.1. *Steps involved in the compression process, mechanisms and principles*

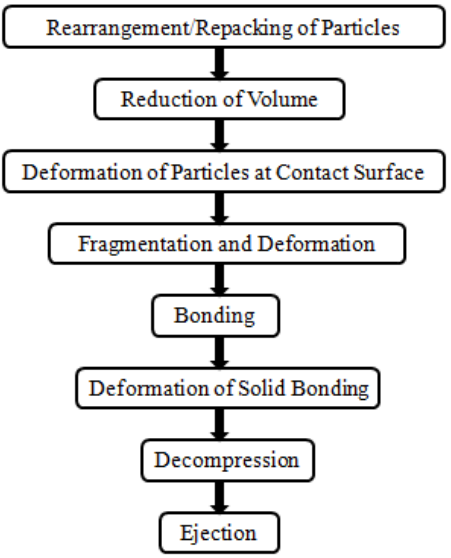


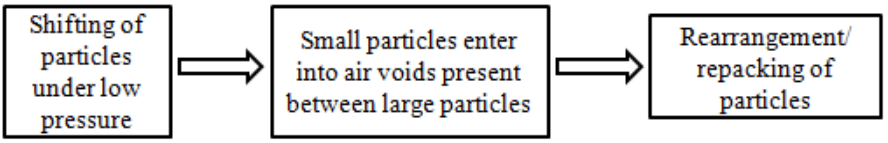
Figure 1.5. *Steps involved in the compression process (prepared for this work)*

1.5.1.1. *Rearrangement/repacking of particles*

When the tablet is formed from a powder solid, the main processes involved are the initial compression of the powdered solid to form a compact tablet leads to consolidation through various stages. Initially, when a powdered solid is compressed under a low compaction load, the small particles are shifted from their position and enter into the air voids present within the large particles in die packing. This gives rise to a closed packing arrangement, and leads to an increase in interparticulate friction as well as interparticulate surface area to increase the particle–particle interaction (Lachman et al. 1986; Mohan 2012). This initial packing of powder solid die cavity is mainly affected by the size and shape of particles. For example, spherically shaped particles are more suitable for tablet compression as compared to irregularly shaped particles (i.e. cubical, flat or needle-shaped particles) because spherical particles involve less rearrangement or repacking (Sahnen et al. 2020).

1.5.1.2. *Reduction of volume*

After the rearrangement or repacking of particles, the compaction load is increased to avoid further rearrangement. The extent of the reduction of the volume of pharmaceutical powder strictly depends upon the mechanical strength of particles as well as the mechanism involved in a reduction under pressure. At this stage, the final reduction of volume is attained followed by the deformation of particles at the surface of contact and fragmentation of particles.

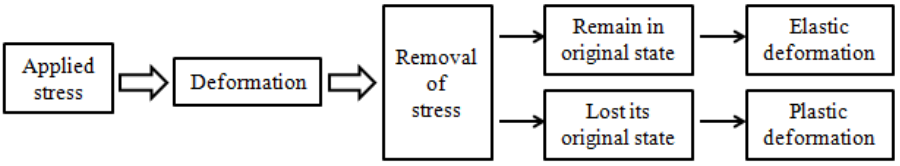


1.5.1.3. *Deformation of particles at contact surface*

When the final reduction of volume is achieved, a further increase in stress does not affect the volume reduction of particle arrangement, as the packing arrangement has already become closed packed and no air void is present there. Hence, the filling of smaller particles into air voids within large particles no longer takes place. Therefore, an increase in compression force leads to the deformation of particles at the surface of contact.

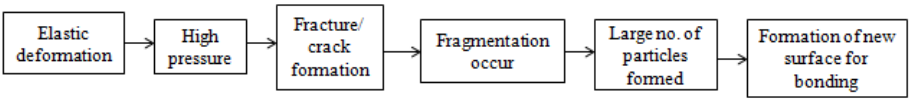
Generally, the particles undergo two types of deformations, i.e. elastic deformation and plastic deformation. The deformation of particles is also dependent on the physical and mechanical properties of the material. Besides this, the amount of applied compression load is also considered.

When a powdered solid bed is enclosed in a die bearing the load of external forces of upper and lower punch, it gives rise to the deformation of particles. After reaching a critical point of deformation, the applied compressive load is removed. Therefore, particles are either deformed elastically, i.e. the particles return to the original shape on the release of stress or the particles deformed plastically, i.e. the particles will remain in their deformed state even after the removal of stress. This plastic deformation of particles leads to the compaction of a tablet.



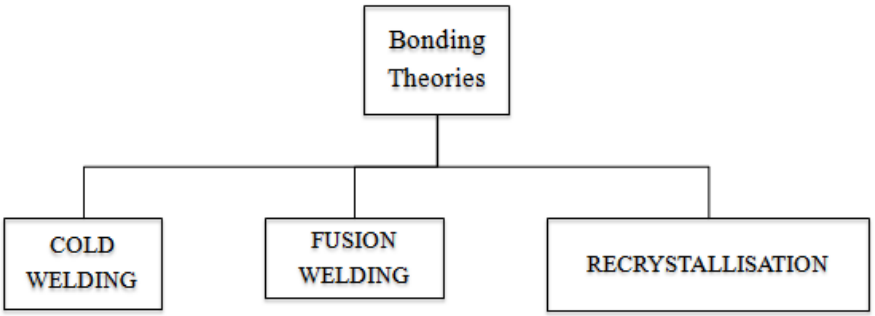
1.5.1.4. *Fragmentation and deformation*

Under the applied stress, particles of powdered solid are not only deformed elastically or plastically, there must be a possibility of fragmentation, and deformation occurs. Fragmentation does not occur if particles are plastically deformed on the removal of stress. If particles undergo elastic deformation, fragmentation occurs under high pressure which results in fractures or cracks on the surface of particles to form new surfaces for bonding (Mohan 2012). Excessive fragmentation occurs in the case of brittle and highly porous material. Hence, more bonding sites will be available, whereas ductile materials that have a low porosity do not undergo fragmentation.



1.5.1.5. *Bonding*

After fragmentation, further increases in pressure cause the formation of new bonds between the available surface sites of particles, increasing the mechanical strength of the powder bed under large compressive force. The bonding can be explained using the following theories.



– *Mechanical theory*: the true volume of the powdered solid can be defined as the total volume of the solid particulate itself except the volume occupied by the inter- and intraparticulate voids.

– *Intermolecular theory*: according to this theory, at this stage bonding between new contact surfaces of particles is only due to the van der Waals forces, because the contact surfaces lie close enough to each other (i.e. 100 nm distance) under high pressure to consolidate the particles.

– *Liquid surface film theory*: this theory deals with the bonding of particles in the presence of liquid thin film, which may result from melting or fusion welding. The necessary condition for this type of bonding is the solubility of the solid material.

1.5.1.6. *Deformation of solid bonding*

As the pressure increases, the strength of the consolidated solid increases followed by a decrease in the density of solid packing within the die cavity.

1.5.1.7. *Decompression*

At this stage of decompression, all kinds of stress or compressive forces are removed for the compaction and consolidation of the tablet. Furthermore, some of the factors must be kept in mind while the tablet is unloaded from the die. As quick loading or unloading of solid bed, brittle fracture, and further plastic deformation may occur. Two main steps have to be considered before studying the decompression process.

1.5.1.7.1. Pre-compression

In the pharmaceutical tableting process, pre-compression is the stage when a small compressive force is applied for the partial formation of the tablet. Compressive forces are further increased slowly in multistage to get better hardness of tablet, especially in the case of brittle and porous material.

1.5.1.7.2. Main compression

Under main compression, there is a formation of interparticulate bonds within the interparticulate contact surface. Initially, particles are rearranged to a more dense structure. Furthermore, an increase in applied force results in fragmentation or deformation of particles.

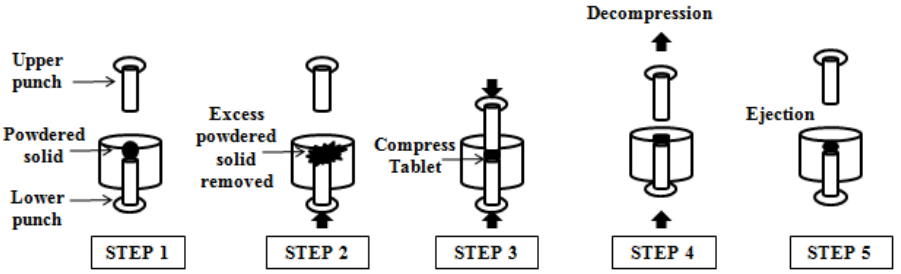
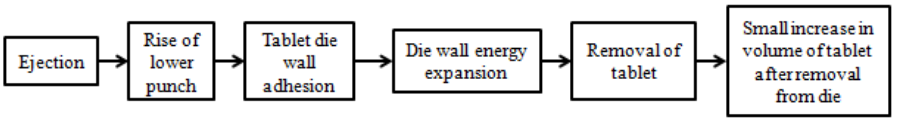


Figure 1.6. *Steps involved in the compression of the tablet (prepared for this work)*

On removal of applied pressure, in the die cavity, elastic deformation occurs on the contact surfaces of the tablet due to elastic recovery. To handle this stress, the tablet must have high mechanical strength. Otherwise, it may result in the fracture of the tablet. If the tablet is more elastic, then capping or lamination may occur. Tablets that undergo plastic deformation are strong enough to hold this stress and do not undergo capping or lamination on decompression. The failure or fracturing of the structure is also influenced by the speed of the process (Mohan 2012).

1.5.1.8. *Ejection*

The last step involved in the compression of the tablet is the ejection of the tablet from the die cavity. In this process, the ejection force of the lower punch must be enough to overcome the adhesion between the die wall and the compact surface of the tablet. Lubricants may help to minimize the effect of the die wall and tablet adhesion, hence reducing the necessity of capping or lamination of material by increasing the tendency of cohesiveness.



1.6. Tablet properties and quality control

1.6.1. *Properties of tablet influenced by compression*

1.6.1.1. *Density and porosity*

As the compressive force increases, the particles of powdered solid beds tend to achieve a limiting density of material. Therefore, an increase in the compressive force increases the density of the tablet. Porosity is inversely proportional to the density of the tablet. The plot shows the relation between porosity and the log of compressive force. As the compressive force increases, particles of solid bed come close to each other to make the material less porous; hence, the porosity decreases (Markl et al. 2018; Wilms et al. 2020). The relation between porosity and density of the tablet is given by

$$porosity = [1 - (tablet\ density/true\ density)]$$

$$= [1-(tablet\ weight/true\ volume)/true\ density\ of\ powder] \quad [1.15]$$

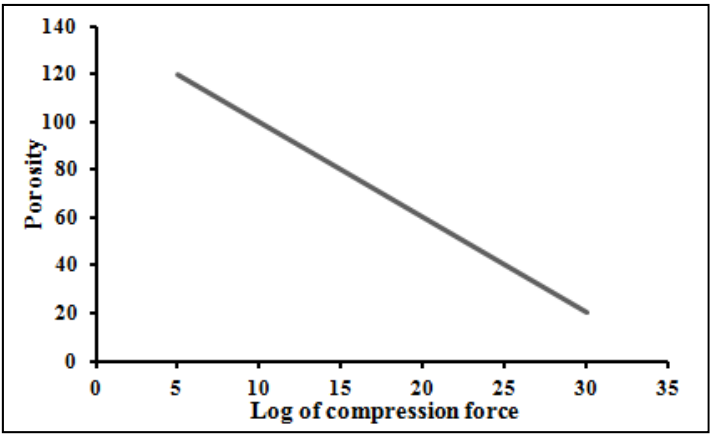


Figure 1.7. *Plot of porosity versus log of compression force (prepared for this work)*

1.6.1.2. *Hardness and tensile strength*

As the compressive force increases, fragmentation and deformation of granules occur, which leads to an increase in specific surface area. Figure 1.8 shows the general behavior of the material with an increase in compressive force. With the increase in specific surface area, there is more availability of sites for bonding. Hence, the hardness and tensile strength of the tablet show a linear relationship with compressive force. Furthermore, an increase in pressure or compressive force may decrease the surface area due to the formation of interparticle bonding.

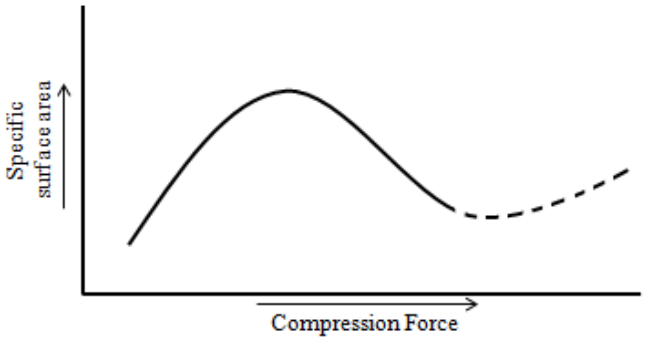


Figure 1.8. *Plot of specific surface area versus compression force (prepared for this work)*

1.6.1.3. *Disintegration time*

Generally, as the applied compressive force increases, the hardness and tensile strength of the tablet also increase, which further increases the disintegration time of the tablet. The case may be different for porous or less dense particles. Exception is also there for coated or non-coated tablets.

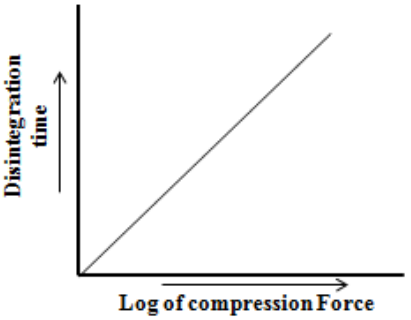


Figure 1.9. *Plot of disintegration time versus log of compression force (prepared for this work)*

1.6.1.4. *Dissolution rate*

As compared to the disintegration time of the tablet, the dissolution rate of the tablet is difficult to predict along with a change in applied compressive force. In the case of a non-coated tablet, the properties of API and excipients also affect the dissolution rate. But generally, if fragmentation occurs while compaction of the tablet, the increase in specific surface area increases the bonding of particles, hence decreasing the dissolution rate of the tablet.

1.6.2. *Factors affecting the strength of the tablet*

1.6.2.1. *Crushing strength of tablet*

Crushing strength (S_T) can be determined easily by applying compressive force (F_c) on the tablet along its diameter until it fractures. It is given by the relation

$$S_T = \frac{2F_c}{DH} \qquad [1.16]$$

S_T is the tensile strength, F_c is the compression force, and D and H are the diameter and thickness of the tablet, respectively.

1.6.2.2. *Friability*

Friability is another parameter to measure the potential and mechanical behavior of tablets while packaging. The friability test measures the weight loss of tablets by revolving the tablets in a standardized plastic wheel at 25 rpm. Compressed tablets having a weight loss of more than 0.5–1.0% of the tablet weight can be acceptable for packaging

$$\%\ friability\ or\ \%\ loss = \left[\frac{(w_1 - w_2)}{w_1}\right] x\ 100 \qquad [1.17]$$

where:

– w_1 is the initial weight of the tablet before the test;

– w_2 is the final weight of the tablet after the test.

1.6.2.3. *Particle size and shape*

Under compression, large particles become fragmented into smaller ones, provide a large number of interparticle contact surfaces and tend to have large bonding sites. Particle shape is also an important factor. For example, spherical particles have good flow properties, whereas cubical or irregularly shaped particles have poor flowability.

1.6.2.4. *Binder and lubricants*

Binders improve the mechanical strength of the tablet during compression, whereas the process becomes reversible during the decompression of the tablet.

Lubricants improve the flow behavior of particles and minimize the die wall friction which helps to prevent the adhesion of particles.

1.6.2.5. *Thickness test*

Thickness is also affected by changing the applied compressive force. Tablet thickness can be determined using an vernier caliper, which further influences the packaging of the tablet. The variation in the tablet diameter should be within ± 5% variation.

1.6.2.6. *Weight variation*

Uneven distribution of the pharmaceutical powdered solid in the die cavity may result in weight variation of tablets. It can be done by weighing 20 tablets

individually, then the average weight of 20 tablets is compared with the individual tablet weight and is given by the relation

$$weight\ variation = \left[\frac{(IW-AW)}{AW}\right] x\ 100\% \quad [1.18]$$

where:

– IW = individual weight;

– AW = average weight.

1.7. Tablet manufacturing challenges

1.7.1. *Capping, lamination and sticking issues*

The main issues that arise during the tableting process under compression force are capping, lamination, sticking and picking (Mohan 2012; Takeuchi et al. 2020). Capping and lamination problem mainly arises during the pre-compression and main compression processes.

1.7.1.1. *Capping*

This problem arises when the upper and lower layers of the tablet separate completely or partially from the main body during ejection from the die wall cavity called capping. The presence of large amounts of fines, low moisture content, and insufficient binders and lubricants cause capping in the tableting process.

1.7.1.2. *Lamination*

When the compression force is rapidly applied and removed on ejection of the tablet from the die, the tablet is separated into two different horizontal layers called lamination of the tablet.

This type of effect is shown by those materials having a high content of oily granules and hydrophobic lubricants.

1.7.1.3. *Sticking*

Sticking may occur, while the ejection of the tablet can be defined as the tablet material, which adheres to the die wall. The granules or particles have moisture content, lesser lubricant, too many binders and soft materials associated with this effect. A rough die wall and too deep a die cavity with rapid compression also affected the sticking of the tablet.

1.7.1.4. *Picking*

Picking refers to the tablet surface material adhesion, only related to the letter, logos or design embossed on the punch faces. The pharmaceutical powder having low melting becomes soft due to the heat of compression. Moisture level is one of the most important factors affecting the picking and sticking process.

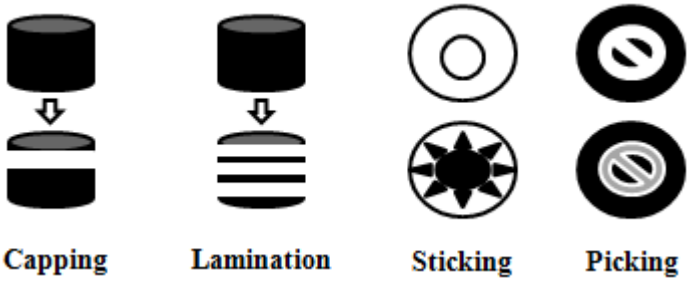


Figure 1.10. *Problems arise in the tableting process (prepared for this work)*

1.7.2. *Solutions and troubleshooting*

The amount of constituents of the pharmaceutical drugs such as API, excipients, diluents, lubricants binders, etc., in the tablet must be considered for the troubleshooting of tableting issues (Mohan 2012).

1.7.2.1. *API modification*

In high-dose drugs, excipients are present in lesser amounts. Therefore, API modification helps to improve the quality of tablets.

1.7.2.2. *Excipient selection and modification*

The amount of excipients present in a tablet is mainly associated with the overall quality of the tablet. Excipients such as diluents and binders have positive effects, whereas disintegrants and lubricants have negative effects on the compaction of tablets.

1.7.2.3. *Diluents*

Diluents are the fillers that help to increase the bulk volume of the tablet. Therefore, diluents improve the cohesion of particles, flow behavior, and direct compression can be applied, for example lactose and mannitol.

1.7.2.4. *Lubricants*

Lubricants help to decrease the friction at the interface of the tablet and die wall during ejection. They also prevent the stickiness of tablet surfaces with punch surfaces and enhance the flow behavior of material by reducing interparticulate friction. Examples of some lubricants are magnesium stearate, calcium stearate and polyethylene glycol.

1.7.2.5. *Binders*

Binders are also known as granulating agents because the addition of binders in the formation of a tablet improves the mechanical or granular strength of the tablet. Water and organic solvents can be used as a binder to form granules from powdered solids. They are cohesive and are important to minimize the problem of capping and lamination, for example, cellulose, methyl cellulose and sucrose.

1.7.2.6. *Disintegrants*

According to the need, some of the drug substances require the desired dissolution rate.

Therefore, disintegration helps to overcome through the cohesion of tablet particles and make the tablet break or disintegrate into primary particles. The main mechanism involved behind the disintegration of the tablet is to take up the moisture from the surroundings and make the tablet initially swallowed, decreasing its tensile strength. The addition of an optimum amount of disintegrants leads to poor compressibility of the tablet. The commonly used disintegrants are sodium starch glycolate and magnesium aluminum silicate.

1.8. Compaction data analysis

Several empirical relationships have been suggested to describe the data, which can be expressed in terms of stress–strain, pressure volume or pressure density. A compaction equation establishes a relationship between a certain characteristic of the powder's consolidation state, such as volume, density, porosity and void ratio versus compaction pressure.

To show a better fit of experimental data to the model, the plot must be transformed into a linear form facilitating comparisons between different data sets. For the given wide range of pressures that can be examined in compaction studies, it is logical and appropriate to plot these pressures using a logarithmic scale. This allows for better visualization and differentiation of the data.

1.8.1. *Heckel equation*

The Heckel equation is derived from the premise that the compaction of the powder under force obeys first-order kinetics (Dudhat 2022). The Heckel equation is formulated as follows:

$$\ln\left[\frac{1}{(1-D)}\right] = KP + A \qquad [1.19]$$

where D is the tablet's relative density at any pressure P, K is the slope and A is the intercept.

A modified Heckel equation (Svačinová et al. 2022) is formulated by Kuentz and Leuenberger and is given as

$$\sigma = \frac{1}{C}\left[\rho_c - \rho - (1-\rho_c)\ln\left\{\frac{1-\rho}{1-\rho_c}\right\}\right]c \qquad [1.20]$$

where σ is pressure, ρ is the relative density, ρ_c is the critical density and C is constant. While Heckel plots can also be used for powder combinations, Mohan (2012) also reported that Hersey & Rees and York & Pilpel categorized powders into three distinct types: A, B and C. The categorization is determined by analyzing Heckel plots and evaluating the compaction behavior of the material.

While using type A materials, we observe a linear connection, where the graphs are parallel (Figure 1.11) as the applied pressure increases, which suggests that the deformation is primarily due to plastic deformation. Sodium chloride is an example of a substance that shows A type of behavior.

Typically, type A materials are soft, can easily deform plastically and have varying levels of porosity based on the packing in the die. This will further affect the size distribution as well as the shape of pharmaceutical powder material.

Type B materials exhibit an initial curved section followed by a linear segment (Figure 1.11), which suggests that the particles are undergoing fragmentation during the initial stages of compression. This may vary due to the brittle fracture of material before plastic flow. It is common for type B Heckel plots to be observed in materials that are more rigid and have greater yield pressures. These materials typically go through the process of compression by fragmentation first, which results in a denser packing with fewer voids. Lactose is a prime illustration of such substances.

A steep linear zone appears at the outset for type C materials (Figure 1.11), but it becomes overlaid and flattens down with increasing pressure. Densification is caused by plastic deformation, which is attributed to the lack of a rearrangement stage.

Furthermore, the compressive strength of tablets can be associated with the K values of the Heckel plot. Higher K values generally suggest tablets that are more resistant to crushing. This information can be used as a criterion for selecting binders for the formulation of tablets. Heckel plots can be affected by various factors, including the duration of compression, the amount of lubricant added as well as the dimensions of the die. Therefore, it is difficult to examine the impact of these variables on the compaction of tablets.

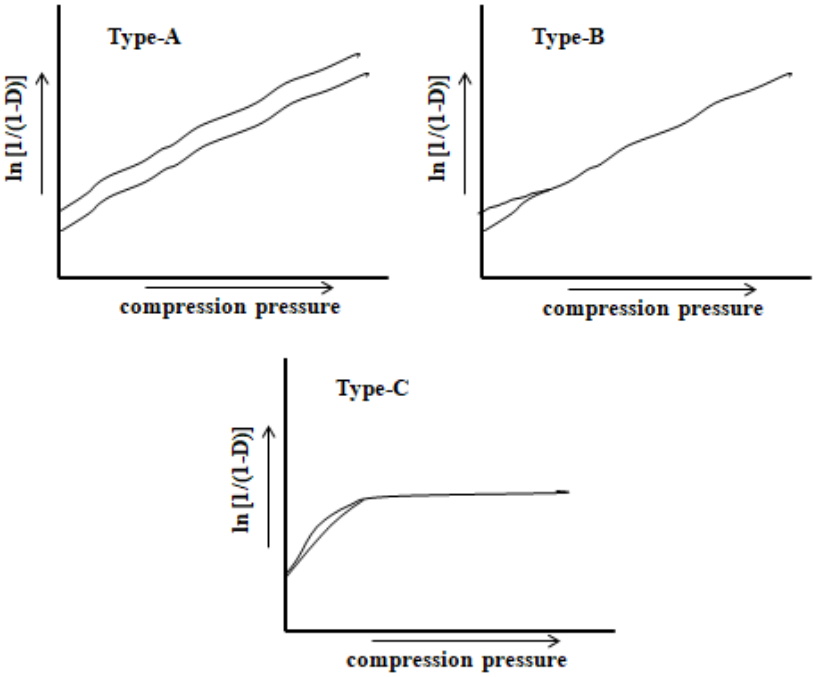


Figure 1.11. *Heckle plot for type A, type B and type C materials (prepared for this work)*

1.8.2. *Kawakita's equation*

Kawakita's equation for powder compression assumes that particles are compressed in equilibrium throughout the process (Dudhat 2022;

Tishkov et al. 2022), resulting in a constant product of pressure and volume. The equation is given as

$$\frac{P_a}{C} = \left[\frac{1}{ab} + \frac{P_a}{a}\right] \quad [1.21]$$

$$C = \left[V_o - \frac{V}{V_o}\right] \quad [1.22]$$

where P_a is the applied pressure axially, a and b are the constants determined from the slope and intercept of the plot, C is volume reduction, V is the compact volume at pressure P_a and V_o is the initial volume of powder. For low pressure and high porosity, this equation fits well with soft and fluffy medicinal powders.

1.9. Conclusion

Characterizing the compaction profiles of pharmaceutical materials necessitates familiarity with the principles underlying compatibility and compressibility. Both events play a significant role in the tablet formulation, whether a hard or soft compact is needed, as well as the brittleness of the materials will determine the relative relevance to depict the compaction process. Using a single equation is unlikely to be sufficient as different materials consolidate through various mechanisms based on their unique feature.

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2

Reactive Chromatography: A Concept of Multifunctional Reactors

High-value chemicals are always of significant importance in various process industries. Synthesizing these compounds has limitations; for instance, low selectivity and limited conversion make the process challenging and time-consuming. The limitations have pushed specific industries to investigate the natural sources of value-added chemicals to purify them further, rather than synthesize them. In this context, reactive chromatography is a novel concept of multifunctional reactors which combines reactors with other unit operations such as distillation, adsorption and stripping. It can enhance the performance and efficiency of chemical processes by reducing capital and operating costs, increasing conversion and selectivity, and overcoming thermodynamic and kinetic limitations. The suitability of reactive chromatography can be addressed through feasibility experiments and theoretical investigations. The mathematical models can then be developed, and experimental validation is performed. The present chapter reviews reactive chromatography's principles, applications and challenges, focusing on the design and optimization methods. We conclude with some future directions and prospects for this emerging technology.

2.1. Introduction

The term multifunctional reactor was coined by German researchers (Agar and Ruppel 1988), who have presented a survey of the possibility of practical examples. Multifunctional reactors are essential to process intensification, integrating reactions and at least another function into a single unit operation. The function can be mass, heat or momentum transfer and even another reaction, i.e. CSTR, conducting exothermic reaction, combined with a cooling jacket or cooling coil, can be termed a multifunctional reactor. In this case, the reaction is combined with heat transfer.

Chapter written by Praveen Kumar GHODKE, Sudip DAS and Rohidas BHOI.

Such integration offers benefits in terms of reduced operating and capital costs and significant energy savings. Process intensification is not concerned with developing new reaction pathways or catalyst formulations, even though they are significant to the performance improvement of the reaction process. The major classifications of multifunctional reactors are multifunctionality by intra-reactor unit processes (integrated reaction and separation units), multifunctionality by inter-reactor units (two or more reactors handling different reactions combined into one) and multifunctionality that involves multi-phase flow of reactants/products in reactions (an integrated chemical reaction process with enhanced interphase transport processes) (Dautzenberg and Mukherjee 2001).

2.2. Concept of multifunctional reactor

Many chemical reactions are observed to be equilibrium-limited. The equilibrium limitation can be overcome by separating one of the product compounds in situ. This concept of the multifunctional reactor, integrating the reaction process with the separation operation, is known as reactive separation. The advantage is fewer separation steps than with a conventional setup. Additionally, the extra degrees of freedom in the multifunctional reactor allow the concentration profiles inside the integrated unit to be controlled appropriately. The continuous separation of the product compounds in the reaction zone benefits in terms of higher reactant conversion. This chapter covers the two most established reactive separation operations, namely reactive distillation (RD) and reactive adsorption (reactive chromatography (RC)). The fundamental difference in RD is that the former works on the principle of volatility and, later, adsorptivity (Baharudin et al. 2021).

2.3. Reactive distillation

One of the classifications of multifunctional reactors is one-pot synthesis, i.e. combining reaction and separation units. Accordingly, RD has become one of the most recognized and attractive units in chemical processing. The RD operation is promising for various reactions, for example, (Trans) esterification, hydrolysis and isomerization. It is helpful due to attainable optimum reactant conversion and product selectivity in an equilibrium-related system involving azeotropes (Muthia et al. 2018). However, the application of RD is limited to the reaction conditions compatible with distillation. Sometimes, it is referred to as catalytic distillation when a solid catalyst is used. RD has been successfully applied to the mixtures wherein at least one product is either the most volatile or the least volatile component. Sometimes, the system's minimum/maximum boiling azeotropes can be

exploited advantageously to achieve in situ removal. Some relevant examples are the esterification of acetic acid by methanol or butanol, MTBE synthesis from methanol and isobutene, etc. (Thotla and Mahajani 2009). The conventional and RD setup is schematically shown in Figure 2.1.

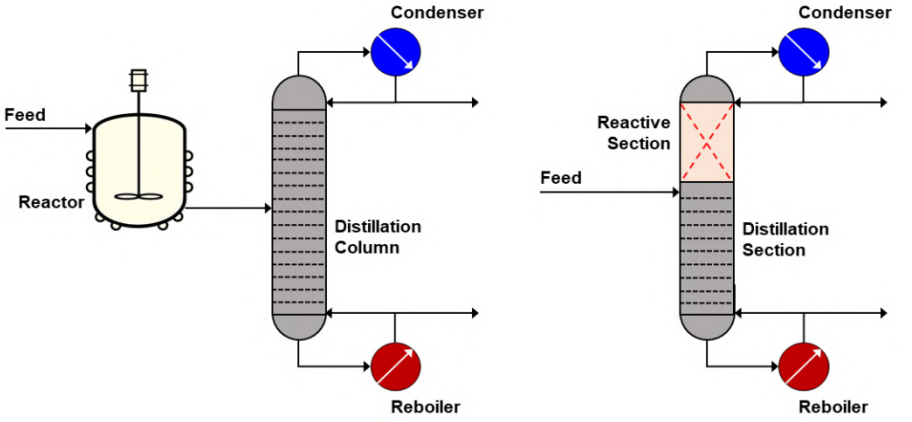


Figure 2.1. *Standard distillation configuration (left) and the reactive distillation (right) (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

2.4. Reactive chromatography

The reaction system, coupled with in situ separation in the presence of a catalyst and an adsorbent, exhibits a multifunctional system. It is known as the sorption-enhanced reaction process (SERP). According to Le Chatelier's principle, the removal of the undesired product in equilibrium limited reaction improves the yield of the desired product in SERP. The chromatographic reactor is preferred over RD when the components are non-volatile, the difference in volatility is small or the system involves heat-sensitive components. The simulated moving bed reactor (SMBR) is a multifunctional reactor that combines continuous counter-current chromatography with the reaction. Due to its ability to overcome thermodynamic limitations, it has been applied to the synthesis of many organic compounds, especially involving reversible reactions. For more details, please refer to the research article by Faria et al. (2022). It may lead to more efficient and economical processes. It is possible to model, design, simulate and experimentally demonstrate the viability of such technology from the knowledge of reaction kinetics and adsorption equilibrium, for example, production of ethyl lactate.

2.4.1. *Theoretical description of chromatographic reactor*

By eliminating one of the products throughout the reaction, RC aids in the completion of reversible processes. The solid phase serves as a catalyst for the response and selectively adsorbs one of the components of the reaction mixture. RC can be run in batch or continuous mode. During the procedure, the solid phase must be shifted to regenerate continuously. Based on how the RC is operated and the properties of phases involved, chromatographic reactors can be classified as shown in Figure 2.2. Among these reactors, fixed bed chromatographic reactors (FBCR) and simulated moving bed reactors (SMBR) are the most extensively used because of the benefits they provide over the other approaches (Noeres et al. 2003). Batch RC is often performed in an FBCR, where a liquid combination runs through a packed bed of catalyst/adsorbent. RC in continuous mode may be achieved easily in SMBR, where solid movement is imitated by switching ports periodically.

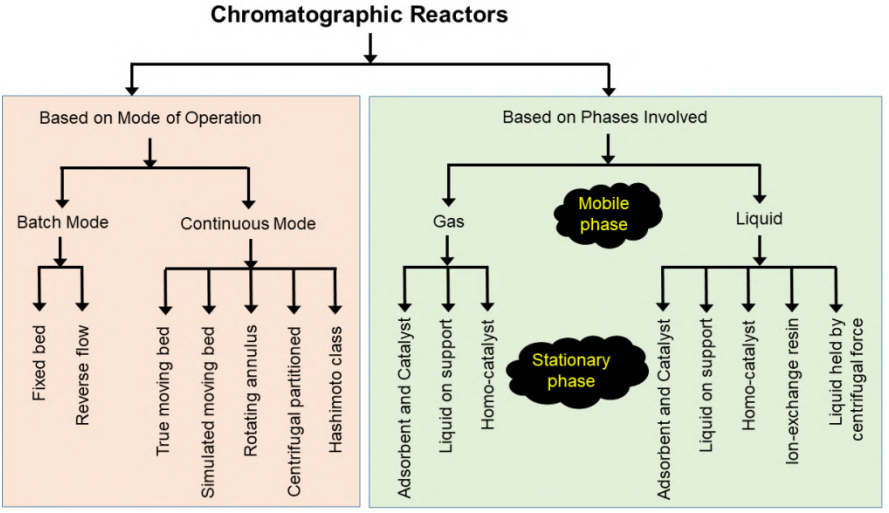


Figure 2.2. *Classification of chromatographic reactors (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

2.5. Types of chromatographic reactors

2.5.1. *Fixed bed chromatographic reactor (FBCR)*

In batch mode, RC is often performed in an FBCR, a packed bed of catalyst/adsorbent through which the reaction mixture flows to produce simultaneous reaction and separation. Figure 2.3 depicts the operation of the FBCR

in pulse mode for a reversible reaction of type A + B ⇋ C + D (Gyani 2010). The stationary phase is chosen in such a way so that it possesses a higher affinity for product C and a lower affinity for the other product D. Consequently, the C front lags and the D front advances, resulting in less concentration of products in the reactive zone to propel the reaction forward. The reaction rates and relative affinities of the components to the resin determine the practicality of RC for a specific reaction. FBCR, operated in either step mode or pulse mode, can be conveniently used to evaluate the feasibility of RC for a specific reaction.

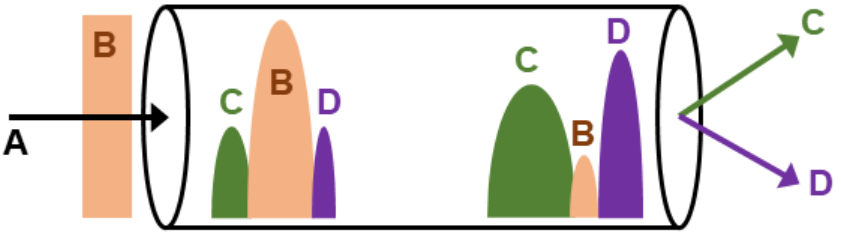


Figure 2.3. *FBCR working principle (pulse mode) for a reversible reaction (Acetic acid (A) + Alcohol (B) ⇋ Water (C) + Ester (D)) (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

2.5.2. *Reverse flow chromatographic reactor (RFCR)*

The RFCR is a primary fixed bed reactor filled with adsorbent/catalyst or a combination of adsorbent and catalyst. In this situation, at least one of the reactants with the highest affinity for the adsorbent is placed in the center of the reactor, and the carrier's direction is altered regularly until the limiting reactant is completely converted. To achieve complete conversion, the reactant should have a greater affinity for the adsorbent and the product should have the lowest affinity.

Figure 2.4 illustrates the operation of RFCR for the reaction A + B ⇋ C. B has the most affinity, whereas C has the least. Reactant B is placed in the center of the reactor, whereas reactant A goes in at one end. Component A reacts with B to form C, and product C elutes at the other end. When B begins to elute at the outlet, the carrier flow is reversed so that B is continuously adsorbed in the bed, ensuring complete conversion. RFCR was first used for NOx reduction with NH_3, in which only NH_3 was found to get adsorbed in the fixed bed (Agar and Ruppel 1988).

2.5.3. *True moving bed reactor (TMBR)*

The TMBR process is a continuous process consisting of a classical four-section configuration, wherein the counter-current movement of liquid phase and solid phases is created. A schematic of TMBR for a reversible esterification type of reaction (Acetic acid (A) + Alcohol (B) ⇋ Water (C) + Ester (D)) is shown in Figure 2.5 (Lode et al. 2001). At the feed and adsorbent ports, feed and adsorbent are introduced. The products are separated and removed at the raffinate and extract ports depending on their affinity for the adsorbent.

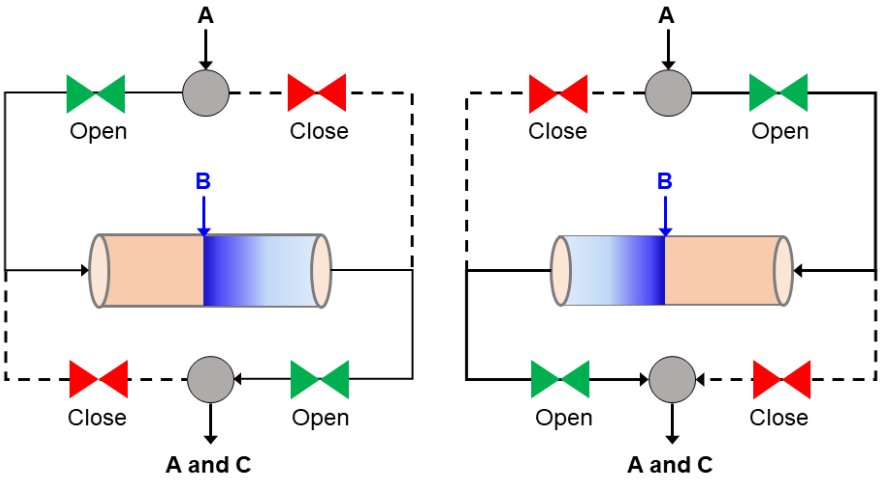


Figure 2.4. *Working principle of RFCR for the reversible reaction A + B ⇋ C (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

In two core zones, II and III, the reaction and simultaneous separation of the products take place. The flow rates are controlled such that the component with the lowest affinity (ester) is transported away with the liquid phase to the raffinate port, and the component with the highest affinity (water) is carried away with the solid phase to the extract port.

The desorbent is inserted at the inlet of section I to desorb the higher affinity component (water) and renew the solid phase. The fresh solid from section I enters section IV and adsorbs the least affinity component (ester) to regenerate the adsorbent, which is recycled back to section I.

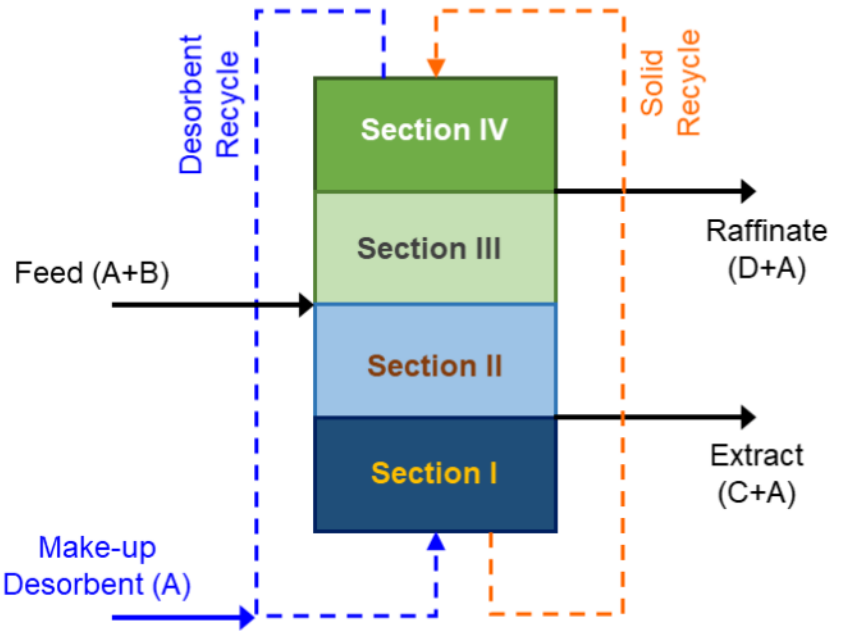


Figure 2.5. *TMBR working principle for a reversible reaction (Acetic acid (A) + Alcohol (B) ⇋ Water (C) + Ester (D)) (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

2.5.4. *Simulated moving bed reactor (SMBR)*

As a practical application of the true moving bed chromatography (TMBC) technique, Universal Oil Products (UOP, USA) presented the concept of SMBC for petrochemical separations in 1961. SMBC replicates the hypothetical TMBC by alternating the intake and output ports to approximate solid movement. TMBR and SMBR have similar principles.

Figure 2.6 shows a schematic of the SMBR method for esterification reaction (Lode et al. 2001). Each portion of the SMBR has a set number of beds linked in series. To ensure the continuous counter-current movement of the solid phase, the intake and exit ports are switched regularly in the direction of the fluid flow by one column concurrently after a specific switch time, simulating solid movement in a discontinuous way. When each section contains many beds and the port switching happens at a sufficiently high frequency, a practically continuous movement of the solid phase may be achieved.

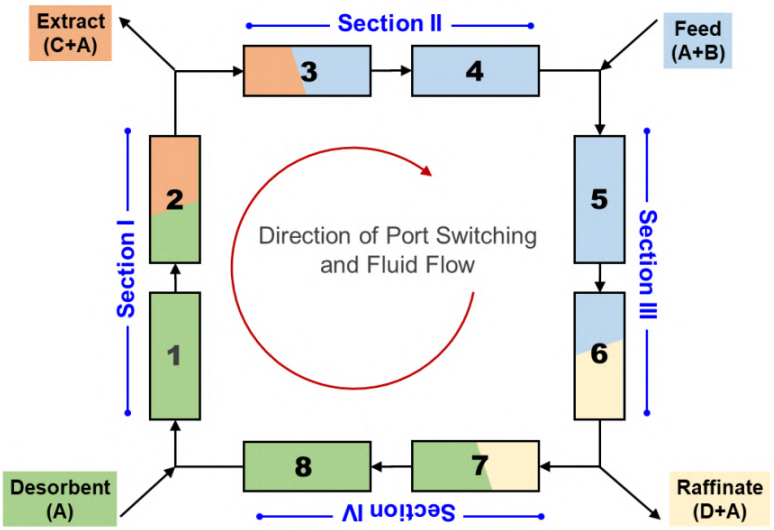


Figure 2.6. *SMBR working principle for a reversible reaction (Acetic acid (A) + Alcohol (B) ⇋ Water (C) + Ester (D)) (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

2.5.5. *Centrifugal partitioned chromatographic reactor (CPCR)*

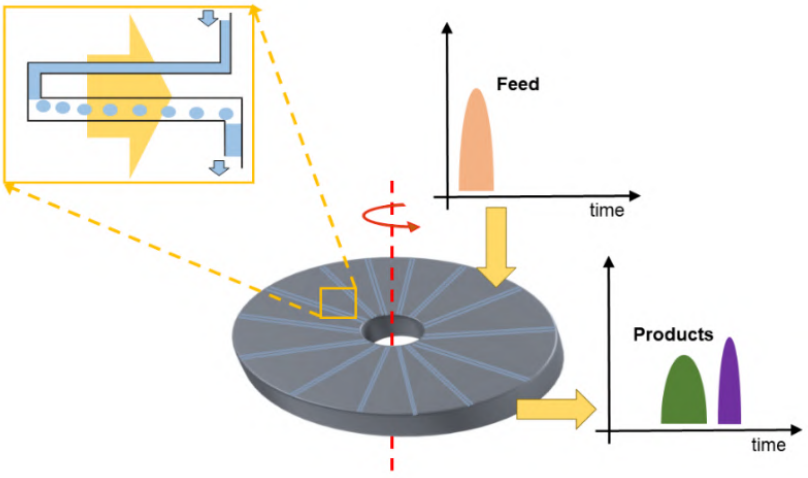


Figure 2.7. *Schematic of centrifugal partition chromatographic reactor (CPCR) (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

CPCR combines reaction, partition chromatography and counter-current distribution without solid support. This is only applicable to liquid-phase processes. This method is based on the dispersion of two immiscible liquids with differing densities. The higher density stationary phase is maintained in the column by a combination of centrifugal force and column geometry, while the mobile phase travels through the column as micro-droplets. In most cases, the stationary phase contains a catalyst for the reaction.

Figure 2.7 explains the CPCR operation. The separation in CPCR refers to liquid–liquid extraction, and the benefit of this approach is its great stationary-phase capacity compared to the traditional technique that uses liquid–solid systems (Hollander et al. 1998, 1999).

2.5.6. *Continuous rotation annulus chromatographic reactor (CRACR)*

The stationary phase is packed in the annular region between the two concentric cylinders that spin around a common axis in CRACR. The mobile phase is injected uniformly throughout the annulus's top cross-section. As indicated in Figure 2.8, a reactant or feed is introduced through the fixed port of the annulus. Due to gravity and pressure differences, the mobile phase goes downward and moves in a tangential direction due to rotation.

Components are shifted tangentially to varied distances depending on their affinity for the bed. As a result, products are separated and eluted from the reactor at various angles in relation to the fixed feed port. This type of chromatographic reactor is particularly advantageous when the mixture involves multiple side products or intermediates, which can be collected in pure form from different locations in the reactor. For more details about CRACR, refer to the book chapter by Fricke et al. (2008).

2.5.7. *Hashimoto chromatographic reactor (HCR)*

This reactor is similar to the SMBR in many ways, although it only contains the first three portions. In the third part, reactors and adsorbers are alternately coupled. Other sections merely have adsorbent columns such as SMBR. This is especially useful for reactions of the form A = B. The solid movement is identical to that of SMBR; however, the reactors are only present in section III. Figure 2.9 depicts the HCR operating concept (Fricke et al. 2008). This method has been used effectively to convert glucose to fructose.

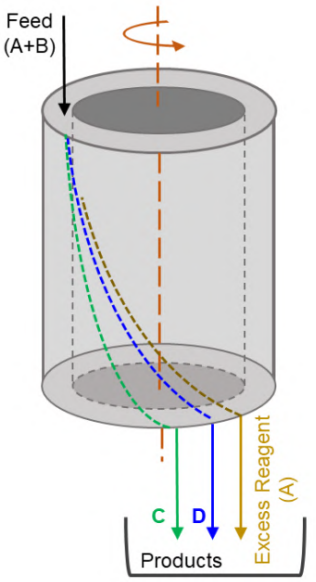


Figure 2.8. *Schematic of centrifugal partition chromatographic reactor (CPCR) for a reaction A + B ⇋ C + D; B is the limiting reagent (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

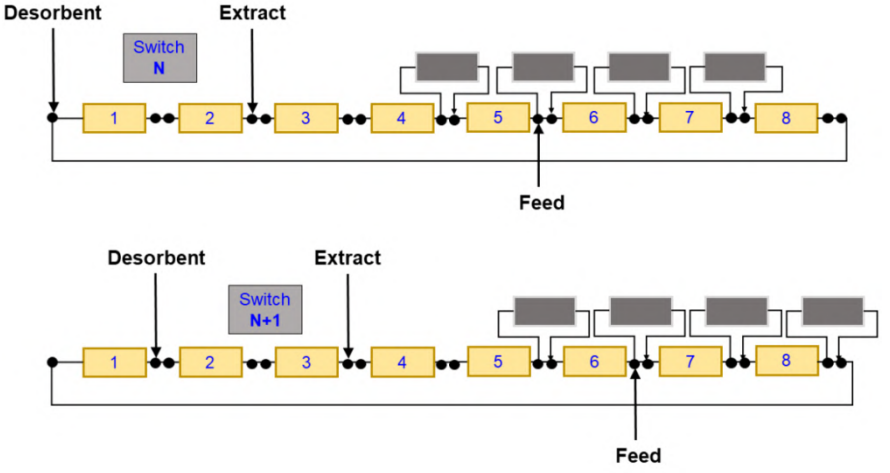


Figure 2.9. *Schematic of Hashimoto chromatographic reactor (HCR) (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

2.6. Comparative discussion

FBCR and SMBR, out of numerous designs of chromatographic reactors described earlier, are widely used because they offer advantages over other techniques. TMBR faces a serious practical shortcoming as the movement of solid cause mixing and attrition; hence, it is difficult to implement in reality. RFCR and SMBR results were compared for hydrogenation of 1,3,5-trimethylbenzene, and it was concluded that similar performance in terms of conversion could be obtained with both systems (Viecco and Caram 2006).

SMBR is better than RFCR in terms of the separation of products, which is a limitation of RFCR. CPCR has been applied to very few systems because of the difficulty in designing columns and selecting the stationary phase. CRACR is useful when the mixture involves several side products or intermediates, which can be collected in pure form from different locations in the reactor. The design and control of the HCR system becomes more complex compared to conventional SMBR, especially when the number of components is large. The mathematical model of FBCR and SMBR is elucidated in the subsequent section of this chapter.

2.7. Applications of chromatographic reactors

By eliminating one of the products throughout the reaction, RC aids in obtaining complete conversion for reversible processes. RC has been effectively used in the past for several heterogeneous reactions such as esterification (Kawase et al. 1996; Mazzotti et al. 1996; Lode et al. 2001; Gelosa et al. 2003; Ströhlein et al. 2006; Gyani and Mahajani 2008; Deshmukh et al. 2009), etherification (Zhang et al. 2001), acetalization (Silva and Rodrigues 2002; Gandi et al. 2006), isomerization (Minceva et al. 2008) and inversion (Azevedo and Rodrigues 2001). A review of all chromatographic reactors is given by Silveston et al. (2013).

Batch RC is often carried out in an FBCR, in which a liquid combination passes over a densely packed bed of an adsorbent and catalyst. In an SMBR, solid movement is replicated by periodically switching ports, making executing RC in continuous mode easier.

An exhaustive list of all SMBR applications is given by Hashimoto et al. (2013). Some of the essential applications of RC for liquid–solid systems and the types of reactors used are summarized in Table 2.1.

Applications	Catalyst/adsorbent	Reactor	Reference
Esterification of acetic acid and b-phenethyl alcohol	Proton-type ion exchange resins	SMBR	Kawase et al. 1996
Esterification of acetic acid and ethanol	Amberlyst-15	FBCR, SMBR	Mazzotti et al. 1996
Synthesis of bisphenol-A from acetone and phenol	Amberlyst-31	SMBR	Kawase et al. 1999
Esterification of iso-amyl alcohol and propionic acid	Lipozyme-IM	SMBR	Mensah and Carta 1999
Synthesis of diethyl acetal from acetaldehyde and ethanol	Amberlyst-15, Amberlyst-18	FBCR, SMBR	Silva and Rodrigues 2002, 2005
Hydrolysis of methyl formate	Dowex 50W-X8	FBCR	Falk and Seidel-Morgenstern 2002
Synthesis of dimethyl acetal from acetaldehyde and methanol	Amberlyst-15	FBCR, SMBR	Gandi et al. 2007; Pereira et al. 2008
p-Xylene isomerization	ZSM-4	SMBR	Minceva et al. 2008
Biodiesel from fatty acids (FA) in used oils and methanol	Silica-supported Nafion resin (SAC-13)	FBCR, SMBR	Kapil et al. 2010
Esterification of 2-ethylhexanol and acetic acid	Amberlyst-15	FBCR	Gyani and Mahajani 2008
Synthesis of ethyl lactate from ethanol and lactic acid	Amberlyst-15	SMBR	Pereira et al. 2009
2-Phenyl ethyl acetate production	Amberlyst-15	FBCR	Graça et al. 2011

Esterification of butyl cellosolve with acetic acid	Amberlyst-15	FBCR	Deshmukh et al. 2009
Esterification of acetic acid with *n*-hexanol	Amberlyst-15	FBCR, SMBR	Patel and Saha 2012
Biosynthesis of dextran from sucrose	Dextran sucrose enzyme, Lewatit TSW (40) in Ca form-adsorbent	SMBR	Zafar and Barker 1988
Hydrolysis of lactose	Lactase enzyme, Dowex 50W-X4 adsorbent	SMBR	Shieh and Barker 1996
Esterification of propionic acid and 2-ethyl-1,3-hexanediol	Lipozyme enzyme, Dowex HCR-W2 adsorbent	FBCR	Migliorini et al. 2000
2,2-Dimethoxy propane production	Amberlyst-15	FBCR	Kawase et al. 2001
Inversion of sucrose	Invertase enzyme, Dowex monosphere 99/Ca adsorbent	SMBR	Azevedo and Rodrigues 2001
Glucose isomerization	Sweetzyme T enzyme, Amberlite CR-13Na adsorbent	SMBR	Toumi and Engell 2004

Table 2.1. *Some important applications of RC for liquid–solid systems*

2.8. Mathematical modeling of chromatographic reactors

Modeling is an important step in chemical engineering design processes. From limited preliminary experiments studied for parameter determination and model validation, validated models allow the virtual prediction of conditions not studied experimentally, optimize and scale up the process. Modeling studies have become increasingly important for designing complicated and expensive processes such as chromatographic separation techniques. In general, models used to describe the performance of chromatographic reactors can be considered extended models of chromatographic separation columns, considering reactions such as esterification, etherification, hydrolysis and hydrogenation. In order to represent chromatographic reactors through mathematical equations, the reaction and the adsorption parameters need to be combined to get the balance of mass or moles. As FBCR and SMBR are the most widely used chromatographic reactors (Gyani 2010, Reddy 2014), mathematical models of FBCR and SMBR have been elucidated as representative examples of batch and continuous chromatographic reactors, respectively, in this section. These models can be used to design chromatographic reactors for a specific target reaction.

A fixed bed chromatographic reactor (FBCR) is a type of reactor that contains a stationary phase packed with a catalytic material. This packing facilitates the continuous transportation of a mobile fluid phase. However, in contrast to the conventional operational mode of a plug-flow tubular reactor with continuous feeding, the reactants are intermittently introduced into the FBCR in the form of rectangular pulses (Falk and Seidel-Morgenstern 1999). The simultaneous occurrence of reaction and chromatographic separation in an FBCR leads to complex processes. Explaining these processes requires a thorough understanding of various factors such as the properties of solid particles, fixed bed, adsorption, diffusion and reaction kinetics. After confirming the feasibility, the reaction can be efficiently carried out in a continuous mode reactor such as a simulated moving bed reactor (Yang et al. 2022).

2.9. Mathematical modeling of FBCRs

The working principle of FBCR is described in section 2.2.1. In FBCR, it is always feasible to achieve complete separation and conversion for the reaction type $A \leftrightharpoons B + C$, regardless of the relative affinity of reactant A. The result of the reaction $A + B \leftrightharpoons C + D$ is always determined by the relative affinity of reactants A and B. In the case of ester hydrolysis reactions ($A \leftrightharpoons B + C$), the presence of extra water can be regarded as a typical reaction ($A + B \leftrightharpoons C + D$), allowing for the prediction of operational feasibilities (Vu and Seidel-Morgenstern 2011).

The modeling of FBCR necessitates the experimental determination of reaction rate constants and all model parameters. The essential parameters for achieving equilibrium include chemical equilibrium constants and adsorption equilibrium constants. However, for specific scenarios such as ester hydrolysis reactions, extended equilibrium models are required. In such cases, the necessary parameters include chemical equilibrium constants, adsorption equilibrium constants and porosity. The adsorption isotherms of all components exhibit linearity during ester hydrolysis processes (Khan et al. 2021). The adsorptivities of the esters are higher than those of hydrolysis products, namely alcohols and organic acids. Due to the increased adsorptivity of alcohols compared to acids, alcohols function as component B, whereas acids function as component C in the example of $A + B \leftrightharpoons C$ (Jogunola et al. 2011).

FBCRs are often classified into two categories of models. The plate models yield sets of ordinary differential equations (ODEs) that depict the mass and energy balances of a finite number of plates, while the continuous models are expressed as partial differential equations (PDEs) (Ranade 2002). While the majority of models focus on the propagation of components primarily in the axial direction (1D), a small number of academics have made efforts to mathematically describe both axial and radial profiles in a column. The radial profiles of concentration and temperature are often insignificant in chromatographic columns filled with relatively small particles, thanks to the uniform packings achieved.

The chromatographic column is regarded as a sequence of interconnected theoretical plates. The mobile and stationary phases in each plate are regarded as being in equilibrium. Axial dispersion is implicitly accounted for in these models based on the number of plates. The influence of mass transfer resistance is commonly disregarded. Two distinct plate models are used to characterize chromatographic separations. The Martin and Synge model can be classified as a continuous plate model, while the Craig model can be classified as a discontinuous plate model. In linear chromatography, the Martin and Synge model produces answers that adhere to a Poisson distribution, but the Craig model yields a binomial distribution. Both models are considered comparable when there is a large number of theoretical plates, as in such cases, the projected elution profiles tend to approach a Gaussian distribution for tiny injections (Felinger 1998).

Plate models, while providing a straightforward means of describing chromatographic processes, possess certain limitations. These models are not readily applicable for individually describing distinct physical kinetic events that result in band broadening. The number of theoretical plates is primarily determined by the unique interactions between each component and the stationary phase. Consequently, using a mean value of theoretical plates for all constituents results in diminished precision of computations.

2.10. Equilibrium-based continuous models

The initial mathematical models of single-component chromatography used the equilibrium theory. This hypothesis is predicated on the suppositions that the establishment of equilibrium between the solution and adsorbent occurs quickly and that the influence of diffusion can be disregarded. Based on the same assumptions, several models have been created to elucidate the interactions between components during percolation in multicomponent chromatography. Typically, the models are expressed as systems of PDEs (Kecili and Hussain 2018). Kienle and his colleagues have expanded the application of the equilibrium theory to RC. The extended equilibrium theory is a powerful tool for assessing feasibility, specifically in determining whether complete conversion of reactants and complete separation of products can be achieved in a chromatographic reactor.

2.11. General rate model and simplified versions

The general rate model enables the simultaneous consideration of all potential factors influencing mass transfer kinetics. Typically, these contributions are represented as a set of PDEs that describe the principles of mass conservation and movement. Despite its intricate nature and numerous input parameters, the model holds the capability to accurately depict non-ideal reactive chromatographic processes. The general rate model can be simplified into simpler models based on the initial assumptions. Aside from the obligatory variables of convection, adsorption and reaction, we may also take into account other words such as dispersion and limiting mass transfer rate. Alternatively, many factors such as dispersion, adsorption kinetics and mass transfer resistances can be combined into a singular effective kinetic parameter. Given the nonlinearity present in the mass balance equations, it is necessary to use numerical methods to solve these models. Nevertheless, it is possible to analytically address specific scenarios involving linear adsorption isotherm and first-order reaction rate expression, such as by using Laplace transform techniques (Wang and Guo 2020).

2.12. Phase distribution

The distribution of phases plays a crucial role in chromatographic procedures, as it is essential for accurate modeling and simulation. The purpose of including definitions of porosities and phase ratios at the start of this section is to provide a clear understanding of these concepts. By using a chromatographic column containing permeable particles and a pore network completely saturated with liquid, the whole volume of the column, V_{col}, can be partitioned into a volume of liquid phase, V^L, and a volume of solid material including the particles, V_{solid}. The volume

of the liquid phase comprises sub-volumes of the interstitial liquid fraction V_{int} and the intraparticle liquid fraction V_{pore}

$$V_{col} = \frac{\pi d_{col}^2}{4} L = V^L + V_{solid} = V_{int} + V_{pore} + V_{solid} \quad [2.1]$$

The volume of the stationary phase V^S is composed of the liquid fraction within the particles and the volume of the solid substance. It can be written as (equation [2.2])

$$V^s = V_{pore} + V_{solid} \quad [2.2]$$

The total porosity ε_t of a fixed bed is determined when the column is uniformly and tightly packed (equation [2.3]):

$$\varepsilon_t = \frac{V^L}{V_{col}} \quad or \quad (1 - \varepsilon_t) = \frac{V_{solid}}{V_{col}} \quad [2.3]$$

The ratio of phase "F" is a significant property of a chromatographic column. It is defined as the ratio between solid-phase volume fraction and total volume of the liquid fractions. The equation is directly linked to the total porosity (equation [2.4]):

$$F = \frac{V_{solid}}{V_{int} + V_{pore}} = \frac{1-\varepsilon_t}{\varepsilon_t} \quad [2.4]$$

2.12.1. *Differential mass balance equations and equilibrium-dispersion model*

The derivation of mathematical models for FBCR often relies on the following fundamental assumptions:

1) The column is uniformly filled.

2) The column does not exhibit any radial concentration or temperature gradients.

3) The volumetric flow rate is constant.

4) The quantification of intraparticle transport can be simplified by using linear driving force formulas.

Let us examine a differential volume element of a column (Figure 2.10), denoted as dV_{col}, which has a differential length dx, a diameter d_{col} and a cross-sectional area A_{col}.

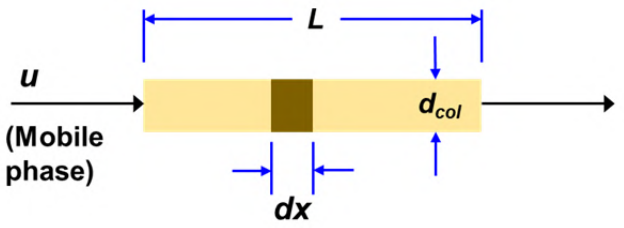


Figure 2.10. *Differential volume element of a column (prepared in this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

The equations governing the conservation of mass for a specific component, denoted as i, in a mixture containing N_C components within a differential volume element of the column can be expressed as (equations [2.5]–[2.6])

For the liquid phase (ε_t):

$$\frac{\partial n_i^L}{\partial t} = -\partial \dot{n}_{conv,i}^L - \partial \dot{n}_{disp,i} + \partial \dot{n}_{mtr,i} + \frac{\partial n_i^L}{\partial t}\Big|_{R,hom} \text{ for i = 1, } N_c \qquad [2.5]$$

For the solid phase ($1 - \varepsilon_t$):

$$\frac{\partial n_i^S}{\partial t} = -\partial \dot{n}_{mtr,i} + \frac{\partial n_i^S}{\partial t}\Big|_{R,het} \text{ for i = 1, } N_c \qquad [2.6]$$

n_i^L and n_i^S represent the quantities of component i present in the liquid and solid phases, respectively. $_{R,hom}$ and $_{R,het}$ are the reaction rates in liquid (homogeneous) and solid (heterogeneous) phases.

If the volumetric flow rate $\dot{V}$ and the total porosity ε_t remain constant, then the linear velocity u will likewise remain constant:

$$u = \frac{\dot{V}}{\varepsilon_t \frac{\pi d_{col}^2}{4}} \qquad [2.7]$$

Therefore, equations [2.5] and [2.6] can be rewritten for the whole column to give the following.

For the liquid phase:

$$\varepsilon_t \frac{\partial c_i}{\partial t} + \varepsilon_t \frac{\partial c_i}{\partial x} = \varepsilon_t \sum_{i=1}^{N_R} v_{i,j} r_j^{hom} + \varepsilon_t D_{ax.i} \frac{\partial^2 c_i}{\partial x^2} + (1 - \varepsilon_t)\beta_i \left[q_{av,i} - q_i^*(\overline{c})\right] \qquad [2.8]$$

For the solid phase:

$$\left(1-\varepsilon_{t)}\right)\frac{\partial q_{av,i}}{\partial t}=\ (1-\varepsilon_t)\sum_{i=1}^{N_R}\nu_{i,j}r_j^{het}-(1-\varepsilon_t)\beta_i\ [q_{av,i}\ -\ q_i^*(\overline{c})] \qquad [2.9]$$

The two conservation equations [2.5] and [2.6] represent a typical 1D heterogeneous two-phase model. c_i is the liquid-phase concentration, $q_{av,i}$ is the average loadings of component i and the axial dispersion coefficient for component i is $D_{ax,i}$. For linear driving force, an internal mass transfer coefficient is βi, and $\nu_{i,j}$ are the stoichiometric coefficients of component i in reaction j.

2.12.2. *Performance criteria*

The primary objectives of a reactive chromatographic process usually include achieving increased conversion, purity, productivity and yield. To enhance the efficiency of this process, it is crucial to have a comprehensive understanding of the correlation between these process factors and the operational parameters.

2.12.3. *Cycle time and productivity*

In the typical periodic dosing performance of an FBCR is the cycle time; the time interval between two consecutive injections is referred to as t^{cyc} (equation [2.10])

$$t^{cyc}=\ t^{end}-\ t^{begin} \qquad [2.10]$$

The time interval between the completion of one injection and the commencement of the subsequent injection might be referred to as the regeneration time. The cycle time can be described in the elution profile by the two times t^{begin} and t^{end}. It depends on the injection time and the spreading of the elution profile under operational conditions.

The two distinct time intervals can be determined by using a specific threshold concentration that indicates the start and endpoints of the elution profile at the column's exit. The threshold concentration is commonly set at 1.0×10^{-9} mol L^{-1}. It might be additionally formulated as a relative fraction of the injection concentration. To prevent band overlapping and ensure complete column regeneration, it is necessary to have a time interval between two injections.

2.12.4. *Conversion*

Conversion is a valuable metric for assessing the efficacy of the reaction process. The conversion of a feed component A in cycle chromatographic reactors can be represented by the following equation (equation [2.11]):

$$X_A = \frac{\dot{n}_A^{in} - \dot{n}_A^{out}}{\dot{n}_A^{in}} = \frac{C_A^{feed}{}_{t^{inj}} - \int_{t_{begin}}^{t_{end}} C_A(t)dt}{C_A^{feed}{}_{t^{inj}}} \quad [2.11]$$

X_A is the conversion, n_A is the moles of A and C_A is the concentration of A. t represents time of injection. For reversible reactions, most reactors cannot convert entire reactants. Based on mass conservation, the conversion can be determined by incoming and outgoing mass flows of the entire process. The integration of the elution profile of the reactant A represents the original or unchanged quantity.

2.12.5. *Yield*

The recovery yield of a desired product is determined by dividing the amount of the product collected in the purified fraction, with the required level of purity, by the maximum amount that could be collected if all of the reactant A was completely converted. It is given by equation [2.12]

$$Y_i = \frac{V_A}{V_i} \frac{\int_{t^{cut\,pt2}}^{t^{cut\,pt1}} c_i(t)\dot{V}dt}{C_A^{feed}{}_{V^{inj}}} \quad [2.12]$$

where Y_i is the yield, v_A is the stoichiometric coefficients of reactant A, v_i is the stoichiometric coefficients of component i, V^{inj} is the injection volume and t_{cut} is the injection time.

2.12.6. *Purity*

The purity of a component i is determined by calculating the ratio of the amount of that component to the total amount of all components in the collected fraction, excluding the solvent. It is calculated as (equation [2.13])

$$Pu_i = \frac{n_i}{\sum_{i=1}^{Nc} n_j} \quad [2.13]$$

N_C represents the total number of components present in the collected fraction. Purity is a limiting factor for the separation process. A result of 99% is generally considered to be below average. The cut-points for fraction collection initiation and

termination are determined by the purity standards. Consequently, they ascertain the amount of output, efficiency and consequently the financial aspects of the procedure.

2.13. Model parameters

The models presented in the earlier section include parameters that define the model. Theories and correlations related to these parameters are summarized here.

2.14. Adsorption equilibrium isotherms

2.14.1. *Thermodynamics of adsorption*

The basic thermodynamic functions for adsorption processes in dilute concentration are directly linked to the adsorption equilibrium constant. The molar Gibbs free energy of adsorption (ΔG_i) is directly linked to the Henry constant K_i given by equation [2.14]. Here, T is the temperature (K), and R is the universal gas constant (J K^{-1} mol^{-1})

$$\Delta G_i = -RT\ lnK_i \qquad [2.14]$$

Adsorption is often an exothermic phenomenon as it releases energy, resulting in a negative enthalpy of adsorption. Van't Hoff's formula can be used to compute the molar enthalpy of adsorption (ΔH_i) since K_i is an equilibrium constant (equation [2.15]):

$$\frac{\partial(lnK_i)}{\partial(\frac{1}{T})} = -\frac{\Delta H_i}{R} \qquad [2.15]$$

The molar entropy of adsorption (ΔS_i) can be determined by using the values of ΔG_i and ΔH_i through the following calculation (equation [2.16]):

$$\Delta S_i = \frac{\Delta G_i - \Delta H_i}{T} \qquad [2.16]$$

2.14.2. *Single component isotherm*

In the context of liquid chromatography, the equilibrium of adsorption is often described under isothermal conditions by the correlations between the solute's loading in the stationary phase (q_i) and its concentrations in the mobile phase (c_i).

These correlations are highly significant for estimating elution times and peak forms.

In the case of a linear isotherm, the slope is given by K_i (Henry constant, equation [2.17]). In an ideal scenario, while performing a rectangular injection, the elution profile of a single component follows a rectangular pulse shape, as described by the equilibrium model. However, due to certain phenomena that cause the spreading of bands, the elution profile in actual linear chromatography exhibits a symmetrical peak that follows a Gaussian distribution pattern. The retention period for the maximum of the peak can be determined by equation [2.14]

$$K_i = \frac{q_i}{c_i} \quad [2.17]$$

$$t_{R,i(max)} = t_0 \left(1 + \frac{1-\varepsilon_t}{\varepsilon_t} K_i\right) \quad [2.18]$$

$t_{R,i(max)}$ is the maximum retention time ε_t and is the bed porosity. The hold-up time of a non-retained component across a column length L is denoted by the variable t_o. It can be ascertained by equation [2.19]

$$t_0 = \frac{L}{u} \quad [2.19]$$

If the highest concentration of the elution band exceeds the linear range of the adsorption isotherm, the slopes of the band can be either convex or concave. This is determined by the interactions between the solute component and the stationary and mobile phases. Convex isotherms exhibit a decreasing slope as the concentration increases. As a result, regions with higher concentrations move faster than regions with lower concentrations. Consequently, the elution profile becomes more concentrated at the beginning and dispersed toward the end. The retention time of the convex isotherm can be determined using equation [2.20], whereas the retention time of the concave isotherm can be determined using equation [2.21]

$$t_{R,i} = t_0 \left(1 + \frac{1-\varepsilon_t}{\varepsilon_t} \frac{\Delta q_i}{\Delta c_i}\right) \quad [2.20]$$

$$t_{R,i\, c_i^*} = t_0 \left(1 + \frac{1-\varepsilon_t}{\varepsilon_t} \frac{dq_i}{dc_i}\Big|_{c_i^*}\right) \quad [2.21]$$

In the case of a concave isotherm, the elution profile exhibits contrasting behavior, with dispersion occurring at the front and compression at the back. The duration for which a scattered front remains in a system is determined by the local slope of the isotherm and can be computed using equation [2.21]. Conversely, the

duration for which a compressed rear remains in a system can be computed using equation [2.20].

Several models exist that describe nonlinear isotherms, such as the Langmuir, Bi-Langmuir, Freundlich and Flowler models. However, the most straightforward and generally realistic model is the Langmuir isotherm (equation [2.22]):

$$q_i = \frac{K_i c_i}{1+b_i c_i} \qquad [2.22]$$

where K_i is the initial slope and b_i is a constant that measures the adsorption energy. The isotherm exhibits convexity when $b_i > 0$ and concavity when $b_i < 0$. The concave isotherm is alternatively referred to as the anti-Langmuir isotherm.

2.14.3. *Retention factor*

The duration for which a component remains in a system is determined by the physical characteristics of the column and the pace at which the mobile phase flows through it. Thus, retention behavior is commonly defined by the retention factor, also known as the capacity factor (equation [2.22])

$$k_i' = \frac{t_{R,i}-t_0}{t_0} \qquad [2.23]$$

The retention factor can be determined by calculating the adsorption equilibrium constant (equation [2.24]):

$$k_i' = \left(\frac{1-\varepsilon_i}{\varepsilon_i}\right) K_i \qquad [2.24]$$

2.14.4. *Multicomponent isotherms*

In multicomponent mixes with nonlinear isotherms, the adsorption of distinct components competes for interactions with the stationary phase. Hence, the adsorption of a solute onto the stationary phase is influenced not only by its concentration in the mobile phase but also by the concentrations of all other solutes present in the mobile phase. The Langmuir theory can be expanded to encompass systems with *n* components, resulting in equation [2.25]

$$q_i = \frac{K_i c_i}{1+\sum_{j=1}^{n} b_j c_j} \qquad [2.25]$$

2.14.5. *Reaction kinetics*

The kinetics of chemical processes are the most crucial information required for their characterization. Equation [2.26] defines the rate of a single reaction as the number of moles of a reactant or product that changes over a specific period and reactor volume

$$r = \frac{1}{V_R}\frac{1}{v_i}\frac{dn_i}{dt} \quad [2.26]$$

n_i and v_i are the mole numbers and stoichiometric coefficients of component i, respectively, whereas V_R represents the reactor volume. The rate of a homogeneous reaction can be defined as equation [2.27] when the volume of the reactor remains constant:

$$r = \frac{1}{v_i}\frac{dc_i}{dt} \quad [2.27]$$

Under the assumption of fundamental formal kinetics rooted in collision theory, the relationship between the rate of a chemical reaction and the concentrations of the reactants can be mathematically represented (equation [2.28]):

$$r = k(T)\prod_{k=1}^{N_K} C_k^{v_k} \text{ for k = 1, N}_\text{K} \quad [2.28]$$

where N_K is the number of reactants and $k(T)$ is the reaction rate constant. v_k is the exponent for the reactant. This temperature dependence is typically expressed using the Arrhenius equation (equation [2.29])

$$k(T) = k_0 e^{-E_A/RT} \quad [2.29]$$

In the Arrhenius equation, the term k_0 is referred to as the frequency factor and shares the same units as $k(T)$, while E_A represents the activation energy. The activation energy is defined as the minimum energy barrier that the reactants must overcome for the reaction to occur.

In a multi-reaction system with N_C components and N_R reactions, the production rate of component i (R_i) can be determined by considering the rate of all reactions occurring (equation [2.30])

$$R_i = \sum_{j=1}^{N_R} v_{i,j} r_j \text{ for i = 1, N}_\text{c} \quad [2.30]$$

Here, $v_{i,j}$ represents the stoichiometric coefficients of component i in reaction j.

The Damköhler number D_a is a significant dimensionless number closely associated with the chemical processes. The term refers to the division of the convection time (as described in equation [2.19]) by a specific reaction time. If only one reaction occurs, a single reactant, A, is sufficient to explain the changes in the concentrations of all other substances. The characteristic response time can be computed by (equation [2.31]):

$$t^{react} = \frac{c_A^{init}}{r_0(c_i^{init})} \quad [2.31]$$

where c_i^{ini} is the initial or feed concentration of A.

For the reaction type $v_A A + v_B B + v_c C + v_D D$, the initial reaction rate is $r_0 = kc_A^{ini} c_b^{ini}$ and $v_A = v_B = -1$. The Damköhler number for this example can be mathematically represented based on the above definition (equation [2.32]):

$$D_a = \frac{t_0}{t^{react}} = \frac{L}{u} k c_B^{init} \quad [2.32]$$

In catalyzed reactions, catalysts decrease the potential energy barrier the reactants need to overcome to generate products. Thus, the rates of reactions are accelerated. The expression of the reaction rate law for homogeneously catalyzed reactions is identical to that of non-catalyzed reactions. Let us suppose a reversible reaction occurring in the homogeneous phase (equation [2.33]):

$$v_A A + v_B B \rightleftarrows v_c C + v_D D \quad [2.33]$$

Based on conventional laws, the rate r^{hom} can be written by the following equation (equation [2.34]):

$$r^{hom} = k_{forw}^{hom} \left(c_A c_B - \frac{c_C c_D}{K_{eq}^{hom}} \right) \quad [2.34]$$

$$K_{eq}^{hom} = \frac{k_{forw}^{hom}}{k_{backw}^{hom}} \quad [2.35]$$

in which k_{forw}^{hom}, k_{backw}^{hom} are the reaction rate constants for the forward and backward reactions, respectively; K_{eq}^{hom} is the homogeneous equilibrium constant (equations [2.35]), and the c_i are concentrations at the equilibrium state.

In the context of heterogeneously catalyzed reactions, the phrase “surface reaction” encompasses the three main steps: adsorption of reactants onto the catalyst

surface, chemical reactions occurring on the catalyst surface and desorption of the resulting products from the catalyst surface.

Surface reaction kinetics can be characterized by many classical mechanisms, such as Langmuir–Hinshelwood (LH), Eley–Rideal (EL) or Hougen–Watson, depending on different assumptions. A plethora of particular models for surface reaction kinetics was created for the example of simple esterification catalyzed by a solid catalyst.

The LH mechanism exclusively involves the reaction occurring through interactions between molecules that are adsorbed on the catalyst's surface. The rate of the reversible reaction in equation [2.33], which is catalyzed by a heterogeneous catalyst r^{het}, can be mathematically represented as (equations [2.36]–[2.37])

$$r^{het,\ LH} = k_{forw}^{het,LH}\left(q_A q_B - \frac{q_C q_D}{K_{eq}^{het,LH}}\right) \quad [2.36]$$

$$K_{eq}^{het,LH} = \frac{k_{forw}^{het,LH}}{k_{backw}^{het,LH}} \quad [2.37]$$

in which $k_{forw}^{het,LH}$, $k_{backw}^{het,LH}$ are the reaction rate constants for the forward and backward reactions, respectively; $K_{eq}^{het,LH}$ is the homogeneous equilibrium constant and the q_i (i = A, B, C, D) are the solid-phase concentrations at the equilibrium state.

Conversely, the EL mechanism postulates that the reaction occurs by collisions between unadsorbed molecules of one reactant (e.g. reactant B) and adsorbed molecules of another reactant (e.g. reactant A). The reaction rate can be represented by the following equation in this scenario (equations [2.38]–[2.39]):

$$r^{het,EL} = k_{forw}^{het,EL}\left(q_A q_B - \frac{q_C q_D}{K_{eq}^{het,EL}}\right) \quad [2.38]$$

$$K_{eq}^{het,EL} = \frac{k_{forw}^{het,EL}}{k_{backw}^{het,EL}} \quad [2.39]$$

If reactions occur in both phases, the overall reaction rate can be expressed as a linear equation that considers both the homogeneous and heterogeneous contributions, considering the volume fractions of the two phases (equation [2.40])

$$r^{tot} = \varepsilon_t r^{hom} + (1 - \varepsilon_t) r^{het} \quad [2.40]$$

2.15. Challenges and future prospect of chromatographic reactors

Chromatographic reactors combine the principles of chromatography and reaction engineering, offering unique advantages in various chemical processes. However, it also poses specific challenges and holds promising future prospects. Chromatographic reactors rely heavily on the efficient mass transfer between the stationary and flowing phases. Achieving large mass transfer rates while retaining acceptable selectivity remains challenging, especially in complicated reaction systems. On the other hand, the pressure loss across the chromatographic column can be large, particularly in high-pressure systems, limiting the scalability and feasibility of chromatographic reactors for certain applications. For best results, the chromatographic column must be packed uniformly with the stationary phase. Maintaining continuous packing density while preventing channeling or cavities can be difficult, especially in large-scale processes. Furthermore, residence time distribution and non-ideal flow patterns might alter the kinetics of processes within the chromatographic reactor. Understanding and managing these kinetic effects is critical for the desired reaction results. Aside from the issues mentioned above, scaling up chromatographic reactors from laboratory-scale to industrial-scale operations while maintaining performance and efficiency presents significant challenges, as issues such as heat and mass transfer, pressure drop and column packing become more prominent at larger scales.

Despite being bottlenecked by these challenges, the RC technology possesses humongous prospects. Continued advancements in materials science may lead to the development of novel stationary phases with enhanced selectivity, stability and mass transfer properties, improving the performance of chromatographic reactors. Moreover, integrating chromatographic reactors with other unit operations, such as membrane separation or catalytic reactions, can intensify the process, reducing energy consumption and improving overall efficiency. Additionally, advancements in computational modeling and simulation techniques enable more accurate prediction and optimization of chromatographic reactor performance, aiding design and scale-up efforts. Moreover, implementing advanced automation and control strategies allows for real-time monitoring and adjustment of chromatographic reactor operations, enhancing process reliability and productivity.

To summarize, expanding the application of chromatographic reactors beyond traditional chemical synthesis to areas such as biotechnology, pharmaceuticals and renewable energy production holds promise for future growth and innovation. Addressing the challenges associated with chromatographic reactors and capitalizing on emerging opportunities are key to unlocking their full potential in various chemical and biochemical processes.

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3

Mathematical Modeling of a Batch Reactor and a Non-Isothermal CSTR with Their Respective Simulation Using MATLAB and ASPEN PLUS

Mathematical modeling and simulation are the most essential tools in chemical engineering, which are more crucial for understanding, optimizing and designing chemical processes. This study delves into the mathematical modeling and simulation of two pivotal chemical reactors: the batch reactor and the continuous stirred tank reactor (CSTR), with a particular focus on non-isothermal conditions. The batch reactor, a closed system, is modeled to capture the dynamics of concentration and temperature over time, encompassing both heating and cooling phases. For the non-isothermal CSTR, a cooling jacket is used to regulate temperature during exothermic reactions, and the system is modeled under the perfectly mixed cooling jacket assumption. The modeling equations incorporate fundamental principles of mass and energy conservation. Computational simulations are conducted using MATLAB and ASPEN PLUS, providing practical insights into reactor behavior. The integration of theoretical modeling with practical simulations enhances the ability to design, analyze and optimize chemical processes across various industrial applications.

3.1. Introduction

Chemical engineering, as a discipline, relies heavily on both theoretical understanding and practical application. At the core of this symbiosis are mathematical modeling and simulation techniques, essential tools that empower

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engineers to optimize and design complex chemical processes. This work explores two major chemical reactors used in industries: the batch reactor and the continuous stirred tank reactor (CSTR). For the CSTR, the focus is on non-isothermal conditions. When exothermic or endothermic reactions occur, temperature regulation becomes critical for operational efficiency. To address this, a cooling jacket is introduced and explored under the perfectly mixed cooling jacket model. This model presents a unique approach to managing reaction heat, providing a comprehensive view of the CSTR behavior.

The study also delves into the batch reactor, an enclosed system where reactants are introduced at the beginning, allowed to react over a specified period and then the final product is removed. This work examines the reactor's mathematical model, aiming to understand the fundamental dynamics of batch processes and provide a basis for practical implementation and optimization. Computational simulations are conducted using MATLAB and ASPEN PLUS to bring these theoretical concepts to life. The outcomes of these simulations add a practical dimension to the theoretical models and offer valuable insights into reactor behavior, emphasizing the importance of accounting for temperature variations in chemical processes. Through this exploration, the study aims to contribute to the optimization of chemical processes, facilitate reactor design and deepen our understanding of non-isothermal reactions, fostering advancements in diverse chemical industries.

3.2. Modeling of a batch reactor

Mathematical modeling of a batch reactor involves establishing relationships between various variables and parameters that influence system behavior. A batch reactor functions as a closed system where reactants are introduced, and the reaction progresses until the desired product is obtained. This modeling is crucial for optimizing diverse chemical processes across industries. In batch reactor modeling, relationships among key variables such as concentration, temperature and reaction time are expressed. These models provide insights into reaction kinetics and system dynamics through governing equations, often in the form of differential equations. These equations capture the complex interactions of chemical and physical phenomena within the reactor. Engineers use these models to predict reaction progress, analyze process conditions and design efficient production strategies. Batch reactors find applications in pharmaceuticals, petrochemicals, food processing and other industries, making accurate modeling essential for enhancing process efficiency, ensuring product quality, and minimizing environmental impact.

The key variables typically involved in batch reactor modeling include concentrations of reactants and products, temperature, pressure and reaction time.

For instance, to model a simple chemical reaction A → B in a batch reactor using first-order kinetics, the material balance equation is used

$$d(C_A)/dt = -r_A$$

where $r_A = k[C_A]$ is the rate of the reaction, $[C_A]$ is the concentration of A, k is the rate constant and t is time. Now, the energy balance is given by the equation

$$\rho \times C_p \times d(T)/dt = \Delta H \times r_A - U \times A \times (T - T_c)$$

where T is the temperature, ρ is the density, C_p is the heat capacity, ΔH is the heat of reaction, U is the overall heat transfer coefficient and T_c is the coolant temperature. Some initial conditions have to be considered such as

$$C_A(0) = C_{A0} \text{ and } T(0)=T_0$$

where C_{A0} is the initial concentration of A and T_0 is the initial temperature. These equations describe the mathematical model for a batch reactor with a first-order, irreversible reaction involving reactant A. The system of ordinary differential equations (ODEs) is solved numerically over a specified time span to simulate the evolution of concentration and temperature.

3.2.1. *Simulation example of a batch reactor using MATLAB and ASPEN PLUS*

In this MATLAB code snippet, a simplistic yet illustrative model of a batch reactor is implemented to simulate the concentration changes of reactant A over time. The parameters include the reaction rate constant, initial concentration and simulation period. The differential equation captures the first-order kinetics of the reaction, where A transforms into products. The resulting plot visually represents how the concentration evolves, illustrating the characteristic exponential decay associated with a first-order reaction. Below is the MATLAB code:

```
% Parameters
k = 0.1;          % Rate constant
A0 = 100.0;       % Initial concentration of A
tspan = [0 10];           % Time span
ode = @(t, y) -k*y;       % Define the differential equation
% Solve the differential equation
[t, concentrations] = ode45(ode, tspan, A0);
```

```
% Plot the results
plot(t, concentrations, '-o');
xlabel('Time');
ylabel('Concentration of A');
title('Batch Reactor Simulation');
grid on;
% Display the final concentration of B
final_concentration_B = concentrations(end);
fprintf('Final Concentration of B: %.4f\n', final_concentration_B);
```

This simulation not only serves as an introductory example of MATLAB's capabilities in modeling chemical processes but also offers a fundamental understanding of batch reactor dynamics. The code's output, the final concentration of A, provides a quantitative measure of the extent of the reaction at the end of the simulation, offering valuable insights into reaction kinetics and system behavior. Overall, this code serves as a starting point for more complex batch reactor simulations and showcases the versatility of MATLAB in chemical engineering applications. From the given input parameters, we obtain the final concentration of B as 36.7879, along with the graph shown in Figure 3.1.

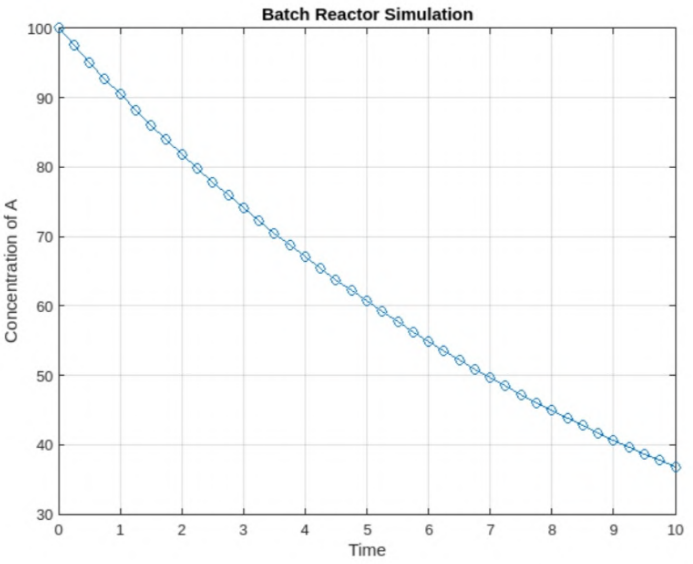


Figure 3.1. *Variation of concentration with respect to time (prepared for this work)*

To perform a batch reactor simulation using ASPEN PLUS, follow a systematic set of steps within the software. Begin by defining the chemical constituents involved in the batch reaction, specifying reactants, products and any intermediates. Next, configure the chemical reactions within the system, detailing reaction kinetics, stoichiometry and thermodynamics. Create a new flowsheet in ASPEN PLUS to represent the process, incorporating a batch reactor unit operation. This unit allows for the specification of batch reaction details, including the reaction time profile. Set initial conditions for the batch reactor, encompassing parameters such as initial concentrations of reactants and temperature. Analyze the simulation results using ASPEN PLUS tools to gain insights into the batch reactor's behavior. Validate the simulation by comparing results with the available experimental data. Adjust reaction kinetics or parameters if needed to enhance alignment between simulation and experimental outcomes. The blocks and process flow diagrams simulated using ASPEN PLUS are shown in Figures 3.2 and 3.3, respectively.

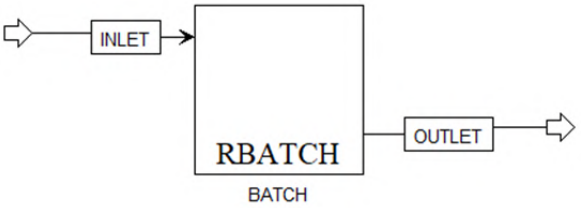


Figure 3.2. *Process block diagram of batch reactor simulated using ASPEN PLUS (prepared for this work)*

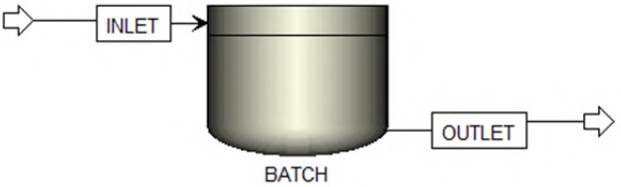


Figure 3.3. *Process flow diagram of batch reactor simulated using ASPEN PLUS (prepared for this work)*

3.3. Modeling of a non-isothermal CSTR

The non-isothermal CSTR described involves an irreversible exothermic reaction with a varying temperature profile over time. This scenario is particularly relevant in industrial processes where temperature control is crucial to optimize reaction rates and selectivity. The reactor is equipped with a cooling jacket to manage the heat

generated during the exothermic reaction. Consider the reaction: $P \rightarrow R$ with rate constant k. The exothermic reaction is assumed to be nth-order for reactant A, and the heat of the reaction is denoted as λ (J/mol of P reacted). The reaction kinetics and thermodynamics are essential factors influencing the reactor's behavior. Negligible heat losses and constant densities are assumed, simplifying the modeling process. To control the temperature rise resulting from the exothermic reaction, a cooling jacket surrounds the reactor. This jacket receives a continuous flow of cooling water at a volumetric flow rate denoted as F_{JT0} and an inlet temperature denoted as T_{JT0}. The volume of water in the jacket, V_{JT}, is held constant, representing a simplified assumption that facilitates the modeling process. The foundation of mathematical models is the inclusion of fundamental physical and chemical laws, notably the laws determining mass, energy and momentum conservation. These basic laws serve as the foundation for detailed mathematical representations, allowing for a systematic and quantitative understanding of complicated systems.

In essence, mathematical modeling entails turning underlying conservation principles into equations and connections that explain the dynamic behavior of physical and chemical processes, so offering a framework for analysis, prediction and optimization. In a perfectly mixed cooling jacket, we assume that the temperature within the entire jacket remains uniform and is denoted as T_{JT}. The exchange of heat between the chemical process operating at a temperature T and the cooling water at T_{JT} is characterized by an overall heat transfer coefficient (U). This coefficient represents an aggregate measure of the effectiveness of heat transfer between the system and the cooling medium. To elaborate further, this overall heat transfer coefficient encapsulates the combined impact of various factors influencing heat transfer, including the thermal conductivity of materials, the thickness of the boundary layers and the flow characteristics of the cooling water. The assumption of a perfectly mixed cooling jacket implies a homogeneous temperature distribution within the jacket, simplifying the modeling approach. This assumption enables the incorporation of the overall heat transfer coefficient into the mathematical framework, facilitating the quantification of heat transfer dynamics in the system. The heat transfer equation for our assumptions is given in the equation

$$Q = U \times A \times \Delta T$$

where $\Delta T = T - T_{JT}$, U is the overall heat transfer coefficient and A is the heat transfer area. The continuity equation expresses the conservation of mass for a given system. For our non-isothermal reactor, we write the continuity equation as the differential equation of mass to time = the mass flow in–the mass flow out.

We know that density is equal to the ratio of mass to volume ($\rho = m/V$). Here, we required mass, so we are rearranging the equation as

$$\text{Mass} = \rho \times V$$

$$\text{Mass flow in} = F_0 \times \rho$$

$$\text{Mass flow out} = F \times \rho$$

On substituting these in the continuity equation, we get

$$d(\rho V)/dt = (F_0 \times \rho) - (F \times \rho)$$

$$d(V)/dt = F_0 - F$$

This is the required total continuity equation for our non-isothermal CSTR. Now similarly, the continuity equation for the reactor component P is given by the equation

$$d(VCp)/dt = (F_0 C_{P0}) - (FC_P) - (V \times k \times (C_P)^n)$$

The reactor energy equation is given by the equation

$$\rho\, d(Vh)/dt = \rho F_0 h_0 - \rho F h - \lambda V k (C_P)^n - U A \Delta T$$

$$\rho C_P\, d(VT)/dt = \rho F_0 C_P T_0 - \rho F C_P T - \lambda V k (C_P)^n - U A \Delta T$$

The jacket energy equation is given by the equation

$$(\rho_{JT} V_{JT})\, d(h_{JT})/dt = F_{JT} \rho_{JT} (h_{JT0} - h_{JT}) + U A \Delta T$$

$$(\rho_{JT} V_{JT} C_{JT})\, d(T)/dt = F_{JT} \rho_{JT} C_{JT} (T_{JT0} - T_{JT}) + U A \Delta T$$

In addition, by the Arrhenius equation, we can obtain the value of k

$$k = k_o\, e^{-Ea/RT}$$

The level controller, acting as a proportional-only feedback controller, is designed to modulate the outflow in response to variations in the tank volume. This means that the controller adjusts the outflow proportionally to the difference between the desired level and the actual level in the tank. Notably, this dynamic regulation ensures that the outflow is completely suspended when the volume reaches its designated minimum threshold, denoted as V_m. This sophisticated control mechanism is integral to maintaining optimal fluid levels within the tank while preventing overflow or undesired depletion

$$F = K_v (V - V_m)$$

With the help of these equations and by knowing certain data, we can model a non-isothermal CSTR.

3.3.1. *Simulation example of a non-isothermal CSTR using MATLAB and ASPEN PLUS*

The following MATLAB code is an example of the mathematical simulation of the non-isothermal CSTR using the modeling equations. The function should be defined at the first and the respective input parameters should be defined. Then, the ODE should be solved, respectively, using the MATLAB functions. The results are generated by plotting a graph. The graphical image shows how concentration, temperature and enthalpy vary over time for the given feed in a non-isothermal CSTR. The resulting graph is shown in Figure 3.4.

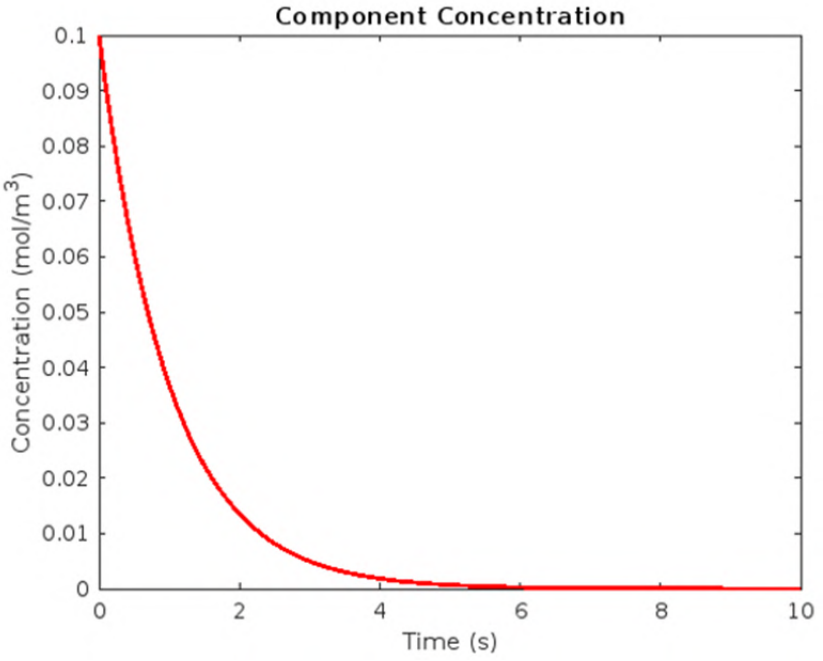


Figure 3.4. *Variation of concentration with respect to time (prepared for this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

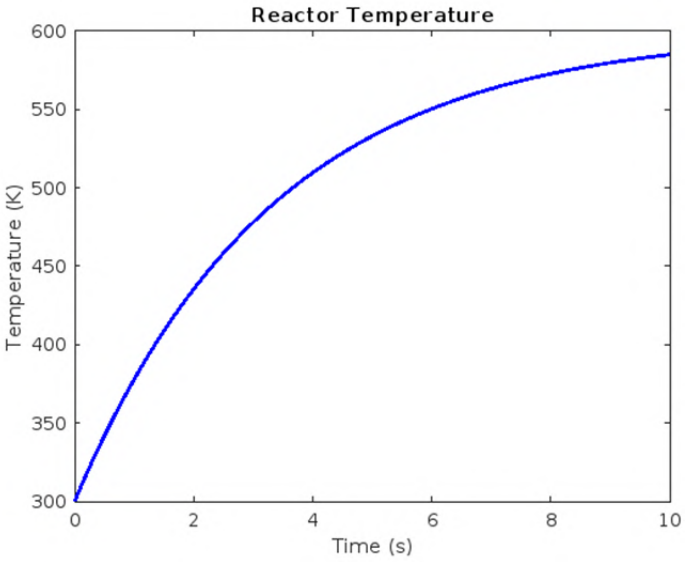


Figure 3.5. *Variation of temperature with respect to time (prepared for this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

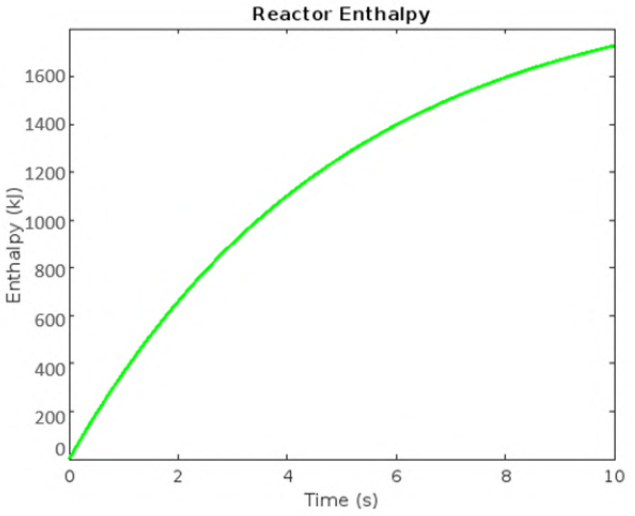


Figure 3.6. *Variation of enthalpy with respect to time (prepared for this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

```
function cstr()     % Define parameters
    rho = 1000;          % Density (kg/m^3)
    Cp = 4;              % Heat capacity (kJ/kg-K)
    k0 = 0.1;            % Reaction rate constant (1/s)
    Ea = 50;             % Activation energy (kJ/mol)
    R = 8.314;           % Gas constant (J/(mol-K))
    delta_H = -20;       % Heat of reaction (kJ/mol)
    UA = 500;            % Overall heat transfer coefficient (W/(m^2-K))
    Vm = 10;             % Maximum volume (m^3)
    VJT = 2;             % Jacket volume (m^3)
    Kv = 0.05;           % Flow rate constant (m^3/(s-kPa))
    F0 = 1;              % Inlet flow rate (m^3/s)
    C0 = 0.1;            % Inlet concentration (mol/m^3)
    T0 = 300;            % Initial temperature (K)
    h0 = 100;            % Initial enthalpy (kJ)
    tspan = [0 10];      % Time span for simulation (s)
    ode_system = @(t, y) your_system_of_equations (t, y, rho, Cp, k0, Ea, R, delta_H, UA, Vm, VJT, Kv, F0, C0);              % Solve the system of ODEs
    [t, solution] = ode45(ode_system, tspan, [C0, T0, h0]);
    function dydt = your_system_of_equations (~, y, ~, Cp, k0, Ea, R, delta_H, UA, Vm, VJT, Kv, F0, C0)
    % Extract variables from the state vector y
    C = y(1);  % Component concentration (mol/m^3)
    T = y(2);  % Reactor temperature (K)
    h = y(3);  % Reactor enthalpy (kJ)
    % Check for negative concentrations or temperatures
    if C < 0 || T < 0
      warning('Negative concentration or temperature detected. Stopping simulation.');
      dydt = [0; 0; 0];
      return;
```

```
    end
    k = k0 * exp(-Ea / (R * T));    % Compute the reaction rate
    F = Kv * (Vm - VJT);            % Compute the flow rate
% Compute the derivatives
    dCdt = F0 * (C0 - C) - F * C - Vm * k * C;
    dTdt = F0 * T0 - F * T - (delta_H * Vm * k * C + UA * (T - T));
    dhdt = F0 * Cp * T0 - F * Cp * T - (delta_H * Vm * k * C + UA * (T - T));
    dydt = [dCdt; dTdt; dhdt];
end
    figure;        % Plot the results
    subplot(3, 1, 1);
    plot(t, solution(:, 1), 'r', 'LineWidth', 2);
    xlabel('Time (s)');
    ylabel('Concentration (mol/m^3)');
    title('Component Concentration');
    subplot(3, 1, 2);
    plot(t, solution(:, 2), 'b', 'LineWidth', 2);
    xlabel('Time (s)');
    ylabel('Temperature (K)');
    title('Reactor Temperature');
    subplot(3, 1, 3);
    plot(t, solution(:, 3), 'g', 'LineWidth', 2);
    xlabel('Time (s)');
    ylabel('Enthalpy (kJ)');
    title('Reactor Enthalpy');
    sgtitle('Non-isothermal CSTR Simulation');
end
```

Simulating a non-isothermal CSTR using ASPEN PLUS follows a structured sequence of actions within the software framework. Initiate the process by commencing ASPEN PLUS and creating a new simulation file. Outline the

constituents of the CSTR by specifying reactants, products and any intermediates. Subsequently, establish the chemical reactions within the system, providing details on reaction kinetics, stoichiometry and thermodynamics. Incorporate a CSTR unit operation into the flowsheet, adjusting parameters such as reactor volume, temperature and pressure. Define the initial conditions, encompassing the starting concentrations of reactants, inlet temperature and pressure. Scrutinize the simulation outcomes by examining concentration profiles and temperature variations. Verify the simulation's accuracy by comparing results against available experimental data. Adjust reaction kinetics or parameters if needed to enhance alignment between simulation and experimental outcomes. The block and the process flow diagrams simulated using ASPEN PLUS are shown in Figures 3.5. and 3.6, respectively.

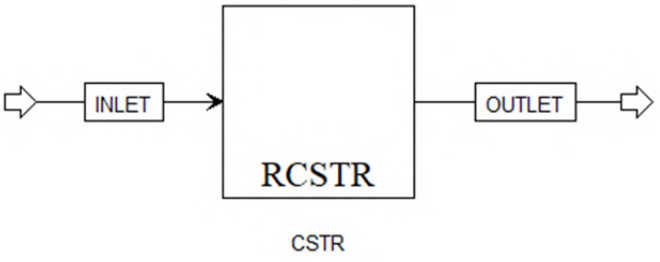


Figure 3.7. *Process block diagram of CSTR simulated using ASPEN PLUS (prepared for this work)*

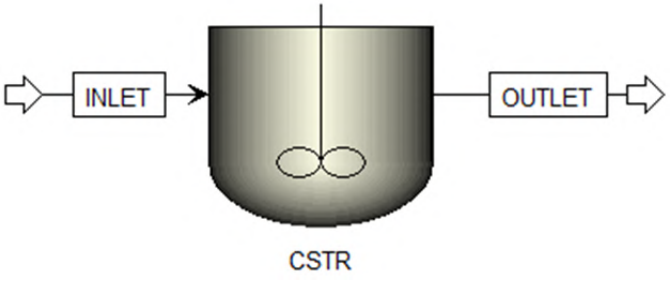


Figure 3.8. *Process flow diagram of CSTR simulated using ASPEN PLUS (prepared for this work)*

3.4. Conclusion

In conclusion, this study provides an exploration of mathematical modeling and simulation for two critical chemical reactors: the batch reactor and the non-isothermal continuous stirred-tank reactor (CSTR). These reactors are essential

in diverse industrial processes, necessitating a comprehensive understanding of their behavior to achieve optimal design and operational efficiency. The batch reactor, modeled as a closed system where reactants undergo reactions over time, was meticulously analyzed to capture the intricate dynamics of concentration and temperature. MATLAB simulations effectively illustrate how these parameters vary over time, demonstrating MATLAB's versatility in chemical engineering applications and providing practical insights into batch reactor dynamics. Similarly, the non-isothermal CSTR was modeled incorporating an irreversible exothermic reaction with a cooling jacket to regulate temperature. This modeling approach, grounded in principles of mass and energy conservation, facilitated a systematic understanding of the reactor's behavior. MATLAB simulations further elucidate the dynamic variations in concentration, temperature and enthalpy, offering valuable insights into the complexities of non-isothermal reactions. Additionally, ASPEN PLUS was used for detailed process simulation and optimization of both reactors. Its comprehensive capabilities in configuring reactor parameters and specifying reaction conditions underscore its role in optimizing chemical processes. Moreover, while recognizing the existence of other software and methods such as computational fluid dynamics (CFD) tools such as COMSOL Multiphysics and process simulation software such as CHEMCAD, MATLAB and ASPEN PLUS were selected for their ease of learning and practical usability. Their integration of theoretical principles with practical simulations enhances our ability to design, analyze and optimize chemical processes, thereby advancing innovation and sustainability in chemical engineering. The integration of theoretical concepts with practical simulations using MATLAB and ASPEN PLUS enhances our ability to design, analyze and optimize chemical processes in diverse industrial settings. The theoretical modeling and practical simulation remain crucial for advancing innovation and sustainability in the field of chemical engineering.

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PART 2

Material Properties and Advanced Applications

4

Properties of Materials and Selection Criteria

The selection of materials is a critical aspect of engineering and design across various industries. This abstract provides an overview of the fundamental properties of materials and the key criteria used in their selection. Understanding the properties and selection criteria is essential for optimizing the overall performance of products and structures. Materials possess a wide range of properties, including mechanical, thermal, electrical and chemical characteristics, and are specifically discussed in the context of the current global demands of chemical industries. Mechanical properties encompass strength, stiffness, ductility and hardness, while thermal properties include thermal conductivity, the expansion coefficient and specific heat capacity. Electrical properties include conductivity, resistivity and dielectric strength, while chemical properties encompass reactivity, corrosion resistance and compatibility with other substances. The compositions of metals and alloys that favor their selection for chemical plants are described, aiming at pressure vessels, storage tanks, reaction vessels and ancillaries. The concern of nonmetals, along with their composition and types, is also discussed in this chapter. Corrosion prevention, chemical equipment linings and case studies are exclusively included to gain insight into the needs of chemical plants and equipment. The correlation between material selection and equipment design considerations is noteworthy for practical implementation.

4.1. Introduction

Understanding material properties and their selection criteria is paramount in the landscape of chemical industries. The intricate relationship between materials and their performance within these industries is pivotal to ensuring safety, efficiency and innovation. This chapter aims to delve into the multifaceted realm of material

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properties, their significance and the meticulous considerations behind their selection within the diverse and demanding scope of chemical production.

The chemical industry plays a pivotal role in modern society, providing essential raw materials for a wide range of products, including pharmaceuticals, plastics, fuels and countless other goods. The success and efficiency of chemical processes within this industry are heavily dependent on the properties of the materials involved. The choice of materials is fundamental in designing chemical processes and equipment. This can be justified by considering several key factors in the field of chemical engineering and process design. The selection of materials that are compatible with the chemicals involved is crucial to ensure the integrity of the equipment and prevent corrosion or degradation (Sinnott and Towler 2013). In addition to this, the materials used in the construction of process equipment must possess suitable thermodynamic and mechanical properties to withstand the operating conditions (Peters and Timmerhaus 2018). Furthermore, the selection of materials must balance the performance requirements with economic considerations, taking into account material costs, fabrication costs and maintenance costs (Sinnott and Towler 2013). Environment and safety considerations cannot be ignored however as they are an important matter for the chemical industries. Materials must meet safety standards and have minimal environmental impact (Turton et al. 2008). Good machinability and weldability also add to this list of criteria for the selection of different materials for practical reasons (Peters and Timmerhaus 2018). Therefore, the choice of materials in the chemical process design is a multidimensional decision.

In this intricate web of chemical process operations, the selection of appropriate materials becomes a pivotal aspect, influencing not just the efficiency but also the safety and longevity of the processes and equipment. Mechanical properties such as strength, elasticity and toughness stand as pillars of structural integrity, ensuring that equipment can withstand the stresses and strains imposed upon them.

Additionally, thermal properties play a crucial role in determining how materials respond to changes in temperature, preventing failures due to thermal expansion or contraction. Chemical properties, particularly resistance to corrosion, oxidation and reactivity, dictate the material's durability and reliability in aggressive chemical environments.

A cornerstone in material selection is to understand the trade-offs between different properties. For instance, while certain materials might exhibit excellent corrosion resistance, they might lack the required strength for specific applications. Balancing these attributes becomes a strategic challenge in material selection, often involving compromises that align with the priorities of safety, efficiency and cost-effectiveness.

Moreover, advancements in materials science have paved the way for innovative materials designed specifically to meet the stringent demands of chemical processes. Composite materials, nanomaterials and surface treatments have emerged as frontrunners in enhancing material properties, offering improved performance, durability and sustainability. The significance of material properties and their selection criteria reverberates throughout various facets of the chemical industry. From designing reactors, pipelines and storage tanks, to selecting instrumentation and safety equipment, the implications of material selection resonate across the entire operational spectrum (Sinnott and Towler 2013).

Safety stands tall as a paramount concern in the chemical industry, and material selection is intricately linked to ensuring a safe working condition. Incompatibility between materials and chemicals can lead to catastrophic consequences, including leaks, equipment failures or even explosions. Hence, meticulous attention to material properties, their behavior under various conditions and their compatibility with chemicals are indispensable in mitigating risks and ensuring operational safety. Regulatory bodies also play a pivotal role in shaping material selection criteria within the chemical industry, which are discussed later in this chapter.

In summary, this chapter aims to unravel the intricate tapestry of material properties and their selection criteria within the realm of chemical industries. From understanding the properties of materials, to navigating the complexities of selecting the right materials for specific applications, this exploration aims to shed light on the critical role that materials science plays in ensuring the success, safety and sustainability of chemical processes and industries.

4.2. Mechanical properties

The mechanical properties of metals used in chemical industries are foundational to the integrity and reliability of equipment and structures. These properties encompass a range of characteristics that define how a material responds to external forces, influencing its suitability for various applications within the chemical sector.

4.2.1. *Strength*

Strength stands as a fundamental mechanical property, indicating a material's ability to withstand applied forces without deformation or failure. In chemical industries, where equipment operates under extreme conditions, strength is critical. Tensile strength, the maximum stress a material can endure before breaking, and

yield strength, the stress at which a material begins to deform plastically, are crucial parameters.

Metals with high tensile and yield strengths are favored for applications where withstanding high pressures or loads is imperative, such as in pipelines, pressure vessels and structural components in chemical plants. Carbon steel (ASTM A106) and titanium alloys (ASTM B265) (ASTM 2023) are known for their excellent strength, which makes them suitable for high-pressure applications, such as pipelines for transporting oil and gas, aerospace components and chemical processing equipment.

4.2.1.1. *Tensile strength and stress–strain relationship*

– Tensile strength: this property measures a material's resistance to breaking under tension. It represents the maximum stress a material can withstand without failing. Engineers often test tensile strength by subjecting samples to gradually increasing forces until they fracture. It is crucial in applications where materials experience pulling forces, such as cables, ropes and structural elements. Stress σ(N/m^2) is defined by the relationship (Ashby et al. 2013)

$$\sigma = \frac{F}{Ao}$$

where F is the instantaneous load applied perpendicular to the cross-section (N) and Ao is the original cross-sectional area (m^2).

– Stress–strain relationship: when stress is applied to a material, it deforms. The stress–strain curve illustrates this relationship (Figure 4.1). Initially, strain increases proportionally to stress (elastic deformation). Once the material surpasses its elastic limit, it experiences plastic deformation, where strain occurs without a corresponding increase in stress. Ultimately, the material fails when it reaches its ultimate tensile strength.

Engineering strain (ϵ) can be calculated by

$$\epsilon = \frac{\Delta L}{Lo}$$

where ΔL is the deformation elongation or change in length at some instant, and Lo is the original length before any load is applied.

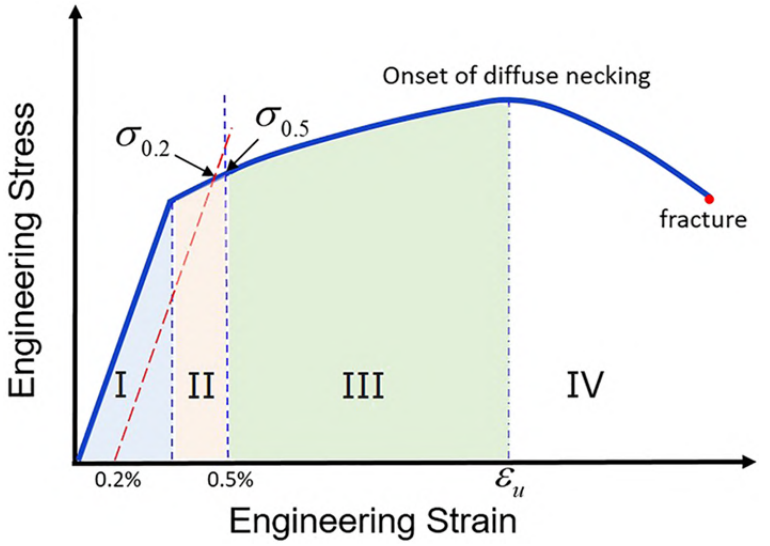


Figure 4.1. *Engineering stress–engineering strain curve (Tu et al. 2020) (Open Access). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

4.2.1.2. *Compressive strength and stability*

– Compressive strength: this property determines a material's ability to withstand forces that compress or squeeze it. Understanding compressive strength is vital in designing load-bearing structures, pillars and columns in construction.

– Buckling and stability: materials under compression can buckle or deform laterally if they are slender. Stability analysis is crucial to ensure structures remain intact under compressive forces without buckling.

4.2.1.3. *Shear strength and material integrity*

– Shear strength: when forces act parallel to the surface of a material, shear stress occurs. Shear strength measures a material's resistance to this type of stress. It is vital in applications involving cutting, fastening and structural stability, such as in rivets and welded joints.

4.2.2. *Hardness*

Hardness (which measures a material's resistance to deformation, abrasion or penetration) is vital in industries where wear and tear are common, as seen in valves,

pumps and components subjected to abrasive chemicals or processes. Hardness also affects a material's machinability and its ability to withstand surface damage, contributing to the longevity of equipment in chemical settings. Various hardness tests, such as the Mohs scale or Brinell, Vickers or Rockwell hardness tests (Figure 4.2), can be used to assess a material's resistance to deformation.

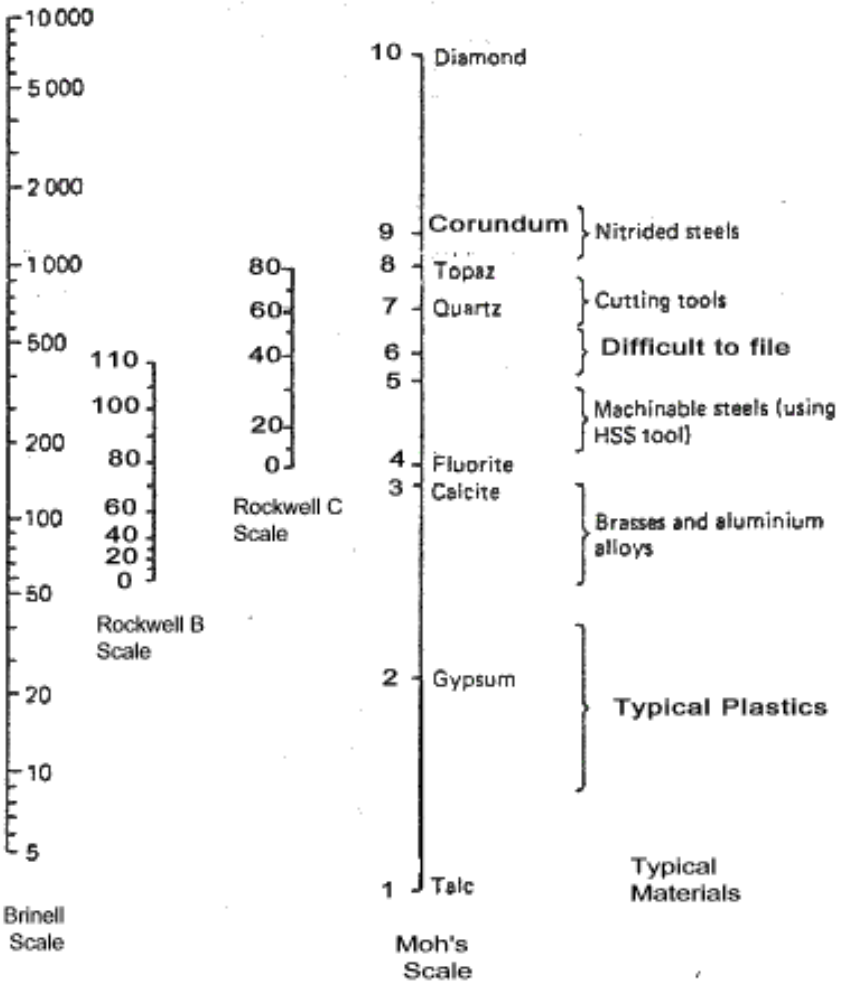


Figure 4.2. *Comparison of several hardness scales (Tubing China 2023) (Open Access)*

Hardness tests are conducted more often than any other mechanical test for various reasons:

1) They are straightforward and cost-effective: usually requiring no special specimen preparation, and the testing equipment is relatively inexpensive.

2) The test is non-destructive: there is no fracture or excessive deformation of the specimen; it only incurs a small indentation.

3) Hardness data can often help estimate other mechanical properties such as tensile strength.

4.2.3. *Plasticity and ductility*

Ductility and toughness are mechanical properties that denote a material's ability to deform plastically and absorb energy before fracturing, respectively. Ductile materials can undergo significant deformation before failure, allowing for shaping processes such as bending or forming, crucial in manufacturing chemical equipment. Toughness is vital for components subject to impact or sudden stress, preventing brittle fracture. Ductility may be expressed quantitatively as either percent elongation or percent reduction in area.

Percent elongation (%EL) is the percentage of plastic strain at fracture:

$$\%\text{EL} = \frac{L_f - L_o}{L_o}$$

where L_f is the fracture length and L_o is the original gauge length.

Percent reduction in area (%RA) is defined as

$$\%\text{RA} = \frac{A_o - A_f}{A_o} x100$$

where $A_o$is the original cross-sectional area and A_f is the cross-sectional area at the point of fracture.

4.2.4. *Fatigue strength and endurance limit*

Fatigue strength represents a material's ability to withstand cyclic loading without failure. In chemical industries, where equipment often experiences repeated stress due to operational cycles or fluctuating conditions, fatigue strength is critical. Components such as rotating machinery, pressure vessels and piping systems need

materials with high fatigue resistance to prevent failure over time. Some materials have a stress threshold below which they can endure an infinite number of loading cycles without fatigue failure. This limit is known as the endurance limit or fatigue limit (Suresh 1998).

4.2.5. *Creep resistance*

Creep resistance is another significant mechanical property, especially in chemical processes involving high temperatures and sustained loads over time. Creep refers to the gradual deformation of materials under constant stress at elevated temperatures. Metals with good creep resistance are preferred in applications such as furnace components, where sustained high temperatures are prevalent.

4.2.6. *Corrosion resistance*

Corrosion resistance is a mechanical property that significantly influences material selection in chemical industries. While it falls more under the category of chemical properties, a material's ability to resist corrosion also impacts its mechanical performance. Corrosion weakens materials, compromising their mechanical properties over time. Stainless steels (ASTM A240), nickel alloys, aluminum alloy (ASTM B209) (ASTM 2023) and titanium are preferred due to their exceptional corrosion resistance in aggressive chemical environments (Roberge and Eng 2005).

The selection of metals for chemical applications involves considering these mechanical properties in conjunction with other factors such as temperature, pressure, chemical compatibility, etc. Metals such as stainless steel, carbon steel, aluminum alloys, nickel alloys and titanium find extensive use in various applications within chemical industries due to their unique combinations of mechanical properties. Each metal offers a distinct set of advantages, allowing for tailored solutions to specific operational requirements. Alloying elements, heat treatments and surface coatings are used to improve strength, hardness, ductility and other mechanical characteristics, addressing the evolving needs of the chemical industry. Ultimately, the significance of the mechanical properties of metals cannot be overstated within the realm of chemical industries.

4.3. Chemical properties

Chemical properties of materials refer to their behavior in reactions or interactions that result in changes in composition or structure. They rely on an

intricate understanding of these properties to develop innovative materials, optimize production and ensure the safety and sustainability of industrial processes (Brady et al. 1990; Atkins and Jones 2007). Chemical properties profoundly impact material behavior. Chemical properties encompass characteristics such as reactivity, stability and compatibility. Reactivity, for instance, defines how materials interact with other substances, leading to corrosion, rusting or other chemical transformations. Stability dictates a material's resistance to changes under different conditions, affecting its lifespan and reliability. Moreover, a material's bonding types and molecular structure, determined by its chemical properties, influence its mechanical, electrical and thermal behaviors (Shackelford 2000; Ashby et al. 2013; Callister and Rethwisch 2020).

a) Atomic structure and composition

At the heart of understanding chemical properties lies the atomic structure. Matter is composed of elements, each having unique properties defined by the number of protons, neutrons and electrons in their atoms. Elements are distinguished by the number of protons in their atoms, known as the atomic number. The arrangement of these elements on the periodic table organizes them by their atomic number, facilitating the understanding of their properties and behaviors. For instance, metals found on the left side of the periodic table generally have high electrical conductivity, while nonmetals on the right tend to be poor conductors. Transition metals, occupying the central portion, often showcase varying oxidation states, enabling diverse applications in catalysis, electronics and materials science. Understanding atomic interactions is crucial in predicting material behavior (Brown et al. 1997).

b) Bonding and material characteristics

Different bonding types – ionic, covalent, metallic – dictate material properties. For instance, metals with metallic bonding exhibit malleability, conductivity and ductility due to the free movement of electrons. Covalently bonded materials often possess high melting points and are typically insoluble in water due to strong molecular structures. Metallic bonding, characterized by a "sea of electrons" flowing between atoms, imparts metals with excellent conductivity and malleability. Ionic bonding results in materials such as salts, typically forming brittle crystals due to the strong attraction between oppositely charged ions. These bonding types directly impact a material's behavior. For instance, polymers often display covalent and weaker secondary bonds, allowing for flexibility and diverse applications in industries such as packaging, textiles and medicine (Brady et al. 1990; Callister and Rethwisch 2020).

c) Reactivity and corrosion

Chemical reactivity is vital in predicting how materials behave in various scenarios and is instrumental in designing processes and selecting suitable materials for specific applications in chemical industries. Materials can exhibit diverse reactions, such as oxidation, combustion or acid–base reactions, based on their inherent chemical properties (Brady et al. 1990; Atkins and Jones 2007). For example, reactive metals such as sodium or potassium readily react with water, producing heat and hydrogen gas. Understanding reactivity aids in predicting these behaviors and potential hazards associated with different materials (Callister and Rethwisch 2020). Polytetrafluoroethylene (ASTM D4894) and Hastelloy (ASTM B622) (ASTM 2023) are highly resistant to chemicals and are often used in the manufacturing of gaskets, seals and linings for chemical processing equipment. They are known for their non-reactivity and low coefficient of friction (Brown et al. 1997).

Corrosion, a common concern, is the deterioration of materials due to chemical reactions with their surroundings. Various corrosion mechanisms exist, including electrochemical reactions, such as rusting in iron due to exposure to oxygen and moisture, or galvanic corrosion arising from the contact of dissimilar metals in an electrolyte. For instance, metals may corrode in the presence of oxygen or moisture, forming oxides that weaken the material over time. The effects of corrosion can be detrimental, compromising structural integrity, causing leaks, reducing efficiency and leading to significant economic losses (Shackelford 2000). Preventing and controlling corrosion involves a range of techniques. Surface coatings such as paints or polymer layers act as barriers, shielding materials from corrosive elements. Cathodic protection methods, such as sacrificial anodes or impressed current systems, prevent corrosion by directing the flow of electrons away from the material (Callister and Rethwisch 2020).

d) Material stability and degradation

Chemical stability refers to a material's resistance to change when exposed to different conditions such as temperature, pressure and pH. Stable materials maintain their properties over time, resisting degradation or decomposition. Environmental factors such as moisture, oxygen, UV radiation, pollutants, temperature, pH and exposure to chemicals can lead to material degradation, altering its properties and performance.

For example, metals might corrode faster in marine environments due to saltwater exposure, while polymers can degrade under prolonged sunlight exposure. This knowledge aids in estimating a material's durability, allowing for better maintenance schedules or replacement plans in various industries.

e) Toxicity and purity

Non-toxicity and purity are critical properties when considering materials for use in various industries, especially in sectors such as pharmaceuticals, food processing, biomedical applications and sensitive chemical manufacturing (Uher 2004). Materials intended for contact with living organisms or for products that enter the human body must be non-toxic (Brown et al. 1997). High purity is essential in industries where even trace amounts of impurities can affect product quality or compromise safety. In sectors where non-toxicity and purity are critical, materials must undergo rigorous testing and certification to ensure they meet safety and quality standards (Kumar et al. 2018). For instance, in pharmaceuticals, ensuring both non-toxicity and high purity is vital to guarantee the efficacy and safety of medicinal products (Huerta-Ángeles et al. 2018).

f) Modification and synthesis

Materials can be chemically modified or synthesized to enhance their properties. Surface modification techniques, such as coatings, plasma treatments or chemical treatments, alter a material's surface properties without changing its bulk properties. Chemical synthesis methods involve creating new materials through processes such as polymerization, precipitation and combustion synthesis. Chemical modification enables the alteration of material properties by introducing additives, dopants or altering molecular structures. For instance, adding carbon nanotubes to polymers can enhance their mechanical strength, conductivity or thermal properties.

Creating materials that are self-healing, resistant to extreme conditions or capable of specific chemical reactions for targeted applications are the current focus. By comprehending how materials interact chemically, scientists and engineers can innovate and develop advanced materials with improved performance and durability. For example, high-strength alloys are used in the aerospace industry due to their superior chemical stability and mechanical properties.

4.4. Other significant properties

In the chemical industries, leaving aside the mechanical and chemical properties, electrical, thermal and optical properties, for example, are also integral not only for process control, safety and equipment reliability but also for product innovation and optimization (Reed 2008). Materials with specific properties play a pivotal role in enhancing efficiency, enabling precise control over processes, and ensuring safety

measures, thereby contributing to advancements and sustainability in the chemical sector (Ashby and Jones 2012).

4.4.1. *Thermal properties*

Materials exhibit varying abilities to conduct heat. Metals such as copper or aluminum boast high thermal conductivity, enabling efficient heat transfer, and are commonly used in heat exchanger tubes or reactor vessels (Uher 2004; Ashby and Jones 2012). In contrast, insulating materials such as wood or foam restrict heat transfer, serving as valuable thermal insulators in various applications (Brown et al. 1997). Materials with high thermal conductivity facilitate rapid heat transfer between the fluids (or gases) circulating in the equipment, and materials with low thermal conductivity such as rubber can be used as insulation which can minimize heat transfer from the outside environment, preserving the temperature inside the heat exchanger, leading to a better overall performance (Kumar et al. 2018; Rao et al. 2020).

The thermal conductivity and heat capacity of materials determine their suitability for heat exchangers, reactors and other equipment. Specific heat capacity defines a material's ability to absorb heat without a significant temperature change. In processes involving variable heat loads or changes in temperature, materials with high heat capacity can act as thermal buffers, helping to stabilize the temperature within the equipment. Water has a high heat capacity, making it suitable for applications where temperature stability is crucial, such as in cooling systems or as a heat transfer fluid.

Thermal expansion, where materials expand or contract with temperature changes, impacts engineering designs that require consideration of structural integrity (Uher 2004). Various thermal resistance materials such as Inconel (ASTM B166) (ASTM 2023), a nickel–chromium alloy, can be used in extreme environments, such as aerospace applications, gas turbine blades and chemical processing plants, whereas graphite (ASTM C564) (ASTM 2023) is used in applications such as crucibles for metal melting and as a moderator in nuclear reactors.

Proper insulation materials are also essential for conserving energy and maintaining optimal operating temperatures. Adequate insulation helps the industry meet regulatory standards, enhance sustainability and maintain optimal operating conditions for various chemical processes. A list of a few such materials is given in Table 4.1.

S. no.	Insulating material	Descriptions	Applications	References
1	Mineral wool	Mineral wool includes materials such as rock wool and slag wool. It is known for its excellent thermal insulation properties.	Suitable for high-temperature applications, such as furnaces and process vessels.	ASTM C612 – Standard Specification for Mineral Fibre Block and Board Thermal Insulation
2	Calcium silicate	Calcium silicate is a rigid insulation material that can withstand high temperatures and is resistant to moisture.	Used in high-temperature piping and equipment insulation.	ASTM C533 – Standard Specification for Calcium Silicate Block and Pipe Thermal Insulation
3	Polyurethane foam	Polyurethane foam is a versatile insulation material with good thermal properties and chemical resistance.	Commonly used for insulating pipes, tanks and equipment in chemical processing.	ASTM C591 – Standard Specification for Unfaced Preformed Rigid Cellular Polyurethane Thermal Insulation.
4	Fiberglass	Made from fine glass fibers and known for its light weight and low thermal conductivity.	Widely used for insulating pipes, vessels and ductwork in various industries.	ASTM C547 – Standard Specification for Mineral Fiber Pipe Insulation.
5	Ceramic fiber	A lightweight, high-temperature insulation material with excellent thermal shock resistance.	Suitable for high-temperature applications such as kilns, furnaces and boilers.	ASTM C892 – Standard Specification for High-Temperature Fiber Blanket Thermal Insulation.
6	Polystyrene foam	Polystyrene foam is a lightweight and cost-effective insulation material with good moisture resistance.	Used in low-temperature applications and where moisture resistance is important	ASTM C578 – Standard Specification for Rigid, Cellular Polystyrene Thermal Insulation.
7	Polyurethane foam	High thermal resistance, lightweight and good for low-temperature applications.	May not be suitable for high-temperature applications.	
8	Polyisocyanurate foam	Good thermal insulation, fire resistance and suitable for high-temperature applications.	May release toxic gases when exposed to fire.	
9	Perlite and vermiculite	Lightweight, fire-resistant and suitable for high-temperature applications.	Considerations: may not provide as high thermal resistance as some other materials.	

Table 4.1. *Various insulating materials (ASTM 2023)*

4.4.2. *Electric properties*

Electrical properties play a pivotal role in enabling precise process control within chemical plants. Sensors, control systems and instrumentation rely on the conductivity and resistivity of materials to monitor, regulate and optimize chemical reactions and production processes. Electrical insulation and grounding systems are crafted from these materials, mitigating electrical hazards and safeguarding personnel and equipment in chemical facilities. Electrochemical processes are fundamental in the chemical industries.

From electrolysis to electroplating, materials with distinct electrical conductivity properties are used to synthesize chemicals, purify substances or deposit metals onto surfaces (Rajoria et al. 2022). These processes, underpinned by electrical properties, drive numerous chemical manufacturing applications. The role of electrical properties in creating safe operating environments cannot be overstated.

4.4.3. *Optical properties*

The optical properties of metals hold substantial importance in various aspects of the chemical industries, contributing significantly to processes, analysis and material selection. Optical sensors have emerged as invaluable tools for monitoring various chemical parameters. Their utilization in detecting changes in substances, monitoring reaction kinetics and ensuring accurate measurements contributes significantly to process optimization and quality control. Optical properties in chemical industries are harnessed for analytical purposes. Spectroscopy and other optical techniques leverage these properties to analyze chemical compositions, monitor reactions and ensure the quality of products. Beyond analysis, optical properties facilitate visual inspection methods critical for assessing product quality and equipment integrity.

4.5. Criteria for material selection with design consideration

Selecting materials in the chemical industry is a critical process that involves careful consideration of various factors to ensure operational efficiency, safety and cost-effectiveness. The materials used in this industry must withstand harsh chemical environments, varying temperatures and pressures, while also meeting regulatory standards and environmental sustainability goals. Here is an in-depth exploration of the selection criteria for materials in the chemical industry.

4.5.1. *Safety and environmental considerations*

The chemical industry must adhere to strict safety regulations. Properties such as flammability, toxicity and reactivity are critical factors in the safe handling, storage and transportation of chemicals due to their potential impact on human health, the environment and overall safety. Here is a justification for the significance of each property:

1) Flammability: understanding the flammability of a chemical is crucial to prevent accidental fires and explosions during storage, handling and transportation. Materials with high flammability can pose serious risks, and appropriate precautions, such as proper storage conditions and fire suppression systems, must be in place to minimize the likelihood of accidents. Options include the use of chemical storage containers made up of high-density polyethylene (HDPE), polypropylene and stainless steel, as well as the use of safety cabinets made up of double-walled steel with insulation.

2) Toxicity: toxicity relates to the harmful effects a substance can have on living organisms, including humans, animals and plants. Proper handling and storage protocols are necessary to prevent accidental releases that could lead to contamination of air, water or soil. The Occupational Safety and Health Administration (OSHA) sets permissible exposure limits (PELs) for many chemicals in the workplace. These limits are often expressed in parts per million. So, if a chemical has a PEL of 50 ppm, it means that the concentration of that chemical in the air should not exceed 50 parts per million in the workplace atmosphere.

3) Reactivity: chemicals with high reactivity can pose risks such as rapid heat generation, gas release or explosions. Understanding a chemical's reactivity helps in selecting appropriate storage containers, segregating incompatible substances and implementing proper handling procedures to avoid dangerous reactions. Reactive chemicals may also require specific storage conditions, such as temperature control or isolation from other substances.

It is important to note that the reactivity of a chemical can depend on its concentration, temperature and the presence of other substances. Always consult safety data sheets (SDS) and follow appropriate safety guidelines when working with reactive chemicals (Ashby and Jones 2012). Some examples are as follows:

1) Hydrofluoric acid (HF): extremely corrosive and can penetrate tissues, causing severe burns.

2) Chlorine (Cl_2): highly reactive and can react violently with various substances.

3) Hydrogen peroxide (H_2O_2): concentrated hydrogen peroxide is a strong oxidizing agent and can react violently with combustible materials.

4) Sodium hydroxide (NaOH): a strong base that is highly reactive and corrosive.

5) Potassium (K): highly reactive metal, especially with water.

6) Acetylene (C_2H_2): highly flammable and can form explosive mixtures with air.

7) Phosphorus (P): white phosphorus is highly reactive and pyrophoric.

8) Chlorine trifluoride (ClF_3): extremely reactive and can react with many materials considered inert.

9) Perchloric acid ($HClO_4$): a strong oxidizing agent and can react violently with reducing agents.

10) Sulfuric acid (H_2SO_4): highly corrosive and can react violently with water.

11) Nitric acid (HNO_3): a strong oxidizing agent that can react with various substances.

12) Mercury (II) fulminate ($Hg(CNO)_2$): highly sensitive and can detonate easily.

13) Bromine (Br_2): highly reactive and can react violently with certain materials.

14) Tetranitromethane (CN_4O_8): highly reactive and explosive.

15) Alkali metals (e.g. sodium, potassium): highly reactive with water, can produce flammable hydrogen gas.

Additionally, government agencies and industry standards often provide guidelines and regulations to ensure the proper management of chemicals. Compliance with these factors is essential to prevent accidents and minimize the environmental impact.

4.5.2. *Reaction kinetics and thermodynamics*

The properties of materials influence reaction kinetics and thermodynamics. For example, catalysts, which are crucial in many chemical reactions, are chosen based on their specific properties to enhance reaction rates and selectivity. Understanding

thermodynamic properties helps in optimizing reaction conditions for maximum efficiency.

The properties of materials play a crucial role in influencing both reaction kinetics and thermodynamics. These properties encompass a wide range of characteristics, including, but not limited to, electronic structure, molecular geometry, surface area and physical state. Justifying this assertion involves considering the impact of these material properties on the fundamental principles of chemical reactions (Uher 2004).

4.5.2.1. *Electronic structure*

a) *Influence on reaction kinetics*: the electronic structure of materials determines their ability to donate or accept electrons, affecting reaction rates. Catalysts, for example, exploit their electronic structure to provide an alternative reaction pathway with lower activation energy, thus accelerating reaction kinetics.

b) *Influence on thermodynamics*: the electronic structure also governs the stability of chemical species formed during a reaction. Materials with specific electronic configurations may exhibit enhanced or diminished thermodynamic stability, influencing the overall energy changes in a reaction.

4.5.2.2. *Molecular geometry*

a) *Influence on reaction kinetics*: the spatial arrangement of molecules affects the likelihood of successful collisions. For instance, reactants with favorable molecular geometries may collide with the correct orientation, increasing the likelihood of effective collisions and faster reaction rates.

b) *Influence on thermodynamics*: molecular geometry influences the enthalpy and entropy changes during a reaction. Well-organized molecular structures may lead to more stable products, impacting the thermodynamic favorability of the reaction.

4.5.2.3. *Surface area*

a) *Influence on reaction kinetics*: in heterogeneous catalysis, the surface area of a catalyst significantly influences reaction rates. A higher surface area provides more active sites for the reaction to occur, leading to increased reaction kinetics.

b) *Influence on thermodynamics*: the exposed surface area can affect the thermodynamics of adsorption and desorption processes, which are critical in reactions occurring on surfaces.

4.5.2.4. *Physical state*

a) *Influence on reaction kinetics*: the physical state of a material (solid, liquid, gas) affects the accessibility of reactants to one another. Reactions in a homogeneous phase generally proceed faster than those involving reactants in different phases.

b) *Influence on thermodynamics*: phase transitions involve changes in energy and entropy, impacting the thermodynamics of a reaction. For example, reactions involving changes in the physical state may have different thermodynamic parameters than reactions occurring solely within the same phase.

Ensuring the above properties, it is said that the properties of materials directly impact both reaction kinetics and thermodynamics by influencing the key factors that govern these processes. Understanding and manipulating these material properties are essential for optimizing reaction conditions, designing efficient catalysts, and advancing our control over chemical transformations.

4.5.3. *Economic considerations*

Optimal material selection can significantly impact the economic viability of chemical processes. By choosing materials that offer the best balance of cost, performance and durability, companies can enhance their competitiveness in the market (Uher 2004).

4.5.3.1. *Example: storage tanks for corrosive chemicals*

Let us consider the selection of materials for storage tanks that will contain a corrosive chemical, such as sulfuric acid. The goal is to balance cost, performance and durability.

Material options:

– Stainless steel: offers good corrosion resistance but can be expensive.

– Fiberglass reinforced plastic (FRP): corrosion-resistant and lightweight but may have higher upfront costs.

– Lined carbon steel: carbon steel tanks lined with corrosion-resistant materials can provide a cost-effective solution.

Comparison:

– Stainless steel: high initial cost, but excellent corrosion resistance and durability.

– FRP: moderate initial cost, good corrosion resistance and lightweight.

– Lined carbon steel: lower initial cost, but the lining may require maintenance over time.

Types of steel	Applications	Properties	Remarks on cost
Carbon steels	Carbon steels are widely used in structural applications, such as buildings and bridges, as well as in machinery and automotive components.	Good strength and ductility, but limited corrosion resistance.	Generally more economical compared to alloy steels
Alloy steels	Alloy steels are used in a variety of applications, including automotive components, machinery and pipelines.	Improved strength, hardness and wear resistance compared to carbon steels.	Higher than carbon steels due to the addition of alloying elements.
Stainless steels	Stainless steels are corrosion-resistant and are used in applications where corrosion resistance is critical, such as kitchen appliances, cutlery, chemical processing and medical devices.	Excellent corrosion resistance, high strength and heat resistance.	Generally more expensive than carbon and alloy steels due to the presence of chromium and other alloying elements.
Tool steels	Tool steels are used for making cutting tools, dies and molds in manufacturing processes.	High hardness, wear resistance and toughness.	Higher than carbon steels, but their specific properties justify the cost for specialized applications.
High-strength low-alloy (HSLA) steels	HSLA steels are used in structural applications, such as bridges and buildings, where high strength and good weldability are required.	High strength, good toughness and improved weldability.	Generally more expensive than carbon steel but offers improved performance.
Maraging steels	Maraging steels are used in aerospace and other high-performance applications where a combination of high strength and toughness is required.	Exceptional strength and toughness, along with good corrosion resistance.	Relatively high due to the special alloying elements.

Table 4.2. *Cost comparison for steel*

If the budget allows, stainless steel might be chosen for its superior corrosion resistance and durability. If cost is a primary concern, lined carbon steel could be selected, with the understanding that the periodic maintenance of the lining may be necessary. In practice, it is also important to consult with material engineers and experts in the field to make informed decisions. Furthermore, a simple comparison is given in Table 4.2, which helps in selecting the type of steel. The selection of steel for various applications in an economic way also involves several factors such as corrosion resistance and heat resistance apart from mechanical properties.

4.5.4. *Other considerations*

a) Temperature and pressure resistance: chemical processes often involve extreme temperatures and pressures (Uher 2004). Materials must maintain their structural integrity and functional properties under these conditions to prevent leaks, ruptures or failures. Thermal expansion coefficients, thermal conductivity and pressure ratings are crucial factors in material selection.

b) Mechanical properties: different applications within the chemical industry require specific mechanical properties such as tensile strength, hardness, flexibility and fatigue resistance. For instance, reactor vessels might require materials with excellent fatigue resistance (Uher 2004).

c) Availability and sourcing: materials must be readily available from reliable sources to maintain a consistent supply chain. Dependence on rare or difficult-to-source materials can lead to production delays or increased costs due to scarcity.

d) Regulatory compliance: the compliances include considerations for safety, health, environmental impact and specific industry certifications to ensure the materials used meet legal requirements. The American Society for Testing and Materials (ASTM) is a global standard body that creates and disseminates voluntary consensus technical standards for a variety of goods and services (ASTM 2023). The American Iron and Steel Institute (AISI) plays a crucial role in the creation and upkeep of standards for items made of steel and iron, such as pressure vessels and storage tanks (ASTM 2023).

e) Lifecycle analysis: a comprehensive analysis of the material's lifecycle – from extraction or manufacturing to disposal or recycling – helps assess its overall impact on the ecological footprint. It considers factors such as energy consumption, emissions and waste generation at each stage.

f) Design considerations: apart from material selection, the design of equipment and structures also plays a pivotal role (Uher 2004):

– Process compatibility: design materials and systems that align with the chemical processes they will encounter. This involves understanding the specific

chemical reactions, temperature ranges, pressures and potential hazards the materials will be exposed to. Ensure compatibility to prevent corrosion, degradation or any adverse effects on the product or the equipment.

– Safety measures: safety is paramount in the chemical industry. Design materials and equipment with built-in safety features such as leak detection and containment systems to prevent accidents or process hazards. Emergency shutdown systems and proper ventilation should also be part of the design considerations.

– Maintenance and reliability: design for easy maintenance, inspection and repair. Accessibility to critical components and routine maintenance points is vital to minimize downtime. Implementing predictive maintenance technologies can enhance reliability by detecting potential issues before they cause significant problems.

– Scalability and flexibility: design systems that can scale up or down easily based on production demands. Flexibility allows for adaptation to changing market needs or technological advancements. Modular designs facilitate easier expansion or modifications without disrupting the entire system.

– Equipment compatibility: consider compatibility with existing equipment and infrastructure. Designs should seamlessly integrate with the current setup to minimize modifications and additional costs (Ashby and Jones 2012). Compatibility ensures smooth operation and reduces downtime during installation or upgrades.

– Heat transfer and insulation: efficient heat transfer is crucial in many chemical processes. Design materials and systems with optimal heat transfer properties to improve energy efficiency. Additionally, proper insulation helps in maintaining process temperatures and conserving energy (Brown et al. 1997).

– Material handling and ergonomics: considering the ease of material handling, especially for substances that may be hazardous, designing equipment and systems with ergonomic considerations to ensure the safety and efficiency of operators plays an important role. Proper ergonomics reduce the risk of injuries and improve overall productivity.

– Waste management and environmental impact: design with a focus on minimizing waste generation and its subsequent environmental impact. Incorporating systems for effective waste treatment, recycling or safe disposal of by-products are indeed parameters to focus on here.

In conclusion, selecting materials in the chemical industry requires a comprehensive understanding of the specific operational requirements, safety standards, environmental impact and long-term economic considerations. Collaborations between material scientists, engineers, regulatory experts and field specialists are pivotal in making informed decisions that balance these multifaceted criteria.

4.5.5. *Metals and nonmetals*

Ferrous metals, which contain iron as their primary constituent, are widely applied in chemical storage tanks and pressure vessels due to their favorable mechanical and corrosion resistance properties. Some common ferrous metals used for these applications include carbon steel and stainless steel. They are described in Table 4.3 along with other such metals.

When selecting ferrous metals for chemical storage tanks and pressure vessels, factors such as the type of chemical involved, operating conditions, required strength and budget constraints must be considered. Additionally, proper maintenance and periodic inspections are crucial to ensure the longevity and safety of these vessels. In general, in the chemical industry, various ferrous metals are commonly used as materials for equipment and infrastructure construction due to their mechanical properties, corrosion resistance and cost-effectiveness. There are several key ferrous metals and their applications in the chemical industry:

– Stainless steel, particularly 316-grade steel, is widely used in the chemical industry for equipment such as storage tanks, piping, reactors and heat exchangers. It offers excellent corrosion resistance, even in aggressive environments containing corrosive chemicals (Rao et al. 2020).

– Carbon steel (grade: A516 (for pressure vessels)) is commonly used in the construction of pressure vessels, storage tanks and structural components. It is cost-effective. However, carbon steel is more susceptible to corrosion than stainless steel and may require protective coatings or linings for corrosive environments (ASTM 2023).

– Alloy steel (reference grade: A387 (for pressure vessels)), which contains additional alloying elements for improved mechanical properties, is used in high-temperature and high-pressure applications. Alloy steel pressure vessels and components can withstand more extreme conditions than carbon steel (Ashby and Jones 2012).

– Cast iron is used in certain applications where its properties, such as good machinability and heat resistance, are advantageous. It may be used in valves, pumps and some types of piping.

– Ductile iron (ASTM A395), also known as nodular cast iron, is valued for its strength and ductility. It is used in piping systems, fittings and pumps in chemical processing plants (ASTM 2023).

– Hastelloy alloys (C-276), although not purely ferrous (they contain a significant amount of nickel), are corrosion-resistant alloys used in highly corrosive environments. Hastelloy C-276, for example, is used in equipment for handling strong acids and corrosive chemicals (ASTM 2023).

S no.	Ferrous metal	Applications and advantages	Technical remarks
1	Carbon steel	Applications: carbon steel is commonly used in chemical storage tanks and pressure vessels for storing a variety of liquids and gases, including corrosive substances. Advantages: 1. Cost-effective: carbon steel is generally more economical than stainless steel. 2. Adequate strength: carbon steel has sufficient strength to withstand the pressure requirements of many applications.	Corrosion susceptibility: carbon steel is prone to corrosion, especially in the presence of aggressive chemicals. Proper protective coatings or linings are often necessary. Limited resistance to certain chemicals: it may not be suitable for storing highly corrosive substances without additional corrosion protection measures.
2	Stainless steel	Applications: stainless steel is widely used in chemical storage tanks and pressure vessels where corrosion resistance is crucial, such as in the pharmaceutical and food industries. Advantages: 1. Corrosion resistance: stainless steel exhibits excellent corrosion resistance, making it suitable for handling a wide range of chemicals. 2. Hygienic properties: stainless steel is easy to clean and maintain, making it suitable for industries with stringent hygiene requirements. 3. High strength: stainless steel offers high strength and durability.	1. Cost: stainless steel is generally more expensive than carbon steel. 2. Specific alloy selection: different stainless steel alloys are available with varying levels of corrosion resistance. The appropriate alloy should be chosen based on the specific chemicals involved.
3	Duplex stainless steel	Applications: duplex stainless steel, which combines the benefits of austenitic and ferritic stainless steels, is used in applications where higher strength and corrosion resistance are needed. Advantages: 1. Improved strength and corrosion resistance: duplex stainless steel provides a balance of strength and corrosion resistance. 2. Cost-effective compared to some high-nickel alloys.	Considerations: Alloy selection: choosing the right duplex stainless steel alloy is crucial based on the specific application and chemical environment.
4	Alloy steels	Applications: alloy steels, which contain various alloying elements, may be used in specialized applications where specific mechanical or corrosion-resistant properties are needed. Advantages: Tailored properties: alloy steels can be designed to provide specific properties, such as increased strength or improved corrosion resistance.	Considerations: Selection based on application: the choice of alloy steel should be based on the specific requirements of the chemical storage or pressure vessel application.

Table 4.3. *Metals and their usages*

On the other hand, we can look at the major pieces of equipment and their preferred construction material. For example:

1) Carbon steel or stainless steel tubes in heat exchangers efficiently transfer heat in chemical processes, and they are used in pumps and valves for handling highly corrosive chemicals.

2) For reaction vessels, carbon steel is used where reactors incorporate chemical reactions involving high temperatures and pressures.

3) The control equipment, structural support, catalyst support, etc., are made up of stainless steel.

Furthermore, non-ferrous metals (aluminum, copper, titanium, zinc, lead and magnesium) and their alloys are chosen based on their specific properties to meet the requirements of different chemical processes. Their roles include providing corrosion resistance, electrical conductivity, thermal conductivity and structural strength in various applications within the chemical industry. The selection of non-metals in chemical equipment and design is driven by their unique properties, including corrosion resistance, electrical insulation, chemical inertness, temperature resistance and specific performance characteristics, all of which contribute to the overall efficiency, safety and longevity of chemical processes.

– Plastic: plastics such as polyvinyl chloride (PVC), chlorinated polyvinyl chloride (CPVC) and polypropylene are commonly used for the fabrication of chemical piping systems. High-density polyethylene (HDPE) and polypropylene are frequently used in the construction of chemical storage tanks and vessels. Plastics such as polytetrafluoroethylene (PTFE) and polyvinylidene fluoride (PVDF) are used in the manufacturing of chemical pumps and valves. Plastics such as polypropylene and polyethylene are used in the fabrication of laboratory equipment such as beakers, flasks and trays. Plastics such as PTFE are used for gaskets and seals in chemical equipment due to their excellent chemical resistance. Fluoropolymers such as PTFE and PFA are used to line the interiors of chemical equipment such as reactors and vessels to protect against corrosion. Plastics such as polyvinyl chloride (PVC) and fiberglass-reinforced plastics (FRP) are used in the construction of ducting and ventilation systems in chemical plants (Mallinson 2020).

– Rubber: the use of rubber in chemical equipment and process plants is driven by its corrosion resistance, chemical inertness, flexibility, sealing capabilities, abrasion resistance and other valuable properties. Rubber components contribute to the overall efficiency, safety and reliability of chemical processes. The diverse applications of rubber in chemical plants highlight its versatility and effectiveness in addressing various challenges posed by corrosive chemicals, mechanical stresses and

environmental factors within the industrial setting (Chandrasekaran 2010). Rubber has applications in lining and coating to protect metal surfaces in equipment such as tanks, pipes and valves from corrosive chemicals. It is also used in gaskets and seals to prevent leaks. Rubber expansion joints are used to absorb movements, vibrations and thermal expansion in piping systems. They help prevent stress on the equipment and maintain the structural integrity of the system. Rubber conveyor belts are used to transport bulk materials within chemical plants. Flexible rubber hoses and tubing are commonly used for the transfer of chemicals within plants. Rubber water is used in the manufacturing of pump components, such as diaphragms and seals, where chemical compatibility and elasticity are essential for efficient pumping and sealing. Rubber is used in anti-vibration mounts to isolate and dampen vibrations produced by rotating equipment, reducing noise and preventing damage to the machinery and surrounding structures (Schaefer 2010). Rubber steel is an effective electrical insulator. In chemical plants, it is used in the production of electrical insulation mats, cable insulation and other components to prevent electrical hazards. Rubber flooring and matting provide a non-slip surface and protect workers from chemical spills and splashes. Rubber linings are applied to the interior surfaces of tanks and other pieces of equipment to protect them from corrosion and chemical attack.

– Glass: the unique properties of glass, such as transparency, inertness and corrosion resistance, make it an invaluable material for ensuring the safe and efficient handling of various chemicals and processes. Chemical reactors, storage tanks and laboratory equipment use glass as their main body constituent. Glass coatings are applied to equipment and vessels to provide a protective layer against corrosion. Glass materials are used in the construction of various sensors and instruments for measuring parameters such as pH, conductivity and temperature. The transparency of glass allows visual inspection of various chemical processes. In photochemical reactions or processes where UV light is needed, glass vessels allow the transmission of light without interference.

– Carbon: carbon materials, such as carbon steel, are often used in chemical processing equipment due to their resistance to corrosion by many chemicals. Catalyst support: carbon supports are used in various chemical reactions, providing a stable and inert substrate for catalyst deposition. Carbon-based electrodes are used in electrochemical processes, including electrolysis and electroplating (Vandeginste 2022). Carbon fibers and composites are used to construct lightweight and high-strength components in chemical equipment, improving efficiency and durability.

– Ceramic materials: ceramic materials, including alumina and zirconia, exhibit excellent corrosion resistance, making them suitable for vessels and equipment exposed to corrosive chemicals (Sakka 2013). Ceramics can withstand high temperatures, making them suitable for chemical process applications, such as furnaces and reactors. They are also used as an insulator in various items of

chemical equipment to prevent heat transfer and maintain temperature control. Ceramics serve as carriers for catalysts in chemical reactions due to their stability and inert nature.

– Graphite: graphite is often used in heat exchangers due to its high thermal conductivity and resistance to corrosion. Graphite electrodes are essential in electrolysis and electroplating. Graphite-based materials are used in seals and gaskets because of their chemical inertness and ability to withstand high temperatures and pressures. The lubricating properties of graphite make it suitable for application in valves and other moving parts within chemical equipment (Dubey et al. 2023).

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5

Hydrogen Production Pathways and Role of Catalysts

The worldwide shift toward decarbonization and energy security has led to a surge in interest in hydrogen as a clean and sustainable energy source. This chapter explores the various methods used to produce hydrogen as well as the underlying mechanisms that power these systems. This encompasses both established and novel techniques, such as photocatalytic water splitting, biomass gasification, steam reforming (SR), membrane reformer, electrolysis and thermochemical cycles. The latest advancements, efficiency, scalability, environmental impact and integration possibilities into renewable energy systems are all considered for each technology. Furthermore, this chapter describes the basic chemical and physical processes involved in catalysis that regulate the production of hydrogen, tackling significant issues including byproduct formation, greenhouse gas emissions, hydrogen yield and resource constraints. This chapter seeks to provide an in-depth analysis of the present and potential hydrogen production paths, catalysts used for different processes as well as insights into the technological breakthroughs.

5.1. Introduction

Hydrogen is a key component for building a sustainable energy future since it is a clean energy carrier that possesses high adaptability. There has been a huge increase in the amount of greenhouse gas emissions, especially COx, that have been released into the atmosphere as a result of the high energy consumption. In addition to this, the combustion of fossil fuels is also a big concern (Muradov 2015). For the energy sector, the concern is whether we will be able to sustain life in the future based on existing energy supplying techniques such as the combustion of fossil fuels. This requires the world to have an efficient energy system by minimizing the

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concentration of harmful gases in the atmosphere due to the combustion of fossil fuels and also needs an alternative and innovative way to produce energy.

To overcome this problem, one of the possible innovative ways of utilizing an efficient energy system is to use a PEMFC (Proton Exchange Membrane Fuel Cell). PEMFCs are promising resources for power applications due to no greenhouse gas emissions (Basile et al. 2008). Hydrogen is considered to be an efficient source of fuel cells for power generation. Natural gas reforming produces approximately 50% of hydrogen gas, 30% is derived from chemical and refinery industries, and 18% is from gasification of coal and other resources (Basile et al. 2008; Muradov 2015). Hydrogen has high fuel density, and only the formation of water takes place after the combustion of it; however, it is difficult to store. Storage of pure hydrogen as a gas requires high pressure, whereas in the liquid phase, it can be stored at –253°C (Lindstorm and Petersson 2002). Instead of storing the highly flammable gas, it can be generated on-site or on-board to avoid storage and transportation limitations. Various methods can be used for the hydrogen generation, including steam reforming of hydrocarbons, electrolysis, biological hydrogen production, photochemical water splitting and pyrolysis. However, when considering on-site or on-board hydrogen generation, steam reforming of hydrocarbons such as methane, methanol, ethanol and glycerol is considered advantageous. Methanol is considered to be one of the most promising chemical commodities due to its high hydrogen–carbon ratio, low reforming temperature, easy availability, easy to store and lower boiling point. The lack of carbon–carbon bonds in the process lowers coke production. Therefore, methanol steam reforming is a practical and promising route for on-board hydrogen generation (Lindstorm and Petersson 2002; Chang et al. 2012). Methane (CH_4) is also a widely used feedstock for steam reforming due to its prevalence as the primary constituent of natural gas which is easily available and inexpensive. Hence, methane steam reforming (MSR) is also promising for hydrogen production which is a well-recognized and economically viable technology for large-scale industrial hydrogen production. Overall, this chapter describes the numerous hydrogen production systems, providing a thorough description of their mechanisms, benefits, limitations and roles in the global energy transition.

5.2. Hydrogen production mechanisms

5.2.1. *Methanol steam reforming*

There are various mechanisms of hydrogen production, each having its own advantages and disadvantages. Hydrogen production by the conversion of methanol includes several processes such as methanol decomposition (reaction 1), methanol

partial oxidation (reaction 2) and methanol steam reforming (reaction 5) (Chang et al. 2012). Methanol decomposition and its partial oxidation produce lower hydrogen yield and high CO concentration in the product stream but methanol steam reforming produces a low concentration of CO and becomes a great source of attraction for supplying hydrogen.

In comparison with other fuels, methanol shows various advantages in hydrogen production such as the presence of only one carbon atom and no C–C bond cleavage. When the reforming temperature of methanol is compared with the other hydrocarbons such as methane, i.e. the reforming temperature of methane is above 500°C, and that of ethanol is 600°C, reforming of methanol is possible even at low temperatures (200–300°C). The methanol steam reforming reaction takes place with two simultaneous reactions: methanol decomposition (reaction 1) and water–gas shift reaction (WGSR) (reaction 4). Apart from the unreacted methanol and water mixture, this process also consists of some small traces of carbon monoxide.

We consider hydrogen production for the application of PEMFCs. The drawback of PEMFCs is that these are useful at CO concentration less than 10 ppm to avoid poisoning of Pt-based catalysts. Carbon dioxide formation should be minimized (Lindstorm and Petersson 2002; Basile et al. 2008; Muradov 2015). CO formation is the primary disadvantage of the methanol steam reforming process. An excess amount of CO generation can also deteriorate the catalyst activity, which can cause poisoning. It can poison the membrane fuel cell catalyst; therefore, this problem is very crucial. Otherwise, it will deteriorate the catalyst with fuel cells of low temperature (Sa et al. 2010). The literature has been proposed for hydrogen production from methanol steam reforming in both conventional reformers and membrane reformers (MR). A remedy is to minimize CO formation using a suitable catalyst with low CO selectivity. So, it leads to the importance of preparation of a suitable catalyst for the methanol steam reforming.

Methanol steam reforming is still a viable method for producing hydrogen, particularly for decentralized, portable and small-scale systems. The process has become much more efficient, scalable and viable after recent developments in carbon monoxide suppression, low-temperature reforming, reactor design and catalytic materials. As interest in using renewable methanol as a feedstock increases, MSR could be crucial to the shift to sustainable hydrogen energy.

5.2.2. *Methane steam reforming*

Methane steam reforming (MSR) is an extensively used process for the production of industrial-scale hydrogen. Due to its well-established technology and abundance of methane-rich feedstock, such as natural gas, it is extremely efficient

and cost-effective. However, it has the considerable disadvantage of emitting carbon monoxide (CO) as a by-product, making it less environmentally suitable. The main disadvantage is that carbon monoxide is produced as a by-product, which contributes to greenhouse gas emissions. The process of steam reforming natural gas is crucial in the generation of hydrogen gas. In recent years, a major portion of hydrogen gas has been generated from MSR. Almost 50% of hydrogen has been recently generated via this process (Kalamaras and Efstathiou 2013). In the initial stage, methane reacts with steam to generate hydrogen and carbon monoxide. The carbon monoxide (CO) generated in the initial reaction reacts with additional steam to yield additional hydrogen and carbon dioxide in the subsequent step. The final mixture contains high hydrogen yield, carbon dioxide and some contaminants of carbon monoxide. MSR (reaction 6) operates under harsh operating conditions such as high temperature (500–900°C) and pressure (up to 20 bar) followed by the water–gas shift reaction (reaction 4).

Recently, the conversion of methane to hydrogen was performed in conventional reactors (CR), which was followed by water–gas shift reactors (WGSR) and was further followed by various H_2 separation and purification units (Iulianelli et al. 2016). Due to exothermic reaction conditions of water–gas shift reaction, it leads to a high concentration of CO (higher than 5%). Therefore, the WGS reactor is required to convert undesired CO into CO_2 and to reduce the amount of CO using WGS reactions. This shift converter is with a high-temperature unit followed by another low-temperature shift unit. HT-WGS is loaded with a high-temperature operating catalyst, whereas LT-WGS is loaded with a low-temperature operating catalyst.

Afterward, hydrogen separation and purification are done by pressure swing adsorption (PSA), cryogenic distillation, etc., as shown in Figure 5.1. Typically, the carbon dioxide is separated and extracted from the mixture using PSA or amine-based solvents. The residual contaminants are eliminated further to obtain high-purity hydrogen. This may include a final purification phase including technologies such as membrane separation.

MSR is a very efficient process that can convert a significant amount of the feedstock into hydrogen. Due to its widespread industrial application and well-established technology, it benefits from economies of scale. As a result, paired with carbon capture and storage (CCS) technology, MSR is environmentally favorable. As MSR uses methane or natural gas as a feedstock, it poses questions regarding long-term sustainability and energy security. Hence, the implementation of process intensification in methane steam reforming through a membrane reformer offers a novel approach that ensures a high degree of selectivity toward hydrogen production while minimizing the yield of carbon monoxide (Dittmar et al. 2013).

Nevertheless, the outlet stream contains high CO content. Therefore, the synthesis of a suitable catalyst with low CO selectivity for MSR is a crucial parameter.

Methanol decomposition

$$CH_3OH \leftrightarrow CO + 2H_2, \Delta H_{298K} = 90kJ/mol \quad [5.1]$$

Methanol partial oxidation

$$CH_3OH + 0.5O_2 \leftrightarrow 3H_2 + CO_2, \ \Delta H_{298K} = 49.4kJ/mol \quad [5.2]$$

Methane dry reforming

$$CH_4 + CO_2 \leftrightarrow 2H_2 + 2CO, \Delta H_{298K} = 247.3kJ/mol \quad [5.3]$$

Water–gas shift reaction

$$CO + H_2O \leftrightarrow CO_2 + H_2, \Delta H_{298K} = -41kJ/mol \quad [5.4]$$

Steam reforming reactions

$$CH_3OH + H_2O \leftrightarrow CO_2 + 3H_2, \Delta H_{298K} = 49kJ/mol \quad [5.5]$$

$$CH_4 + H_2O \leftrightarrow 4H_2 + CO2, \Delta H_{298K} = 165kJ/mol \quad [5.6]$$

$$C_2H_5OH + 3H_2O \leftrightarrow 6H_2 + 2CO_2, \Delta H_{298K} = 174kJ/mol \quad [5.7]$$

$$C_3H_8O_3 + 3H_2O \leftrightarrow 7H_2 + 3CO_2, \Delta H_{298K} = 122.89kJ/mol \quad [5.8]$$

Under high-temperature and -pressure conditions, catalyst deactivation could take place due to the fouling of a catalyst.

Another problem of methane steam reforming is carbon deposition which affects the catalyst performance and can also lead to catalyst breakdown and carbon deposits which can result in a shutdown of the plant (Rostrup-Nielsen and Bak Hansen 1993). This problem can be controlled by improving the catalyst activity.

One of the main areas of the present study has been the development of extremely active catalysts for low-temperature methane steam reforming (below 700°C).

The goal of these catalysts is to increase hydrogen yields and methane conversion rates at lower temperatures.

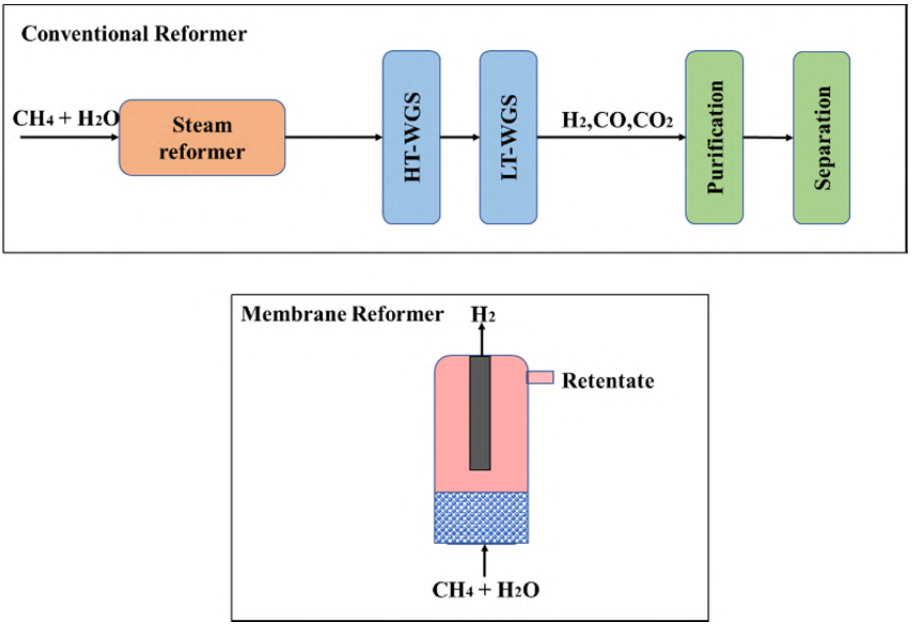


Figure 5.1. *Conventional reformer versus membrane reformer technology for hydrogen production via methane steam reforming. For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

5.2.3. *Ethanol steam reforming*

Ethanol steam reforming (ESR) is an attractive and economical process which is used for hydrogen production. It is easily available from biomass, non-toxic and easy to store. The CO_2 emissions generated during steam reforming can be absorbed through the growth of biomass (Biswas and Kunzru 2007). Steam reforming of ethanol is an endothermic process. Therefore, high heat energy is required for hydrogen production. Hence, the main challenge is to minimize the heat energy. Catalysts play a crucial role in minimizing the amount of heat energy required. Various parallel reactions occur such as the decomposition of ethanol, dehydration, dehydrogenation, methane reforming, water–gas shift reaction, etc. One of the major disadvantages of steam reforming of ethanol is again the coke deposition on the surface of the catalyst which may occur via the cracking of ethylene and ethanol decomposition. The C–C bond in the ethanol is responsible for the highly endothermic nature of the reaction. The high-temperature conditions enhance the CO formation, but for PEMFCs, the concentration of CO is a major issue; it should be less than 10 ppm to avoid the poisoning of Pt electrodes. So, this needs a final purification unit. Research has shown that the primary reaction for noble metal

catalysts used in ESR is the dehydrogenation of adsorbed ethanol (reaction 7) (Panagiotopoulou and Verykios 2012).

In conclusion, more effective and sustainable hydrogen production is being made possible by the most recent developments in ethanol steam reforming, notably in the areas of reactor design, process integration and catalyst development. With the increasing availability of renewable ethanol, ESR may be crucial in facilitating the shift to a low-carbon hydrogen economy.

5.2.4. *Glycerol steam reforming*

Biodiesel is a high-quality fuel that can be produced by transesterification of triglycerides. Glycerol is a by-product generated during the process of producing biodiesel. The transesterification process yields a total of 1.4 million tons of glycerol. Various techniques have been considered for glycerol usage such as hydrogenolysis, gas phase reforming and etherification.

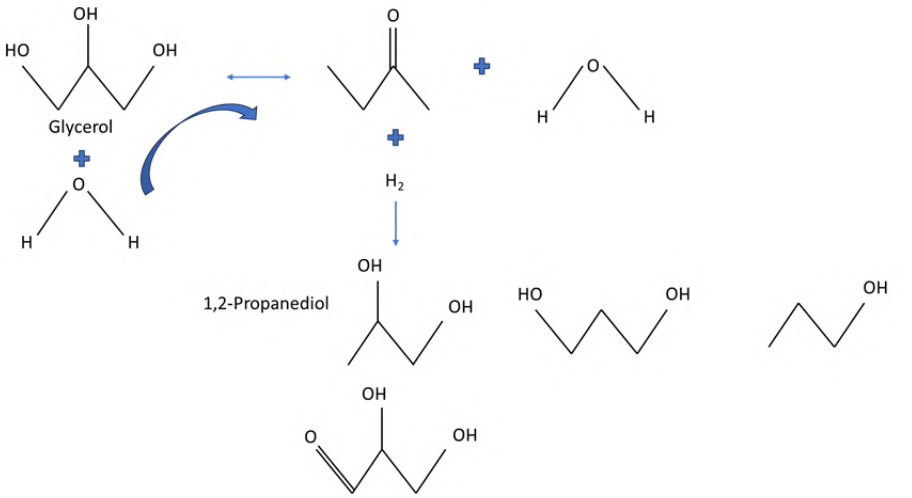


Figure 5.2. *Possible products of glycerol*

The various products that can be produced from glycerol conversion are represented in Figure 5.2. Glycerol is converted to products such as ethylene glycol, 1,2 propanediol and 1,3 propanediol through different routes such as steam reforming, hydrogenolysis, dehydration, dry reforming, etc. (Papageridis et al. 2016; Soares et al. 2016). Due to some impurities present in crude glycerol, it cannot be used directly in applications. Therefore, the purification process for crude glycerol is

a crucial step for most of the applications. However, in biodiesel production, glycerol faced a crisis due to its too-expensive purification processes. Purification through distillation is an expensive process. The steam reforming process is the common and favorable process because of the direct removal of hydrogen. This process has an endothermic nature and operates at high temperatures and pressure. The process of steam reforming of glycerol involves the decomposition of glycerol and then reaction with water–gas shift. The overall reaction of glycerol steam reforming (GSR) is represented in (reaction 8) (Dou et al. 2014).

In previous studies, GSR has been catalyzed with different types of metals such as transition and noble metals. Among transition metals, the catalyst based on nickel (Ni) was discovered to be the most effective catalyst for the process of glycerol steam reforming. The GSR is strongly affected by glycerol/water ratio, temperature and pressure.

Due to the increasing availability of glycerol from the manufacturing of biodiesel, recent advancements in glycerol steam reforming (GSR) have concentrated on increasing its efficiency for hydrogen production. The synthesis of novel catalysts and process condition optimization are two of the main developments. Although the majority of research has been carried out in laboratories, there has been a recent focus in testing GSR at semi-industrial scales. This involves optimizing gas flow and hydrogen mole ratios by assessing the effects of temperature and catalyst loading. These kinds of research are crucial for advancing the technology to practical uses.

5.2.5. *Pyrolysis*

Pyrolysis is a thermal decomposition process that can be used to produce hydrogen from organic feedstocks such as hydrocarbons, biomass or polymers. It produces hydrogen-rich gases by operating at high temperatures in the absence of oxygen. Pyrolysis can efficiently use waste materials, addressing waste management as well as energy generation. It also has the potential for carbon collection and utilization, which makes it an appealing choice for long-term hydrogen generation (Shafizadeh 1982). It is still not commonly used, and research is being conducted to improve its efficiency, scalability and cost-effectiveness. The selection of appropriate reactor materials might be difficult when operating at high temperatures.

The development of environmentally friendly hydrogen generation technology is critical to the global effort to battle climate change and transition to clean energy sources. Each technique presented in this chapter has its own set of benefits and drawbacks, making it ideal for specific applications and conditions. The process of producing hydrogen is influenced by parameters such as feedstock availability,

energy supply, efficiency and environmental concerns. As technology advances, a mix of these technologies will almost certainly play a critical part in establishing a greener, more sustainable future fueled by hydrogen. Continuous research and development are required to overcome existing obstacles and realize hydrogen's full potential as an energy carrier. Using catalysts to enhance product quality is one of the most significant developments, especially for bio-oils. In order to improve the conversion efficiency and lower the oxygen content of bio-oils and increase their compatibility with conventional fuels, catalysts such as silica alumina and HZSM-5 are used. Under the umbrella of the circular carbon economy, this process – known as catalytic pyrolysis – is being investigated as a platform technology for the value-adding of waste products such as plastic and biomass.

5.3. Renewable production methods

Hydrogen has become an essential component in the worldwide energy shift, providing a sustainable substitute for fossil fuels. As hydrogen only yields water as a byproduct when consumed, it is a perfect fuel for lowering greenhouse gas emissions. However, the processes used in its manufacture have a significant impact on how sustainable hydrogen is. While there are many ways to produce hydrogen, renewable energy sources stand out for their capacity to produce clean, sustainable energy. The main renewable hydrogen production techniques are examined in this chapter, along with their benefits, drawbacks and prospects for the future. Here is a discussion of the most promising approaches.

5.3.1. *Electrolysis*

Electrolysis is a versatile and environmentally friendly way of hydrogen production that involves the splitting of water molecules into hydrogen and oxygen using electric current. Its ability to produce high-purity hydrogen and compatibility with renewable energy sources make it particularly attractive toward hydrogen production. The two basic types of electrolysis are alkaline electrolysis and proton exchange membrane (PEM) electrolysis. The electrolyte in alkaline electrolysis is an alkaline solution, most often potassium hydroxide (KOH). It operates at relatively high temperatures and pressure, often between 50 and 70 degrees and 5–30 bar, respectively. The procedure is comprised of two major reactions. Water (H_2O) is reduced at the cathode by the addition of electrons (e-) to generate hydrogen gas (H_2) (reaction 9). Hydroxide ions (OH-) are oxidized at the anode to produce oxygen gas (O_2) and water (reaction 10). Alkaline electrolysis is well known for turning electrical energy into hydrogen with a reasonably high efficiency. It is a well-established technology that has been used in a variety of industrial applications. Over time, the use of alkaline electrolytes, particularly KOH, can cause corrosion

and degradation of materials and components. It can be difficult and expensive to scale up alkaline electrolysis systems for large-scale hydrogen generation (Mohammadi and Mehrpooya 2018). A solid polymer electrolyte membrane is used in PEM electrolysis that selectively enables protons to pass while separating hydrogen and oxygen. The operating temperature is lower, often between 60 and 80°C, and the system operates at near ambient pressure

$$\textit{At cathode} \quad 2\mathrm{H}+ \ +2\mathrm{e}- \ \rightarrow \ \mathrm{H}_2 \qquad [5.9]$$

$$\textit{At anode} \quad 2\mathrm{H}_2\mathrm{O} \rightarrow \ \mathrm{O}_2 \ + 4\mathrm{H}+ \ +4e- \qquad [5.10]$$

As PEM electrolysis systems are highly efficient, especially at partial loads, they are well suited for intermittent renewable energy sources. PEM electrolyzer's compact size enables decentralized applications, making them appropriate for a variety of contexts. They can start and stop quickly without causing considerable performance reduction. When compared to alkaline electrolyzers, PEM electrolyzers can be more expensive to construct and run. Materials used in these electrolyzers must tolerate high temperatures as well as chemical reactions, which might be difficult. The decision between alkaline and PEM electrolysis is influenced by parameters such as efficiency, system size and cost, with each approach having advantages and disadvantages (Zhang et al. 2022).

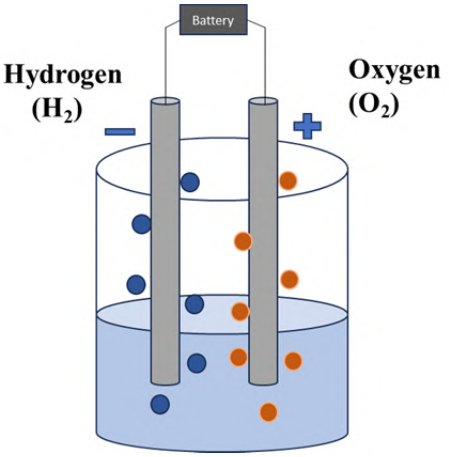


Figure 5.3. *Water electrolysis. For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

Electrolysis is predicted to play an increasingly crucial part in the transition to a greener and more sustainable energy future as technology advances. However, electrolysis is a highly energy-intensive process with high-cost limitations.

This makes hydrogen produced by electrolysis less cost-effective as compared to hydrogen produced in other ways (Kalamaras and Efstathiou 2013). The infrastructure required for large-scale hydrogen synthesis by electrolysis is less developed than that required for more common methods such as methane steam reforming.

Solid oxide electrolysis cells (SOECs) are high-temperature electrolysis devices that produce hydrogen by splitting water vapor into hydrogen and oxygen, similar to solid oxide fuel cells (SOFCs) but in reverse mode. SOECs are energy-efficient and may run on a variety of heat sources, such as waste heat from industrial processes or renewable energy sources. They possess the capacity for generating hydrogen on a large scale. The main issue is that these operate at high temperatures, which can reduce material durability and increase expenses. SOECs are still in the process of development and commercialization.

5.3.2. *Biological hydrogen production*

Biological hydrogen generation involves the use of microorganisms such as algae and cyanobacteria to produce hydrogen through the photosynthesis or fermentation processes. Microorganisms such as algae and cyanobacteria are used in biological hydrogen generation to produce hydrogen via photosynthesis or fermentation. Biological hydrogen production is still in the experimental stages, and it faces hurdles such as low production rates, scaling difficulties and the necessity for ideal microbe growth conditions.

5.3.2.1. *Photobiological hydrogen production*

Photosynthesizing microorganisms, such as algae and cyanobacteria, have the ability to spontaneously create hydrogen under certain conditions. This process is known as photobiological hydrogen generation. By using photosynthesis, these organisms use sunlight to fuel chemical reactions. They are able to redirect energy in order to split water into hydrogen and oxygen in specific environmental circumstances. This process has low efficiency and rates of hydrogen production. The oxygen sensitivity of hydrogenase enzymes prevents large-scale synthesis. A significant amount of research is required to enhance scalability and optimize the process for the stage of development.

5.3.2.2. *Dark fermentation*

In order to make hydrogen, a biological process known as “dark fermentation” uses specific bacteria to break down organic materials (such as food waste, biomass or agricultural waste) in the absence of light. Microorganisms ferment sugars, polysaccharides and other organic materials in this anaerobic process to produce

organic acids and hydrogen. This process has various challenges such as lower hydrogen yields than with other techniques. Synthesis of byproducts such as organic acids, which could require additional handling, needs ongoing study to determine the optimal bacterial strains for hydrogen production and to increase efficiency.

5.3.2.3. *Limitations of biological production of hydrogen*

The economic practicality of biological hydrogen production systems is currently limited due to several limitations, notwithstanding their potential. When compared to more conventional production methods such as steam methane reforming or electrolysis, many biological processes yield less hydrogen. Biological systems are sensitive to their surroundings; they need careful regulation of variables such as pH, temperature and nutrition supply. Although biological processes show promise in small-scale applications, it is still difficult to scale these techniques up to meet the world's demand for hydrogen.

5.3.3. *Photoelectrochemical water splitting*

Photoelectrochemical (PEC) water splitting combines photochemistry with electrolysis. When exposed to sunlight, specialized materials from electron–hole pairs drive the water splitting mechanism. As PEC directly harnesses solar energy for hydrogen production, it is a renewable and sustainable solution. It has off-grid and distributed application possibilities. The efficiency of PEC cells, cost-effectiveness and the availability of sufficient materials are all challenges. Continuous materials science and engineering research are required to increase PEC system performance and durability.

High-temperature chemical reactions are used in thermochemical water splitting to break down water molecules into hydrogen and oxygen. Concentrated solar energy or nuclear heat sources can be used to power this technology. Thermochemical water splitting is extremely efficient, particularly when using high-temperature heat sources. It is appropriate for large-scale, continuous hydrogen generation and can use a variety of heat sources, making it adaptable. The intricacy of reactor design, material selection and the high operating temperatures necessary are significant challenges. High temperatures can affect the durability of materials, necessitating research into improved materials. PEC water splitting produces hydrogen directly from solar energy without the need for a middle step. If technology can be tuned, there is a chance for great efficiency. This is currently in the experimental stage; there are still problems with material stability, cost and efficiency that need to be resolved before being widely used.

Renewable hydrogen production has a bright future ahead of it, with governments, businesses and academic institutions all over the world showing an

increasing interest in (and willingness to invest in) it. Green hydrogen technologies are developing more quickly as a result of the drive to achieve net-zero emissions by 2050. Several nations have launched national hydrogen programs to encourage the production and use of hydrogen. Renewable hydrogen is anticipated to become increasingly important to the world energy grid as technology advancements drive down costs and boost efficiency. As it may be used as a clean fuel, energy transporter and storage medium, hydrogen is a vital component of a sustainable energy transition.

5.4. Conventional and membrane reformers

The synthesis of hydrogen through steam reforming is a conventional method. Moreover, for high-grade hydrogen, a multistep integrated system is commercially used to produce pure hydrogen which generally consists of a CR followed by WGSR to promote the water–gas shift reaction for minimizing CO content (Figure 5.1). Furthermore, hydrogen separation and purification units are also used to get high-purity hydrogen. In the CR, steam and hydrocarbon initially react under the desired operating pressure and temperature conditions. These operating conditions depend on the exothermic and endothermic nature of the reaction. To carry out MSR, CR with a Ni-based catalyst is used, as explained in the Introduction. This process requires both high temperature and pressure for the reforming reaction to occur. Whereas, for methanol steam reforming, methanol and steam react in a CR over a Cu-based catalyst. However, the CO concentration is still high during steam reforming reactions in the outlet stream. Therefore, a WGSR is to be followed by a steam reformer. Two WGS reactors in series are arranged in the conventional system as shown in Figure 5.1. The first high-temperature WGS reactor was catalyzed by iron oxide catalysts for steam reforming. On the other side, the second low-temperature reactor was catalyzed by zinc oxide (Ledjeff-Hey et al. 2000). Scrubbing methods are used industrially to separate CO_2 from the outlet gaseous stream; other techniques such as PSA, temperature swing adsorption and cryogenic distillation can be adapted to produce high-purity hydrogen. However, all these processes have some limitations. Cryogenic distillation does not process for high-purity hydrogen but its advantage is its low operating temperature. Therefore, the PSA process is a suitable process for producing high-grade hydrogen (Adhikari and Fernando 2006). As discussed above, steam reforming of hydrocarbons is affected by certain limitations such as heat transfer problems and thermodynamic constraints in CR due to the endothermic nature of steam reforming reaction. Therefore, to obtain an adequate heat transfer rate, the catalyst must be packed in narrow tubes in a CR (Rostrup-Nielsen et al. 2002).

In previous years, many efforts have been made to improve the efficiency of steam reforming reactions in CR. One piece of research is to modify the catalyst

properties in terms of the type of support, catalyst deactivation, coke formation, use of promoters, etc., to make it more durable (Trimm 1997). Some studies toward the preparation method of catalyst and support type to improve the performance have been studied. Development with a new research field is membrane reformer technology. Mostly palladium membranes are used widely in this research field. Then, a new and advanced technology came with an integrated system in which both hydrogen production and separation take place in a single unit. This is also termed as process intensification (Basile et al. 2015). Many researchers found that MR is an advanced technology which has a realistic approach to the reforming process with a high yield of hydrogen production. The utilization of membrane reactors showed better performance than CR in terms of high pure hydrogen yield. Membranes are the barrier that allow the transfer of some components of a mixture while retaining some of them in terms of selectivity. The components that pass out through the membrane are called permeate, and components that do not pass are called retentate, as shown in Figure 5.1. For the separation of hydrogen, membranes should have some characteristics such as flux, which should be high, low cost and high mechanical strength. There are many advantages to membrane reactors over CR. As an MR generates and separates hydrogen in a single unit with high hydrogen purity, it reduces the number of units required which makes the system compact and can be used for on-site or on-board hydrogen generation. Additionally, there is conversion enhancement due to the Le Chatelier principle. Therefore, MR is better than the conventional reformer in terms of high performance and compact size.

In previous years, the research interest was in the application of Pd-based membranes because of the permeation selectivity of hydrogen (Lu et al. 2007). However, in the case of palladium membrane at temperature > 300°C, the major drawback is embrittlement which takes place after the phase transition of pure palladium (Pd). Although palladium membranes produce high-purity hydrogen unsaturated hydrocarbons, certain compounds can also foul the membrane surface. Therefore, a certain improvement is also required in the field of membrane technology by making it cost-effective without the deactivation of membranes.

5.5. Catalysts for hydrogen production technologies

The catalyst is of critical importance in the production of hydrogen. They accelerate the reactions by decreasing their activation energy. A catalyst is widely used to make the system more efficient and lower the temperature of the reaction. One of the primary concerns in steam reforming reactions is the deposition of coke, which has the potential to degrade and deactivate the catalyst. Moreover, a deactivated catalyst can cause blockage of reformer tubes which can further lead to the shutdown of the plant (Rostrup-Nielsen and Bak Hansen 1993). Catalyst resistance plays an important role in avoiding this problem. As already discussed, noble metal

catalysts are less associated with coke formation. However, high cost makes noble metal catalysts less attractive. Therefore, Ni-, Cu-, Fe- and Co-based catalysts are more active by modifying the promoters, supports and additives to make them durable (Trimm 1997), whereas supports such as Al_2O_3, CeO_2 and ZrO_2 are highly active for steam reforming reactions. The supports help in stabilizing the metal catalyst by preventing the agglomeration and sintering of particles. The support also provides the surface area for metal dispersion. Therefore, metal support interaction is crucial in influencing the catalytic performance. Other parameters such as metal dispersion on catalyst support, surface area, catalyst particle size and catalyst durability also affect the catalytic performance. For methanol steam reforming, copper-based catalysts are very selective (Breen and Ross 1999; Lindstorm and Petersson 2002). Group 8–10 metals also show high stability and selectivity for methanol steam reforming. Some studies show the incorporation of promoters, while some of them focus on the preparation method of catalyst. For highly active copper-based catalysts, smaller particle size, high copper dispersion and surface area of metal are the points to be considered for steam reforming reaction. Several preparation methods for the copper-based catalyst are found in the literature review (Table 5.1).

It can be concluded that alloy formation takes place due to metal–metal interaction. Lindstorm and Pettersson (2002) reported that monolithic catalysts for methanol steam reforming potentially work for the on-board production of hydrogen. They observed that the best result with the perspective of high hydrogen yield, Cu60/Zn40 shows a 60% hydrogen yield at 210°C and CO concentration below 1%. None of the catalysts achieved complete conversion. Yang et al. (2011) studied that the ZnO–Al_2O_3 catalyst was found to exhibit good catalytic activity at high temperatures and promising catalyst because of its high thermal stability for steam reforming of methanol. The incorporation of zirconium in the catalyst was observed by Agrell et al. (2003). They observed that the incorporation of ZrO_2 enhances catalytic performance, whereas, with the addition of copper, the metallic surface is easily oxidized.

Das et al. (2015) reported that copper-impregnated ceria–zirconia catalyst prepared by surfactant-assisted co-precipitation method for steam reforming of methanol shows better activity for the Cu10/CZ60 composition. For methanol steam reforming, the Ni/ceria-based catalysts are extremely active. Although Ni/ZrO_2 produced a high H_2 production, it did not convert all of the methanol, where the Ni/CeO_2 catalyst showed a selectivity of up to 45% (Hernandez et al. 2011). Agrell et al. (2003) reported that methanol molecule adsorption is preferable on the copper surface, which is responsible for the subsequent formation and increase in the amount of CO_2. It can be concluded that a higher amount of copper contributes to better oxidation of methanol.

Catalyst	Preparation	T(°C)	BET (m^2/g)	Conversion
15Cu/7ZnO/78Al_2O_3 (Agarwal et al. 2005)	WI	200–240	129	~ 50%
10Cu/5ZnO/85Al_2O_3 (Agarwal et al. 2005)	WI	200–240	158	~ 90%
3Cu/12ZnO/85Al_2O_3 (Agarwal et al. 2005)	WI	200–240	132	~ 20%
Cu/20Ce/Al (Patel and Pant 2007)	CP	280	102	100%
Cu/10Ce/Al (Patel and Pant 2007)	CP	280		78%
Cu/Zn/Zr/Al (Breen and Ross 1999)	CP	255–345	78	100%
Cu/Zn/Zr/Al (Breen and Ross 1999)	SP	345	103	100%
12Cu/4Zn/4Zr/80Al (Patel and Pant 2006)	WI	260	153	60%
12Cu/4Zn/4Zr/80Al (Patel and Pant 2006)	CP	260	98	97%
Cu–Fe/Al_2O_3/Zn/ZrO_2 (Sharma et al. 2019)	IWI	350	167	48%
Cu/ZnO (Agrell et al. 2003)	CP	220	48.6	57%
Cu/ZnO/Al_2O_3 (Agrell et al. 2003)	CP	250–300	91.9	-
Cu/ZnO/ZrO_2 (Agrell et al. 2003)	CP	250–300	81.8	-
Cu/ZnO/ZrO_2/Al_2O_3 (Agrell et al. 2003)	CP	220	116.2	33.2%
Ni0.8–Cu0.2/ZrO_2 (Lytkina et al. 2015)	SI	300	180	100%

Table 5.1. *Catalysts used for methanol steam reforming*

It is known that noble metal catalysts and VIII group non-noble metals have less sensitivity toward coke formation. Indeed, their high cost makes the nickel-based catalyst a source of attraction for methane steam reforming. Industrially, it is the most commonly used owing to its cheap cost. As shown in Figure 5.4, it can be concluded that nickel shows the highest percentage among all of the metals used for MSR.

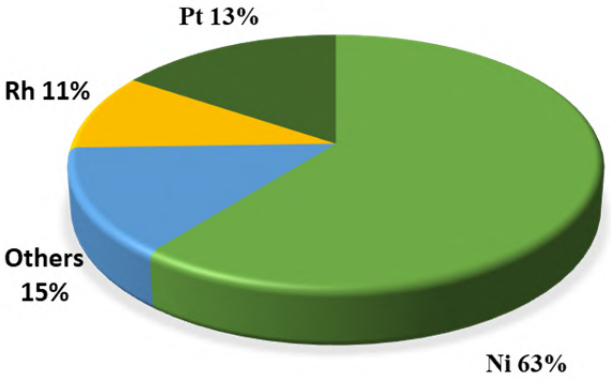


Figure 5.4. *Qualitative percentage distribution for different catalysts used for methane steam reforming. For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

John et al. (2008) identified the following catalytic order in terms of methane steam reforming Pt < Ir < Rh < Ru as it is clear that Pt is the less active catalyst among all the metals. Nieva et al. (2014) reported that Ni-based catalyst activity depends on the type of support which plays a key role in catalysis. Various support properties are responsible for the metal dispersion, sintering resistance, etc. Some authors concluded the catalyst activity of Ni-based catalysts in the following order: Ni/SiO_2 < Ni/Al_2O_3 < $Ni/ZnAl_2O_4$ < $Ni/MgAl_2O_4$ during MSR at 600°C. Due to carbon deposition, Ni/SiO_2 deactivated easily as compared to other catalysts, whereas $Ni/ZnAl_2O_4$ shows a high catalytic activity due to high sintering resistance and low carbon deposition. At 500°C, supports such as Al_2O_3 and SiO_2 allow for the oxidation of Ni-based catalysts, whereas ZrO_2 helps to stabilize the Ni-based catalyst and helps to obtain high methane conversion among all other supports owing to favoring the hydroxyl group formation during MSR. If we take into account the oxygen storage capacity, CeO_2 has been considered as a highly active support for Ni-based catalysts.

Both noble and non-noble metals are reported for ethanol steam reforming. Cu, Ni and Co were reported to be most active among non-noble metals. Liguras et al. (2003) reported the catalytic order among noble metals in the following order: Ru < Pt < Rh over Al_2O_3 support. Batista et al. (2003) studied that coke formation is mainly responsible for catalyst decay in steam reforming reactions. High conversion (> 90%) was obtained for steam reforming of ethanol with all catalysts. Results indicated that methane formation is determined by the decomposition of ethanol and

cobalt is the key component for the catalyst performance. Due to their strong catalytic activity on C–C and C–H bonds, Ni-based catalysts are the most commonly used catalysts. However, due to the sintering of Ni particles, there is insufficient tolerance for carbon deposition. This is the main barrier for ESR in industrial applications. Konsolakis et al. (2016) demonstrated that Co/CeO_2 showed excellent catalyst activity in the 400–800°C temperature range. A catalyst stability performance was observed in the order of Co > Ni > Cu > Fe. Co-based catalysts showed enhanced performance as compared to Ni-based catalysts toward steam reforming of ethanol. Lopez et al. (2012) studied that ESR and separation of hydrogen from other gases using Pd-based membranes are most attractive and 100% selectivity was measured through the membrane.

Biswas et al. (2007) reported that after the impregnation of nickel, the catalyst support area decreased. Catalysts with CeO_2/ZrO_2 showed a higher surface area as compared to CeO_2 samples. Impregnation of zirconia into the ceria lattice increased the active surface area of the mixed oxide catalyst.

By comparing the TPR profiles, it is clear that for 30% $Ni/Ce_{.41}Zr_{0.59}O_2$ and 30% $Ni/Ce_{.16}Zr_{0.84}O_2$, the reduction peak was not present at higher temperatures. They also reported that the reduction of nickel was highest (78.1%) for 30% $Ni/Ce_{.74}Zr_{0.26}O_2$ catalyst.

Catalysts based on nickel have recently gained popularity due to their accessibility and affordability. Ni-based catalysts showed high catalytic activity for C–H, O–H and C–C bonds. Moreover, Ni-based catalysts showed deactivation due to the blockage of active sites of nickel because of coke deposition. For glycerol steam reforming, a Ni-based catalyst supported on SiO_2 was found to be efficient with high glycol conversion. Soares et al. (2016) reported that Al_2O_3 is a suitable support for glycerol hydrogenolysis. Ruthenium copper bimetallic catalyst shows an alternative for 1,2 PDO production. There is a greater frequency of $Ru–Cu/ZrO_2$ than the Al_2O_3 catalyst. Similar to the work of Soares et al. (2016), Papagerisdis et al. (2016) reported that higher glycerol conversion has been achieved for Ni/Al_2O_3 catalysts as compared to that for Co/Al_2O_3 and Cu/Al_2O_3.

5.6. Conclusion and future prospects

This chapter provides a comprehensive overview of hydrogen production technologies and mechanisms, catalysts describing the various mechanisms that are focused on the development of hydrogen as an environmentally friendly and crucial energy carrier. This chapter provides an overview of their practical implementations and associated drawbacks. Electrolysis has various advantages such as high-purity hydrogen production and versatility. However, challenges include infrastructure

issues, higher costs and energy-intensive processes. Therefore, overcoming all these factors is a major concern toward the electrolysis process in the hydrogen economy, whereas pyrolysis of fuel is a highly energy-intensive process with low hydrogen yields as compared to the other processes. Photochemical water splitting (PEC) is a promising technology which converts sunlight into hydrogen fuel with less efficiency and stability. Hence, it requires some advancement in large-scale implementation. Moreover, steam reforming is a cost-effective process with a high hydrogen yield. It is also integrated with carbon capture and storage technology. Steam reforming of alcohol is the best mechanism of hydrogen production due to its low cost, no C–C bond cleavage and being economically favorable. Steam reforming of methane is also a well-established method with high hydrogen yield and economical process as methane is abundant and cheaper than other fuels. Similarly, ethanol, glycerol and other hydrocarbon steam reforming can also be used industrially but their highly endothermic nature and high coke formation make these processes limited for commercialization. On the other hand, the steam reforming process is also favorable for on-site and on-board hydrogen generation by using membrane reformer technology. Transition metal catalysts were mainly used for steam reforming such as Ni, Co, Cu and Fe with widely used supports Al_2O_3, CeO_2, ZrO_2 and MgO. Bimetallic Cu- and Fe-based catalysts on AZZ (Al_2O_3, ZrO_2, ZnO) support is the most efficient catalyst for steam reforming of alcohols. Ni and La metals on Al_2O_3 and CeO_2 supports are mostly used for MSR reactions with low CO selectivity. Various promoters can also be used with the combination of metals to enhance the catalytic activity. Hence, the steam reforming process is the most efficient process with carbon capture technology. However, the major challenge is to enhance the catalyst properties to make the steam reforming process more efficient to be used for membrane reformer technology.

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6

Maximizing Vinyl Chloride Production: An ASPEN PLUS Simulation Approach

In the current scenario, numerous chemicals are manufactured in the chemical industry. Among these, vinyl chloride ($C_2H_3Cl_2$) is characterized by its flammable, unstable and colorless nature. Vinyl chloride's major product is polyvinyl chloride (PVC), which has extensive applications in contemporary lifestyles. This work primarily focuses on optimizing the mass yield production of vinyl chloride. To achieve this, we use the ASPEN PLUS software to simulate the production process. Two categories of feedstock are used: the first is acetylene, and the second is ethylene. Temperature and pressure variations are implemented within reactors to maximize efficiency. Additionally, the deactivation of the catalyst is considered, and a normal stoichiometric reactor is used in the simulation process to attain the desired yield. The main objective of this project is to compare the results obtained from these two disparate feedstocks acetylene and ethylene within a single simulation flow process, to achieve a high yield of vinyl chloride ($C_2H_3Cl_2$).

6.1. Introduction

The chemical industry plays a pivotal role in the current world, producing various combinations of substances that influence our day-to-day lives. The conventional production of PVC from vinyl chloride remains the predominant method in the industry due to its established processes and infrastructure. Vinyl chloride (C_2H_3Cl), characterized by its flammability, instability and colorless nature, stands out as a crucial component within this society. Various research efforts are ongoing to replace vinyl chloride as the primary material in substances such as polyvinyl chloride. However, due to its established processes and infrastructure, the conventional production of vinyl chloride remains unchanged (Bartsch et al. 1975).

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Derivatives such as polyvinyl chloride (PVC) find extensive applications in modern lifestyles due to their increased demand, signifying the need to optimize the mass yield production of vinyl chloride, for which we use ASPEN PLUS simulation software to simulate the detailed production process. Enhancing efficiency can alleviate the stress of vinyl chloride production and its impact on nature. The two feed categories – acetylene and ethylene with chloride – are used in this process. Parameters such as temperature and pressure with reactors are optimized accordingly to find the best pathway with increased efficiency to produce vinyl chloride without any losses.

We will verify whether ethylene exists to obtain vinyl chloride. These changes are carefully observed and analyzed in the stream outputs and equipment to understand the deviations restricting the smooth production of vinyl chloride. The effect of catalyst deactivation is also considered in this study. The core objective of this study lies in the comparative analysis of results obtained from these disparate feedstocks within a unified simulation flow process. By subjecting acetylene and ethylene with chloride to the simulation environment, insights into their contributions to vinyl chloride production are the focus. The overarching goal is to identify the feedstock that can yield the highest production efficiency, aligning with the industry's ongoing quest for sustainability and economic viability.

The outcome of this study focuses on the strengths and limitations of using acetylene and ethylene with chloride as feedstocks for vinyl chloride production. It provides valuable insights for optimizing vinyl chloride synthesis, thereby enhancing the efficiency and sustainability of the chemical industry.

6.1.1. *Vinyl chloride*

In several chemical productions, the unique chemical production is vinyl chloride. The chemical universal formula of vinyl chloride is $H_2C = CH – Cl$. It has a 62.5 relative mass with a sickly sweet odor in nature. Also, it is a colorless and flammable gas at ambient temperature. The boiling point of vinyl chloride is -13.4°C to -13.8°C and a melting point of -153.8°C with a density of 0.911 g/mL at 25°C. Vinyl chloride is little soluble in H_2O and very highly soluble in organic solvents. It is also known as chloroethene and chloroethylene and monochloroethylene. The vapor density of vinyl chloride is 2.16, which makes it heavier than air, so inhalation, ingestion or skin absorption can affect it negatively in humans (Cowfer et al. 2006)

In the case of the latter last century, vinyl chloride is produced from the ethylene dichloride (EDC) with alcoholic caustic potash, initially by dehydrating ethylene dichloride (EDC) with alcoholic caustic potash. These industries were moved to the

hydrochlorination of acetylene. In the 1940s, ethylene became more abundant. In commercial processes, specifically the balanced ethylene route, the current menu is that 98% of the polyvinyl chloride (PVC) production is used by polyvinyl chloride and also after a huge percentage of the remaining production of polyvinylidene chloride and chlorinated solvents from polyvinyl chloride. Therefore, this production is very critical and needed in chemical industries (Braun et al. 2003).

In an acetylene-based process, a catalyst, often mercuric chloride deposited on active carbon, is used where feed gases are purified, dried and mixed before entering tubular fixed bed reactors packed with the catalyst. A slight excess of HCl is typically used to achieve a near-maximal acetylene conversion, resulting in over 98% HCl conversion with excellent selectivity towards vinyl chloride. The significant challenge with this method is the volatility of the catalyst, mercuric chloride, where deactivation of mercury-based catalysts poses a challenge to a decrease in activity in addition to the potential problem of mercury leaching from the catalyst, which can be problematic due to its toxic nature, making the acetylene route commercially less important.

Efforts to remodify another compound, ethane, are used in the production of vinyl chloride because of the very low cost of ethane in the market and the molecular symmetry of ethane poses challenges, resulting in a broad spectrum of products when chlorine is added. Now, the most promising routes involve ethylene, ethyl chloride and EDC. These are the side products and are achieved by a high incineration temperature oxychlorination that by a 100% good catalyst is used to bring a maximum level of vinyl chloride. Despite its feasibility, the main focus is on the design of the material for the oxychlorination process. The critical thing about the high-temperature reaction design is having a severe challenge. The temperature can be up to 500^{o}C, making chlorine highly aggressive to most materials. Common issues with direct production routes include poor selectivity because vinyl chloride production not only yielded a single product, but also many major side components were extracted in the production process of vinyl chloride, some with significant impact (Zichittella et al. 2021) (Wagoner et al. 1983).

Vinyl chloride burns quickly and is unstable at high temperatures. Therefore, we use compounds such as trichloroethane, trichloroethylene and tetrachloroethylene to facilitate the reaction. The transportation of vinyl chloride is a main thing that must be noted off with low loss. So, vinyl chloride is usually shipped in pressurized liquified cylinders to maintain its vapor pressure. The long-term storage of vinyl chloride poses a risk due to the formation of unstable polyperoxides. These can increase in concentration and become hazardous when exposed to atmospheric oxygen, especially in the presence of contaminants. This can result in the explosive polymerization of chlorides. The first toxicity on vinyl chloride was reported in 1970. Exposure to the unconfined liquid can cause frostbite due to evaporative

cooling. In addition to the production of vinyl chloride, the safety process should also deal with the major part when vinyl chloride has decomposed large amounts of carbon dioxide, carbon monoxide, hydrogen chloride and phosgene (carcinogenic), as these can cause damage to the human respiratory system and liver, as reported in Kielhorn et al. (2000), leading to angiosarcoma and hepatocellular carcinoma diseases, which can have long-term effects. Exceptionally high levels of vinyl chloride can accidentally cause damage to human internal organs, so safety should be a concern during its decomposition (Kielhorn et al. 2000).

Materials such as copper and steel are used for piping in the petrochemical product. Here, the steel piping material is for storage purposes and equipment handling of vinyl chloride. Also, at this particular temperature, the mixed moisture of vinyl chloride damages and corrodes the pipe. Mostly, copper is not used for vinyl chloride because the reaction between acetylene in vinyl chloride can produce an explosive acetylide when exposed to copper. The gaskets in fittings and connections are made of asbestos, Teflon, lead and carbon (Cowfer et al. 2006).

6.1.2. *Applications of vinyl chloride*

Globally, the demand for vinyl chloride is crucial as it is used to make numerous materials for the market. The chemical product is beneficial for other engineering processes. They also produce construction products, electrical products, wires, cables and fitting insulation parts, especially polyvinyl chloride, for various uses such as pipe production, coating and insulation (Carroll et al. 2011).

Approximately 95% of the world's polyvinyl chloride (PVC) production uses vinyl chloride as the raw material. PVC is used in the manufacture of pipes, medical devices and automotive parts, as well as in the manufacture of similar materials other than plastic. Only 12% vinyl chloride is used in the manufacture of plastics worldwide. It is used for flooring and ceiling coverings, as well as electrical applications such as insulation, coating of wires and in the transport sector for the upholstery of vehicles and consumer goods. In addition to being a large process, vinyl chloride is also used in a small type of daily usage products such as automotive parts and wall coverings. In addition to polyvinyl chloride production, it is also used in the manufacture of chlorinated solvents such as 1,1,1-trichloroethane as a degreasing solvent for metal equipment and for the manufacture of resins from the production of ethylene diamine (Carroll et al. 2011).

Along with the raw material, vinyl chloride produces a vinyl acetate (VA) or vinylidene chloride (Vdc) as co-monomers and major manufacturing of polyvinyl acetate (PVA) and polyvinylidene chloride (PVC), respectively. Also, it has major uses in drug production, cosmetic production and aerosol production in the market.

Vinyl chloride was once used as a refrigerant and coolant, but it is now banned due to its adverse effects on humans and environmental pollution (Cowfer et al. 2006).

6.2. Methodology

6.2.1. *Production of vinyl chloride*

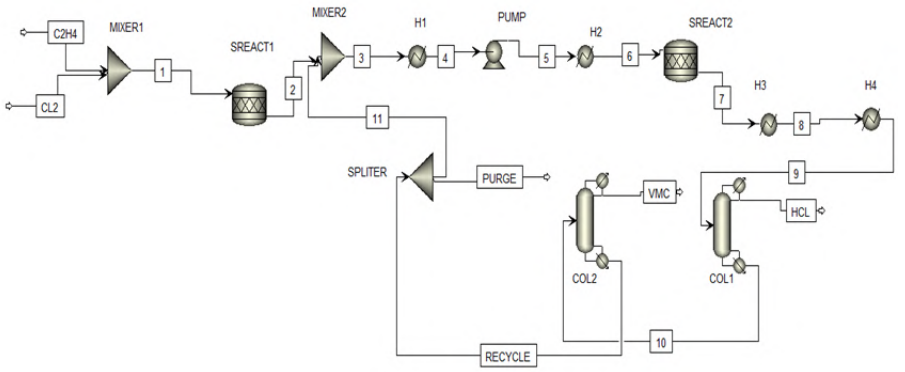


Figure 6.1. *Flowsheet of vinyl chloride from ethylene feedstock (prepared for this work)*

The production of vinyl chloride or any other product was calculated by hand before the technology was developed. We have now started to use high-technology simulation software. So, here the ASPEN PLUS software simulated the process and achieved a higher yield of vinyl chloride (Figure 6.1). The process begins with the raw materials ethylene (C_2H_4) and chlorine (Cl_2) being injected into the feed in a mixer. In the mixer, one feed is mixed at a certain temperature, with slight fluctuations occurring during the mixing process. The feed is entered into the mixer at optimum temperature (750°F) and pressure (950 psi). Then, the feed is completely mixed and, in mixer 1, the feed is mixed with a certain temperature that has some variation in the mixing, and the (1) product flows into reactor 1. The stoichiometric reactor is used in this process (Rstoic), where the catalyst was not mentioned in the reactor. In this process, the flowsheet shows two reactors for two types of reactions: endothermic and exothermic. This is because we have both cracking and chlorination reactions. Reactor 1 has an exothermic reaction in the process: in reactor 1, we have a chlorination to convert the product of ($C_2H_4Cl_2$). The exothermic reaction emits more heat energy in the reactor, resulting in a higher temperature. After the reaction, the resulting product is dichloroethane ($C_2H_4Cl_2$) with a mole fraction of 0.93.

Then, the resulting dichloroethane is fed into the mixer. Another mixer feed is recycled from the distillation column heavy key that mentions the remaining components of vinyl chloride in the column. The mixing is approximately (2 atm) and the pressure is controlled. After the mixed feed is introduced into heater 1 at 300 K, the temperature may vary slightly due to the direct heat exchange during the mixing process. The product is sent from mixer 2 to the discharge pump to increase the pressure of the feed. The discharge pump is optimized to 30 atm in the process plant. Increasing the pressure affects the flow rate, a critical factor for the vinyl chloride production reaction at high temperatures. Therefore, the pump is set to increase the pressure accordingly. Heater 2 operates at 515 K, which is higher than heater 1. The high temperature in heater 2 facilitates catalytic cracking during the heating process. Reactor 2 involves an endothermic reaction in the process.

Heater 3 and heater 4 exchange heat, as mentioned in the flowsheet. The two heaters continuously heat the feed because the stable heating before heating is used to provide good production efficiency in the field. Therefore, we use a simultaneous heater after the reactor process. After the feed is entered into column 1 and the HCL is separated, a light key is 88%. The heavy key is given to the next column 2 to separate the vinyl chloride. The vinyl chloride is separated in column 2. Column 2 is operated in 20 stages and at 10 atm pressure. The achieved efficiency of vinyl chloride is 92% in the process plant. The separation of vinyl chloride is in the high-pressure column. The reactions for the manufacture of vinyl chloride are as follows:

$$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$$

$$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$$

6.2.2. *Recycling process*

The main goals are waste reduction, resource conservation and environmental impact reduction. Industries can reuse resources through recycling, which lowers the demand for virgin raw materials. This lessens the negative effects of resource extraction on the environment and contributes to natural resource preservation. The recycling process is used to increase the efficiency of the product.

Through recycling, we can reduce energy consumption and improve the economic efficiency of the plant. Research indicates that process engineers should ensure economic strength across the industry. We should also minimize the waste of the outcome product as much as possible. This approach may help save the environment and improve the efficiency of industries. A splitter is used here to separate the purge, and the remaining material is reused for vinyl chloride production.

6.3. Results and discussion

The result is from the simulated flowsheet using an ethylene feedstock. The results show the heater 1 outlet, reactor 2, column 1 and column 2. These unit operation conversions demonstrate how efficiency has been achieved. Table 6.1 shows the heater outlet. It demonstrates that the maximum expected conversion of $C_2H_4Cl_2$ in reactor 1 is achieved due to the exothermic reaction. Heater 1 exchanges the heat with reactor 1. The efficiency began with $C_2H_4Cl_2$ used in good conversion and heat exchange.

Component	Mole fraction
C_2H_4	**0.013**
Cl_2	**0.006**
HCl	**0.000**
C_2H_3Cl	**0.005**
$C_2H_4Cl_2$	**0.974**

Table 6.1. *Result of dichloroethane after heater 2 from ethylene feedstock*

Component	Mole fraction
C_2H_4	**0.008**
Cl_2	**0.003**
HCl	**0.387**
C_2H_3Cl	**0.391**
$C_2H_4Cl_2$	**0.208**

Table 6.2. *Result of dichloroethane after the reaction at SREACT 2 from ethylene feedstock*

Table 6.2 shows the conversion of vinyl chloride and HCL from the reactor. As mentioned, reactor 2 has an endothermic reaction. Here, the high-temperature reaction is endured. Through that reaction, the main product is converted in the process field. There are various products formed in a main reactor such as mole fraction HCl (0.387), C_2H_3Cl (0.391) and $C_2H_4Cl_2$ (0.208). These are the rate reactions taken in this work result.

The result of column 1 is the separation of HCL from the raw material of the chlorine and ethylene process. In this process plant, almost better efficiency is achieved in HCL recovery. Table 6.6 shows the result of HCL. After the reactor, the

two heaters maintain the temperature gradually for better efficiency. Here, the high-temperature reactant will be fed to the column. The reactant feed is entered in the center of the distillation column to avoid flooding and leakage of the unit operation in the column. By a suitable column design, the recovery of HCl is 88% or 0.88 of the mole fraction.

Component	Mole fraction
C_2H_4	**0.019**
Cl_2	**0.003**
HCl	**0.886**
C_2H_3Cl	**0.090**
$C_2H_4Cl_2$	**0.000**

Table 6.3. *Result of column 1 light key HCL from ethylene feedstock*

Component	Mole fraction
C_2H_4	**0.000**
Cl_2	**0.006**
HCl	**0.010**
C_2H_3Cl	**0.927**
$C_2H_4Cl_2$	**0.055**

Table 6.4. *Production of vinyl chloride from the process plant from ethylene feedstock*

Table 6.4 shows the expected vinyl chloride achieved in the process. It shows that 93% of vinyl chloride is achieved in column 2. Column 2 has a certain design and a different temperature at the point. The expected vinyl chloride efficiency is achieved through a stage used in a distillation column. The results show vinyl chloride as a mole fraction of (0.927).

In the process mentioned above, the flow sheet of acetylene feedstock for vinyl chloride production was taken and compared to the ethylene process. In the acetylene feedstock process, a significant amount of energy is consumed, but it achieves high efficiency in producing vinyl chloride. The HCl and acetylene reaction were performed at a very high temperature in the reactor. The plant design is systemized in a full configuration for efficient product quality. The operating temperature and pressure are high enough. The rich steam of vinyl chloride also

existed at a low temperature of -16°C. The same simulation process is completed in that work. Table 6.5 shows the conversion of HCl and acetylene in the reactor (Akintola et al. 2020).

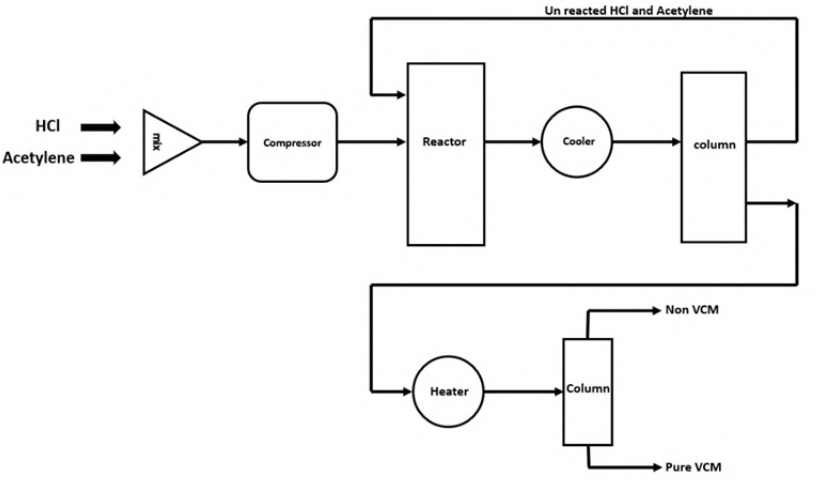


Figure 6.2. *Process of vinyl chloride production by using an acetylene feed (prepared for this work)*

Component	Mole fraction
C_2H_2	**0.980**
Cl_2	**0.000**
HCl	**0.900**
C_2H_3Cl	**0.000**
$C_2H_4Cl_2$	**0.000**

Table 6.5. *Conversion of acetylene and HCl in acetylene feedstock vinyl chloride production*

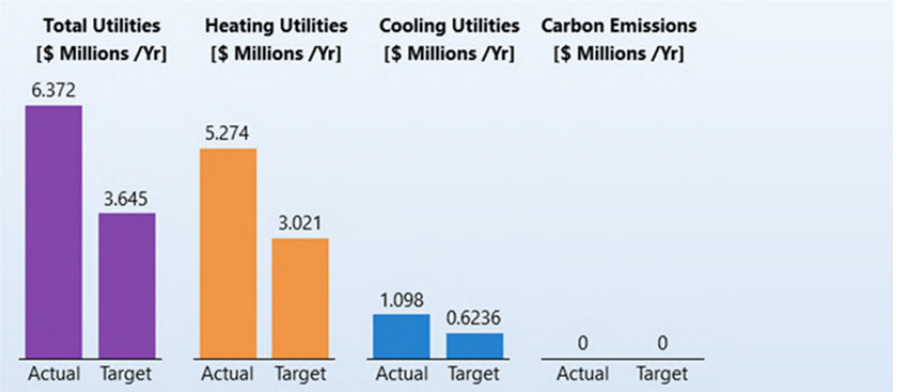
Component	Mole fraction
C_2H_3Cl	**0.99–0.10**

Table 6.6. *Production of vinyl chloride from the acetylene feedstock*

The production of vinyl chloride using acetylene feedstock yields excellent results. The work shows good conversion in an energy consumption process. Table 6.6 shows a 99% conversion of vinyl chloride. The process field is ideal.

6.4. Energy used

The ASPEN PLUS software analyzed energy utilization and the amount of energy used in producing vinyl chloride. Plant management should focus not only on the production of components but also on the economic aspects of the process plant. Figure 6.3 shows the result of the financial balance in the ethylene feed, revealing some additional lag in the design. Ethylene feedstock's actual energy is used in the process of vinyl chloride monomer (vcm). The savings are minimal, and the research will clarify the economic rate. In the simulation, the financial performance is relatively good and the market shows a very cheap product of ethylene feedstock as a production of vinyl chloride.



Summary Table

	Actual	Target	Available Savings	% of Actual
Total Utilities [$ Millions /Yr]	6.372	3.645	2.73	42.80
Heating Utilities [$ Millions /Yr]	5.274	3.021	2.25	42.72
Cooling Utilities [$ Millions /Yr]	1.098	0.6236	0.47	43.21
Carbon Emissions [$ Millions /Yr]	0	0	0.00	0.00

Figure 6.3. *Graph showing the actual and target cost to produce vinyl chloride from ethylene feedstock (prepared for this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*



6.5. Conclusion

Feedstock has a marked influence on the manufacture of vinyl chloride, affecting whether the process is energy-efficient or economical. Though science shows that acetylene allows a striking effectiveness of 99% to vinyl chloride and 90% in the case of HCl, practical and economic factors can dictate the choice of ethylene reagents. Regarding the results acquired in the ASPEN PLUS simulator, ethylene has a slightly lower conversion efficiency of 93% for vinyl chloride and 88% for HCl. Still, the presented numbers can be considered as efficient compared to the commercial standard. Another factor that makes ethylene preferred to acetylene is that it is relatively cheaper. Ethylene is usually less pricey and more accessible than acetylene; therefore, using ethylene entails reduced costs of raw materials to synthesize vinyl chloride. The lower conversion efficiency can be partially balanced by cost savings, which makes the entire process more economically viable in the long run.

Additionally, the production facilities and safety aspects also favor ethylene. Ethylene-based plants are generally more straightforward and offer fewer operational risks than acetylene plants, which use highly reactive acetylene and require several safety precautions. Other factors that add to the economic advantage of ethylene plants include cheap operational and maintenance costs. In real-world industrial scenarios and electricity generation, achieving a 99% conversion efficiency is often idealistic, and the actual efficiency is typically close to this ideal. Users of engineering services and personnel in industries should be aware of the following economic implications: the cost of raw materials, plant construction and layout, safety and overall maintenance expenses. This is slightly inferior to the efficiency of ethylene production, but the latter's economic feasibility confirms that it can be used effectively for vinyl chloride production Therefore, although acetylene, in terms of theoretical conversion efficiency, converts to vinyl chloride to a higher degree, using ethylene as a feedstock for the economical, safe plant construction and less expensive plant operation appears to be effective and viable for the large-scale production of vinyl chloride.

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7

Process Intensification and Advanced Materials

Process intensification (PI) is a fast-expanding area of study and business that has so far brought about an array of innovations within the chemical process sector. PI concentrates on a lot more small, environmentally friendly and energy-efficient devices. In addition, PI strives to develop innovation in a sustainable and less hazardous manner. Its instruments include miniaturization, novel energy methods, new separation approaches, integrated optimization and control strategies, reducing the number of tools (i.e. multiple functions into a single device), improving heat and mass transfer via advanced mixing methods as well as shorter dispersion routes, and miniaturization. Centrifugal force fields, ultrasonics, revolving electrodes and rotating cells, which can operate with or without the use of magnetic fields, are a few of the methods used for process intensification. In principle, electrolytic may be carried out with these tools without an outside potential or current. Another approach that was considered was the use of light. The synergies between process intensification (PI) and new materials are examined in this chapter, which additionally explains how their integration could end up in manufacturing procedures which are both efficient and sustainable. The developing framework for the integration of Industry 4.0, Process Intensification and Circular Chemistry will be emphasized and addressed in this chapter. It will also discuss how the data collected through this integration will be essential to the development of the next wave of Process Intensification strategies. By combining these two innovative strategies, the objectives are to increase production, minimize the effect on the environment and optimize resource use.

7.1. Introduction

Process intensification (PI), is an entirely new notion used in process design and chemical reaction engineering. PI is frequently understood as an umbrella strategy or a collection of devices designed for strengthening the effectiveness of processes in terms of improved environmental sustainability, lower output or system expenses,

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and energy efficiency. Therefore, the application of PI seeks to benefit from various tools (such as contactors, reactors and separators) and methods, such as the use of phases and alternative fluid, severe operating environments, multipurpose devices and different forms of energy, including centrifugal fields, solar, ultrasonic, light, microwave, electric and magnetic fields (Reay et al. 2013). Many reaction systems, such as chemical, catalytic and mass transport mechanisms, and, to a lesser degree, electrochemical mechanisms have seen the use of process intensification. Several definitions of process intensification from the last 25 years can be found in Table 7.1.

As far as the author is aware, a Polish magazine published the first use of the term "process intensification" (Leszczynski et al. 1973). Ramshaw et al. (1983) provided PI with an edge at Imperial Chemical Industries (ICI) in the 1980s (Law et al. 2017). There is not yet a consensus-driven definition of PI. There are also numerous additional definitions which have already been circulated in the literature. Four guiding theories for PI are given by Van Gerven and Stankiewicz (2009): 1) to achieve kinetic regimes with better conversion and selectivity, dynamically alter circumstances to maximize the efficacy of intramolecular and intermolecular events; 2) provide every molecule with an identical processing experience (e.g. uniform, gradient-free heating in a plug-flow reaction); 3) optimize the particular areas of surface where driving forces apply and optimize them at all scales (e.g. improve transfer surface area through microchannel designs); 4) make use of the synergistic effects of unfinished processes (multifunctional reactors, for instance). Although they have received little attention from the PI community, Van Gerven and Stankiewicz (2009) contend that the first item mentioned above will be the most important in the future.

The catalyst supports' topological structure (shape-selective structures, functionalized surfaces, optimized pore radii distributions and pore connectivity) and chemical routes and kinetics may all be changed at the molecular level. These things have a lot of influence on catalysis. Static mixers are one way to provide the molecules with an identical processing experience. They improve the particular interfacial area for mass transfer, while offering an almost ideal plug-flow with intense mixing. Local mixing may also be improved by using structured packings in reactors, such as foams, gauzes, monoliths and different kinds of micromixers. One possible method for achieving localized, gradient-free heating in a plug-flow reactor is using microwave heating. Better mass and heat movement (diffusion and convective transport) is the subject of the third argument raised above. Mass transfer conditions may be boosted by pressured flow in membrane-based reactors (MRs) and multiphase flow in reactors of phase-transfer catalysis aided by ultrasound. Higher mass transfer rates are also a result of shorter diffusion routes in microreactors and pore structures that are optimized for transport (Keil et al. 2007; Trogadas et al. 2016).



On an enormous scale, multifunctional devices may offer synergistic effects. A popular instance is reactive distillation (RD), which blends separation and reactions into a single column with catalytic packing. Reactant and product separation drives equilibrium-limited reactions towards greater yields. Any liquid-to-liquid separation cannot be accomplished with this procedure since the pressure and temperature requirements must be met. Chemical process engineering (CPE) uses mathematics, physics and chemistry – particularly quantum chemical approaches, as well as classical molecular simulations, classical and statistical thermodynamics, transport phenomena (such as heat and mass transfer, diffusion and fluid flow), classical mechanics, electrodynamics, chemical kinetics and numerical mathematics.

Definitions of process intensification	Definition by
System level modifications are enabled using the Process Intensification 4.0 framework. Process Intensification 4.0 boosts equipment design, predictive control and optimization by using data-driven algorithms to comprehend more physical and chemical processes.	López-Guajardo (2022)
Any development in chemical engineering that results in substantially smaller, safer, cleaner and more energy-efficient technology, or consolidates several operations into fewer devices (or an individual apparatus) can be referred to as process intensification.	Baldea (2015)
Process intensification (PI) is a comprehensive overall system-based intensifying in comparison with the conventional method of process intensification that relies on the application of methods and techniques to achieve dramatic enhancement of the effectiveness of one component or gadget.	Portha et al. (2014)
In chemical engineering, research and development, process intensification relates to an integrated approach for manufacturing and process innovations with the goal of retaining a profit, even in the face of increasing uncertainties.	Becht et al. (2009)
Technologies that consolidate numerous tasks into fewer devices (or a single apparatus) or that combine massive, costly and highly energy-intensive equipment or processes with compact, affordable and more effective ones are often referred to as process intensification.	Touris and Porcelli (2003)
The concept of decreasing the chemical plant's size needed for achieving a certain output aim is referred to as process intensification.	Cross and Ramshaw (1986)
Process intensification is the design of a very compact plant that reduces the cost of the "primary plant component" and installation.	Ramshaw and Arkley (1983)

Table 7.1. *Selected definitions from the last 25 years concerning process intensification*



In the context of productivity enhancement in the industry, productivity is defined as the relationship between the output's production and all of the inputs that are needed to complete the work at hand. This encompasses the capital value-based evaluation that was conducted throughout the development phase. Implementation and a favorable view inside the sector can only occur if a strong economic advantage can be obtained (Becht et al. 2009; Raghavan and Reddy 2014). Process safety is also very important to PI, and better process safety performance is crucial to the long-term viability of the chemical and energy industries. However, using engineering for sustainable development is a challenging endeavor due to the complexity and constant alterations of processing plants. Process safety engineering is the science of including an in-depth knowledge of the intricate interactions between chemical process technology, mechanical and process design, process control and process safety management systems in everyday engineering procedures, according to Mannan et al. (2015, 2016), who provide an overview of trends and challenges in process safety. Process intensification methods and how they can be used in different areas are presented in this study. Promises and difficulties for the future are also covered.

7.2. Process intensification technologies

The ultimate objective of process intensification is to boost the performance of procedure operations by optimizing numerous operational variables. This method may minimize energy, waste and operational costs while enhancing product quality, safety and impact on the environment. Heat transfer intensification, reaction intensification and combination intensification are a few of the instruments and techniques obtainable for process intensification (Dutta et al. 2023). Process intensification is frequently accomplished by using one of many approaches, including fluid dynamics, chemical engineering, management system engineering, simulation and modeling. Process intensification attempts to decrease the amount, cost and energy consumption of process tasks, while improving the quality and yield of the end outcome. This technique has become increasingly common in various industries where it is possible to lessen the negative environmental effects of present operations (Jadhav et al. 2023).

7.2.1. *Microreactors*

According to Moulien et al. (2004), microreactors belong to the sub-millimeter class of chemical reactors that may achieve higher reaction rates, reduced volumes and higher product selectivity. Even with extremely viscous fluids, they assist in complete mixing at high rates of flow. Increased heat and mass transfer rates in addition to precise control over the reaction volume under consideration allow for



the possibility of alternative reaction paths (Wörz et al. 2001). Catalysis, steam reforming, organic synthesis and multiphase reactions are a few of the typical uses (Jensen et al. 2001; Lin et al. 2015). Another example is the reversible polymerization manufacturing poly (vinyl butyral) at 90°C using cross-flow micro-channel reactors, which is a highly sought-after product for the fabrication of safety glasses in the automotive sector (Jensen et al. 2001). It involves the presence of an acid catalyst and viscous fluids such as poly (vinyl alcohol) and n-butanal. Phase change and precipitation issues are typically the result of the batch process's minimized reaction rate, resulting in a product yield of 20–30% (estimated in terms of butyral group concentration). A well-controlled reaction occurs at 50°C in just 56 seconds when 1,000-µm long by 500-µm wide micro-channels made of stainless steel and PTFE (Teflon) are used in a cross-flow pattern and submerged in water. After an hour of aging, the product yield has been reported to be as high as nearly 75% (Jensen et al. 2001). Good mixing performance was attained with an optimum flow-rate at a 5% solution of PVA with a maximum limit of 80 ml/min (Jensen et al. 2001). The financing requirements for different utilities could be reduced as a result of the catalyst's enhancement of the process. The insignificance of gravitational forces, scale formation resulting from material incompatibility and the expense of microfabrication are a few of its main drawbacks.

7.2.2. *Membrane distillation*

Due to its capability of minimizing throughput and energy consumption, membrane technology has served a vital role in boosting mass transfer efficiencies. It is a hybrid technique which combines conventional distillation with membrane separation (Stankiewicz et al. 2000). Approximately 60% of plants currently in operation globally use desalination units based on osmotic pressure differential (Driol et al. 2011). Yet, the brackish feed water with a high salinity level detracts from their performance. According to recent reports, approximately 100% inorganic rejection of salt was accomplished with direct contact membrane distillation with conductive heat transfer – all without requiring any additional energy (Hickenbottom et al. 2014).

7.2.3. *High-gravity processing*

Counter-current gas–liquid flow via a rotating packed bed with continuous feeding of one phase is rendered feasible by the addition of a high-gravity field through a high-speed rotor (Srivastava et al. 2023). It provides shorter interaction times over rotor packing with an improvement in mass and heat transfer rates, minimum area needs, less maintenance and lightweight equipment (Moulijn et al. 2004). The utilization of high-gravity processing techniques may meet the demand



for de-aerated seawater in oil fields for re-injection, thus avoiding blocked pipe-works near rocks producing oil. To reduce the oxygen content to the parts per billion (ppb) concentration level, a traditional vacuum stripper with a 3 m diameter and 10 m height and enormous auxiliary would be required (Peel et al. 1998). Rather, a smaller alternative would be required. For a high-gravity processing deaeration operation, a minimum pressure of 2.2 bar must be maintained to achieve successful momentum transfer to feed salt water (500 m^3 annually). To allow for the rotor's tip speed to be roughly comparable to the liquid velocity in the radial direction, the energy requirements for high-gravity processing technology have a direct connection to this process time. The oxygen level of processed saltwater samples is anticipated to have an intensification factor of 1,000 (Peel et al. 1998). Energy consumption was found to have decreased by 90% when a 400-RPM, 2.8-m long, 1.0-m diameter rotor was enclosed with inexpensive reticulated metal foam. Back mixing issues and a consequent significant pressure drop are the main downsides of this "virtual" separation column with uniformly distributed bubbles maintained throughout a 10-mm thick packing.

7.2.4. *Spinning disc reactor*

With the use of the thin liquid film creation unique to its spin disc design, spinning disc reactor (SDR) technology finds use where issues with back mixing, as in stirred tank reactors, and higher power requirements, as in high-gravity field process reactors, are eliminated. The intention is to accomplish uniform mixing in the laminar area (assumed) and an extremely brief residence period by intensifying the spatial domain (Oxley et al 2000; Moulijn et al. 2004). A liquid layer with a micrometer thickness normally lies over a spinning disc with "spiral grooves" that are exposed to high circumferential velocity (up to 1,000 RPM) in an inert atmosphere (usually nitrogen below 1 bar pressure) (Hickenbottom et al. 2014). For the purpose of keeping disc operating temperatures constant, coolants such water or ethylene glycol are used. A multiphase reaction called Darzen's reaction, which has been helpful in the development of drugs, is a prime instance. In contrast with typical batch reactors that operate at 0°C with approximately 1.5% impurity, it occurs in less than a second at 20°C with less than 0.1% impurity (Oxley et al. 2000).

7.2.5. *Compact heat exchangers*

Compact heat exchangers (CHE) increase the useable heat transfer area in relation to exchanger volume, thus decreasing the exchanger's size and investment costs. Its values vary between 300 and 700 m^2/m^3 for the liquid phase and are significantly higher for the gas phase. Common instances of hybrid reactor-heat



exchanger combinations built on printed circuit boards that improve heat transfer rates are plate or plate-fin heat exchangers (Reay et al. 2002). Heat pumps and HVAC (heating, ventilation and air conditioning) systems represent two applications for this kind of heat exchanger, (Reay et al. 2002). Over the course of the last 10 years, two noteworthy CHE designs have come into existence: Alfa Laval, Sweden's Compabloc heat exchanger, and Chart Marston, the UK's "Marbond" heat exchanger. The Compabloc plate heat exchanger is composed of laser-welded corrugated steel and has multiple passes arranged in an alternating cross-flow pattern at high turbulence. Compared with traditional shell-and-tube heat exchangers, an intensification factor of 3.5 provides a lower plant footprint for the same thermal load. Since 2001, a Slovakian ammonium nitrate production plant has been using Compabloc technology in an evaporator unit. As a result, fouling problems have lessened, heat transfer rates have risen and steam energy consumption (~ 5 MW) has dramatically dropped. The "laptop-sized" "Marbond" heat exchanger works well for multiphase chemical systems, owing to its sub-millimeter hydraulic channels and high voidage design. A significant 95% capacity drop compared with current traditional shell-and-tube heat exchangers can be obtained if a world free of corrosion is maintained (Reay et al. 2002). The CHE technique has certain limitations, notably poor inertial force participation, substantial pressure drops when using especially viscous fluids and fouling issues.

7.2.6. *Alternative energy sources*

The ability of multiple irradiations to generate significant localized heating, turbulence and chemical effects makes them suitable for use in process intensification (Stankiewicz et al. 2006). In the context of chemical engineering, we will discuss all three of them briefly here: microwave, ultrasound and plasma irradiation. We will additionally discuss some of the most recent discoveries in science that have made use of these methods.

7.2.6.1. *Microwave*

The precise and concentrated heating that takes place whenever microwave radiation is used is one of its greatest benefits. Microwaves are frequencies that sit between the infrared and radio wave segments, in the gigahertz (0.1–300 GHz) range. Microwave ovens commonly operate at 2.45 GHz. Here, the absorbance of a specific molecule influences how it behaves. Because more polar materials absorb radiation more effectively than less polar ones, when cooking in a microwave, for instance, water heats up quickly, whereas oil heats up considerably more slowly and does not heat up at all on the ceramic plate underneath. Although using a microwave to heat food can save energy usage, there are other advantages.

The extraction of various elements and real reactions such as transesterification processes are just a few examples in chemical engineering where this type of selective heating could prove useful. Probably the most controversial topic in process intensification in the past 10 years has been microwave-assisted reaction intensification. The discussion has centered on whether the kinetic reaction rate is actually increased by microwaves, or if the rise is only because of the Arrhenius effect, resulting in a local temperature increase that speeds up processes. On the other hand, local hotspot formation and selective heating are responsible for the observed increases.

In the discussion surrounding this issue, emphasis has been placed on temperature measurement accuracy. Priecel and Lopez-Sanchez (2018) provide an insightful critical review on this subject. When at least two substances are present that have distinct absorption responses to MW, selective heating is achieved. The reaction rate is frequently accelerated whenever one of the components serves as a catalyst and heats up much beyond the surrounding bulk temperature. If a particular metal or carbon substance is added to active carbon, such as Pd, which substantially absorbs microwave radiation, this property can be successfully improved (Horikosh et al. 2011).

However, exercise caution while choosing the MW field strength, as overheating can have unfavorable consequences such as deactivating the catalyst. It is therefore advised to carefully measure the real temperature that is generated by particles that are heated by microwave radiation, for instance, by using thermal cameras with fiber optic probes/thermocouples (Gangurde et al. 2017). Kappe et al. (2013) presented a rationale for the effect of microwaves on organic synthesis, highlighting that the majority of the consequences could be explained as bulk thermal phenomena. The researchers performed a comprehensive analytical definition and examination of the phenomena, evaluating cases where microwave radiation is extremely helpful (such as in the manufacturing of 2-methylbenzimidazole) or ineffective. They arrived at the conclusion that non-thermal microwave effects are non-existent.

7.2.6.2. *Ultrasound*

The word “ultrasonification” refers to the usage of ultrasound in a process that will boost mass transfer, dissolve solid reactants more easily or improve reaction efficiency. The formation of reactive intermediates in cavitating “bubbles” during their impending collapse is triggered by high local temperatures and pressures, which is where the ultrasonic effect originates. Two British shipbuilders named Thornycroft and Barnaby observed unusual erosion on a propeller in 1895, which led to the first account of cavitations resulting from ultrasound. The engineering elements of chemical synthesis using ultrasound technology have recently been

reviewed by Sancheti et al. (2017). According to the phases involved, the study classified the reaction system: homogeneous reactions benefit from US solely in radical mechanisms, while heterogeneous reactions are affected by physical consequences of cavitation, such as improved mass transfer and particle shrinkage. Increased intensification is highly probable if the radical reaction and many phases are coupled.

7.2.6.3. *Plasma*

The third unconventional source of energy addressed in this investigation is plasma-assisted process intensification. A fourth state of matter, called plasma, is an ionized substance that becomes sufficiently electrically conductive so that long-range magnetic and electrical forces govern its motion. When it comes to technology, using plasma reactors seems more novel and interesting than using microwave and ultrasounds. But it has found usage in many different applications, such as naphtha-cracking, ethanol reforming with steam, biomass pyrolysis and the decomposition of carbon dioxide along with other volatile organic matters, in addition to the removal of environmental pollutants. Undoubtedly, because plasma techniques have the potential to accelerate methane activation and other reactive intermediates, their use in carbon dioxide reduction in chemicals and fuels is now receiving a lot of research attention (Abiev et al. 2020). Differentiating between various kinds of plasma may be useful in this case. Although the term “plasma” typically evokes images of an extremely warm fluid, plasmas can actually occur in a broad range of temperatures, contingent upon their energy level, temperature, electronic density and classification as either a high temperature (thermal) or a cold (non-thermal or non-equilibrium) plasma. Many reactions cannot be carried out in extremely hot temperatures, so they may have a negative or “scary” sound. Due to this, writers often refer to processes that take place at ambient temperature as non-thermal plasma (NTP) technology. NTP has applications in the elimination of volatile organic compounds (VOCs). Adsorption, membrane separation, thermal and catalytic oxidation, photocatalysis and bioreaction are some of the methods that have traditionally been used to regulate VOC emissions (Vandenbroucke et al. 2011). In contrast to most traditional gas treatment technologies, NTP has been shown to be more energy-efficient and efficient. It may additionally ionize compounds in gaseous form, which could lead to developments in many chemical synthesis reactions in the future, particularly in the field of pollution control (Penetrante et al. 2013). Recently, a wide range of plasma technologies have been developed, such as gliding arc discharge, corona, microwave, radio frequency (RF), glow discharge and dielectric barrier discharge (DBD) (Du et al. 2012). In both thermal and non-thermal plasma research, carbon dioxide is a prominent subject. It turns out that in a pulse discharge field, carbon dioxide can be activated. The momentum of the impact of electron dissociation can be reduced from 11 eV to 5.5 eV when plasma increases the vibrational levels of carbon dioxide molecules (Chung et al. 2016).

7.2.7. *Alternative fluids*

The development and use of solvents to alter volatile organic compounds is now getting a lot of attention, with the goal of improving processes that use solvents that are less damaging to the environment, including water, super critical fluids and ionic liquids (Forsyth et al. 2004). The salts that melt below 100°C create ionic liquids that are composed of both anions and cations (Welton et al. 2004). Ionic liquids are growing increasingly common due to their numerous applications, including as electrolytes in batteries and capacitors, as a replacement for traditional solvents and in catalytic reactions where component solubility and solvent–solute interactions are critical since they affect the solutes' reactivity (Gordon et al. 2001; Forsyth et al. 2004; Welton et al. 2004). The ions that make up an ionic liquid and the properties of the solute decide whether a material is miscible with it. Miscibility with water in particular is fascinating. In certain circumstances, two distinct layers happen, yet in other cases, some ionic liquids are miscible in water in all compositions. Strong hydrogen bonds between water and the anions in the ionic liquid cause this occurrence; short-chain alcohol can be added to the biphasic systems to promote mixing and change the solubility of water in the ionic liquid (Gordon et al. 2001). Ionic liquids share some interesting characteristics. Firstly, they are non-flammable, which is important when they are used as solvents in exothermic reactions. In addition, they have a low vapor pressure, making them useful in separation techniques such as sublimation and distillation, where low-boiling solvents cannot be used. Ionic liquids are also known for their thermal stability across a broad temperature range, which enables applications in temperature-dependent processes such as extraction and crystallization, as well as effective kinetic control over chemical reactions (Forsyth et al. 2004). The supercritical fluids provide an additional intriguing option. When a fluid's temperature and pressure are higher than the critical values, it is referred to as supercritical. The characteristics of supercritical fluids lie in the middle of those of gases and liquids. By altering the pressure and temperature, these properties can be changed. They exhibit a density akin to liquids and a diffusivity and viscosity similar to gases (Cansell et al. 2003). The ability to distinguish the product and recycle the gas without needing extra purification stages is the main advantage of using supercritical fluids in industrial operations. These advantages are especially noticeable when using CO_2 and water, the two most significant supercritical fluids. They are thermodynamically stable, harmless and nonflammable. Moreover, they exhibit superior heat transfer qualities, which make them a respectable substitute for the fluids used in refrigeration systems (Knez et al. 2014). While the use of CO_2 as an industrial solvent has gained a lot of attention since it does not require additional resources for the treatment of waste and the byproduct from the process is a highly valuable byproduct, other solvents such as hexane, propane, butane and ethanol in hypercritical condition are also receiving

increasing attention (Knez et al. 2014). Supercritical fluids find many applications, including the synthesis of novel materials, serving as an encouragement for novel catalysts, helping as a reaction medium in multiple reactions (e.g. Friedel–Crafts alkylation, hydroformylation and transesterification) (Brunner et al. 2010), as well as being used in separation techniques such as chromatography and extraction processes (Knez et al. 2014).

7.3. Integration of process intensification and advanced materials

Process intensification (PI) approaches combined with advanced materials provide a revolutionary approach for enhancing sustainability, product quality and process efficiency in a variety of industries. In many different industries, advanced materials serve as crucial to enhancing process intensification (PI). Advanced material for process intensification is shown in Figure 7.1. With the goal of maximizing yields, eliminating waste production and consuming less energy, process intensification involves reconfiguring and optimizing unit activities. With unique characteristics such as enhanced surface area, selectivity and durability, advanced materials – such as catalysts, membranes and nanoparticles – offer previously unattainable control over reaction kinetics and separation processes. For example, in chemical synthesis, accurate oversight of reaction variables leads to higher selectivity and shorter reaction times if microreactors and advanced catalysts are used. Similar to this, the use of innovative membranes into processes of separation improves efficiency by allowing the desired chemicals to permeate selectively while lowering energy consumption and waste generation. Additionally, the design of flexible and compact process units is likely to be made simpler by the use of new materials in process intensification, enabling more flexible and decentralized manufacturing setups. The combination of PI and advanced materials has potential applications outside of chemical engineering, including biotechnology, renewable energy and medicines. For example, the use of customized catalysts and microfluidic devices may speed up drug synthesis procedures in pharmaceutical manufacturing, increasing the yield and purity of active pharmaceutical ingredients.

Advanced materials such as high-performance membranes and tiny catalysts may enable improved conversions and purification processes in fuel cell technology and manufacturing of biofuel, thus contributing to the development of renewable energy. All things considered, the combination of process intensification and advanced materials indicates a paradigm change towards environmentally conscious, productive and adaptable manufacturing processes. This integration has the ability to spur innovation and solve global scarcity of resources and environmental impact challenges.

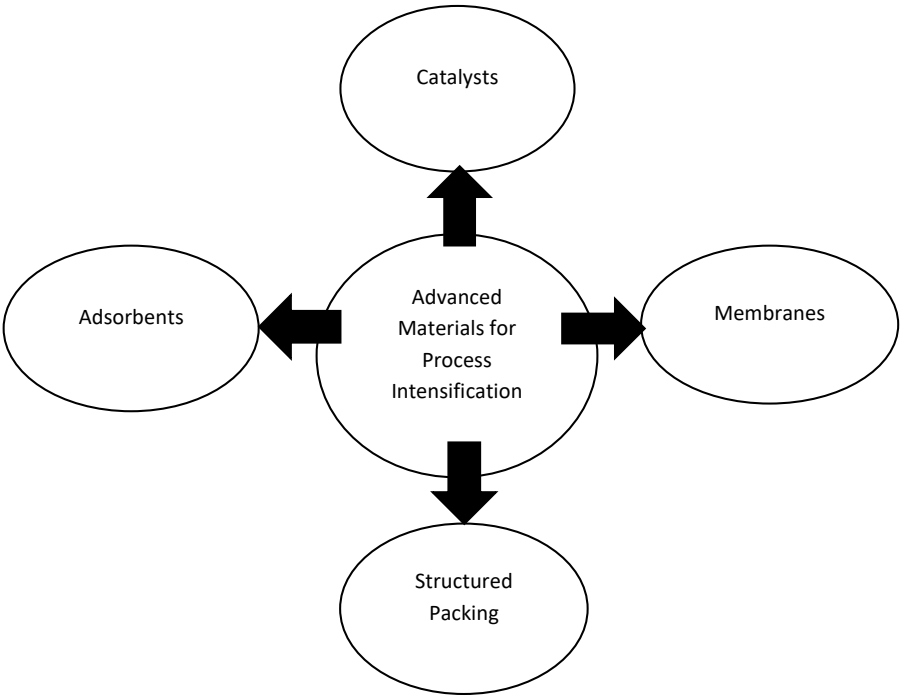


Figure 7.1. *Advanced material for process intensification (figure complied by the author)*

7.3.1. *Advantages and disadvantages of process intensification*

Improved execution of interactions between molecules under ideal driving force and synergistic effect circumstances has been the guiding premise of process intensification. Chemical plants can achieve an elevated level of safety by maintaining lower pressure levels with fewer energy requirements, even while gradient-free concentration and temperature profiles can be attained with a reduction in residence time. Fewer degrees of freedom and enhanced process control are the consequences of merging different unit operations.

The use of PI techniques increases plant costs by approximately 20% (Costello et al. 2004). Consumables, process utilities and plant maintenance amount constitute nearly all of the operating costs. With PI approaches, these parameters can be adapted for better output yield and turnaround time. Table 7.2 provides a summary of the choices that PI offers.

1) Reduced need for raw materials
2) Diminished energy usage
3) Decreased output of waste byproducts
4) A smaller footprint for plants
5) Safer procedures
6) Lower plant equipment expenses

Table 7.2. *Advantages of process intensification*

Although a number of PI technologies have shown promise in the labs such as the European Process Intensification Centre (EUROPIC), Centre for Process Systems Engineering (CPSE) at Imperial College London, Sustainable Process Technology (SPT) Group at the University of Twente and Chemical and Biological Engineering Department at the University of Wisconsin–Madison, their industrial applications are still in the beginning stages of development. Plenty of barriers stand in the way of PI's industrial adoption, as illustrated in Table 7.3.

1) Process engineers lack in-depth expertise and understanding of PI.
2) Pilot-scale facilities for PI are insufficient for the current production lines.
3) There are high risks in developing prototypes and retrofitting current processes, both technically and financially.
4) Top management is unaware of the potential advantages of PI technologies.
5) There is a lack of process control systems that can accommodate new PI modules.

Table 7.3. *Disadvantages of process intensification*

In the chemical industry, development and research operations focus primarily on novel goods (chemistry) and less so on novel methods of production (chemical engineering). While equipment makers and engineering firms are not doing much to encourage process intensification, chemical manufacturers exhibit little interest in developing new kinds of machinery or processing methods.

The high expense of retrofitting PI technologies in existing plants, which raises the stakes for commercializing revolutionary technology, is another obstacle. Major challenges arise when PI techniques are taken up from lab, pilot, to commercial scales. Long development paths are required for PI technologies, necessitating efficient IP cooperation among various R&D labs, universities and industry partners.

7.3.2. *Applications of process intensification*

7.3.2.1. *Process intensification of distillation column*

In distillation, process intensification pertains to improving conventional distillation methods in order to get increased productivity, lower energy usage and a smaller equipment footprint. Reactive distillation, membrane distillation, dividing-wall columns and other techniques can be used to enhance distillation operations for improved separation efficiency. These innovations improve product purity, decrease environmental effects and save operating expenses, all of which have a beneficial impact on several kinds of industries, including food processing, petrochemicals and pharmaceuticals. In the long run, distillation process intensification offers a route to more affordable and environmentally friendly manufacturing processes. Using a "heat mass integration strategy" (HMI), Jiang et al. (2018) intensified multicomponent distillation and offered methods for intensification in "divided wall columns (DWC)". They used heat-migration isolation (HMI) on thermally connected distillation columns, which substantially lowered both the number of columns needed and the quantity of heat needed. This tactic minimized the quantity of reboilers and condensers required for multicomponent multiple distillation towers, hence reducing the heat duty on both exchangers. They tested with HMI on six component distillation, which generated a variety of distillation column designs. They discovered that when side streams were used in place of sub-mixture heat exchangers after two columns had been merged, the number of heat exchangers decreased from 10 (in conventional distillation) to six. Moreover, a very energy-efficient model was developed when sub-mixing streams were swapped out for thermal coupling, cutting the number of heat exchangers to four. The capital cost was 30% lower when DWC distillation was used in place of conventional distillation. When thermal coupling was changed to "liquid transfer" solely and used with DWC, operational configurations were achieved. This tactic reduced the problems that impeded its widespread use, such as the desired vapor split in DWC. Process intensification was introduced to reactive distillation (RD) by Kiss and Jobson (2018) via the combination of RD with other intensive distillation technologies, including DWC, heat-integrated distillation and cyclic distillation. By mixing microwaves with traditional reactive distillation, Ding et al. (2016) discovered an efficient process intensification method. This approach enhanced the product purity in addition to reaction time. Spasojevic et al.'s (2010) novel approach to reducing entropy creation along the column expedited the distillation process. Adiabatic columns, which require condensation chambers and reboilers for heat exchange, were used in the previous method. Nevertheless, they used the diabatic distillation method, which involves introducing heat during the stripping process and withdrawing it from the rectifying portion. Heat exchangers are not required because heat exchange happens independently on each tray. In the conventional method, the temperature of the trays dictated how much heat could be exchanged on them. To

minimize the development of entropy, they use the amount of heat to be exchanged as a control variable rather than temperature. This method was tested for the separation of feed mixtures including 0.5 mole fractions of each of the hydrocarbon's benzene and toluene. In the adiabatic column, the created entropy was 2.998 J/s K, while the minimal value for the diabatic column's produced entropy was 1.056 J/s K. They were able to conserve about 64.77% of the energy needed by using this tactic.

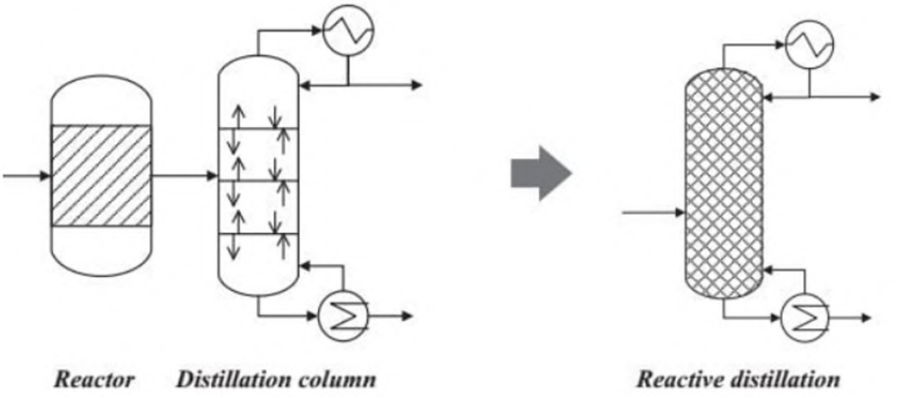


Figure 7.2. *Process intensification of distillation column (open access: https://epicsysinc.com/blog/what-is-process-intensification/)*

7.3.3. *Process intensification in biodiesel production*

To boost productivity, reduce expenses for energy and improve overall sustainability, the biodiesel production process has been made more efficient and optimized through process intensification. To increase reaction rates, boost yield and use fewer catalysts and resources, techniques such as enzymatic transesterification, microreactor systems and reactive distillation are used. By combining these techniques, the production of biodiesel becomes more affordable, sustainable and scalable, advancing the use of renewable energy sources and diminishing reliance on fossil fuels. "Ultrasonic cavitation reactors" were used by Dhanke et al. (2019) to boost the production of biodiesel. They experimented with the cottonseeds and methanol esterification reaction technique. They investigated the effects of variables on the synthesis of biodiesel, including reaction time, temperature, concentration of the catalyst and oil-to-alcohol mole ratio. By altering the parameters, such as the oil-to-alcohol mole ratio (1:6–1:15), the concentration of the catalyst (NaOH) from 0.5 to 2 weight percent, the reaction temperature from 30 to 60°C and the reaction time from 10 to 40 minutes, they conducted a series of experiments. Ung et al. (2016) used the "Hydrodynamic Cavitation Reactor" (HCR) to carry out process

intensification in the production of biodiesel. In an effort to increase the production of biodiesel, Samniang et al. (2014) used a supercritical process that involved the interaction of methanol, krating oil and jatropha oil without the use of a catalyst. 90% of pure biodiesel was generated by maintaining a reaction pressure of 8–18 MPa, a methanol-to-oil ratio of 30:1, and a reaction period of 5–15 minutes. Jiang and Tan (2012) produced biodiesel from coconut oil using the supercritical process in the presence of several co-solvents. By using these co-solvents, the biodiesel results were able to reach 72% compared to 41% when none was used. They found that this method produced excellent outcomes in an environmentally benign manner with very little byproduct production. Using microwaves to speed up the process, Khemthong et al. (2012) synthesized biodiesel from palm oil and methanol with the help of Cao acting as a catalyst.

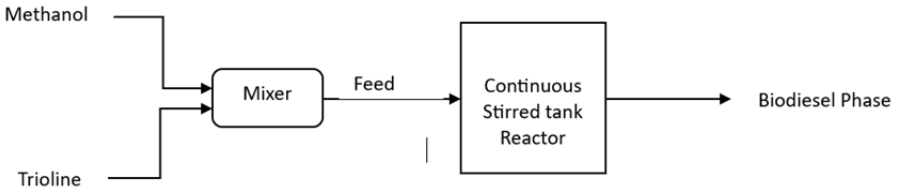


Figure 7.3. *Conventional production of biodiesel using CSTR (figure complied by the author)*

7.3.4. *Process intensification in extraction*

Process intensification in extraction minimizes environmental impact, improves efficiency and cuts down on energy usage, consequently modernizing conventional techniques for extraction. It entails using cutting-edge methods such as microwave-assisted extraction, ultrasonic extraction and supercritical fluid extraction. These methods significantly boost mass transfer rates, resulting in increased yields, quicker extraction times and less solvent consumption. Moreover, process intensification offers up new possibilities in sectors such as pharmaceuticals, food and beverage, and cosmetics by facilitating the extraction of high-value compounds from a variety of raw materials, such as plants, biomass and waste streams. Overall, the use of process intensification in extraction holds the potential to promote cost-effectiveness, sustainability and innovation in a range of manufacturing processes. Petroleum products were extracted from aqueous solutions using sorbents more forcefully by Vialkova and Malyshkina (2019). A technique for addressing oil spill-related water pollution is sorption, which has been shown to have a 99% accuracy rate. Activated carbon, pine sawdust, polyurethane foam loading and other natural sorbents generated from plant wastes have been used to prevent issues such as the expensive price and high toxicity of synthetic and inorganic sorbent. They only discovered the

shortcomings of plant materials' inadequate sorption capabilities as a natural sorbent. The results showed that heating pine sawdust in the microwave to 40°C enhanced its sorption capacity by 10%. Microwave heating enhanced the sorption capacity by two to five times, ozone treatment raised it by 1.5 times and microwave heating of a solution containing low concentrations of petroleum compounds increased it by 1.5 times. Tang et al. (2016) improved the extraction procedure of tiopronin (TPN), a free thio derivative containing glycine (CAS No.-1953-02-2). TPN is applied to treat linear function cells, heal linear injuries induced by ethanol and treat linear tissue. After removing it from its aqueous solution via ethyl acetate, TPN developed as an extract phase by crystallizing and drying. Three stages of cross-current extraction with a 30% ethyl acetate loss were used in the conventional production process. Despite using cross-current extraction, they used counter-current extraction to increase the synthesis of TPN. They noticed that the amount of ethyl acetate required in every stage was 370–430 for 800–900 kg of TPN aqueous solution (70–80 kg TPN). Three- to five-step counter- and cross-current extractions were simulated and computed using MATLAB programming.

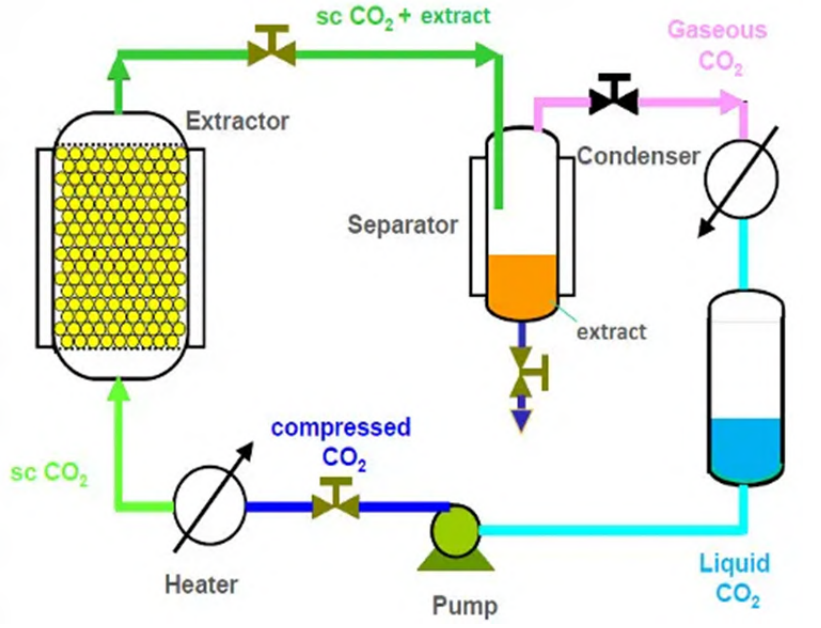


Figure 7.4. *Supercritical fluid extraction unit (source: NPTEL). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

7.3.5. *Process intensification on catalyst development*

In the field of catalyst development, process intensification refers to a deliberate endeavor to improve catalytic processes through the optimization of catalyst properties and reaction conditions. This entails developing multifunctional catalysts that can catalyze numerous reactions at once, using sophisticated reactor designs for enhanced mass and heat transportation, and nanostructuring catalytic materials to boost surface area and reactivity. By integrating these strategies, scientists hope to increase yield, selectivity and catalytic efficiency – all of which will aid in the development of environmentally friendly and lucrative chemical processes. Research by Lind et al. (2020) focused on using 3-D printing to design and produce multipurpose structural catalysts. It was found that this multifunctional structured catalyst exhibited both rapid and effective mass transfer, and low pressure drops. For demonstration, an iso reticular foam composed of 10 mg of Al Si has been produced and tested by 3D printing. The catalyst's capacity to oxidize NO to NO_2 was investigated. The two primary procedures that took place in the production and design process were the anodization technique and catalyst impregnation. Both low- and high-voltage concentrations of electrolyte were used in their anodization process experiments. By adjustment of the anodization conditions, it was found that the SiO_2 content in the outermost coating of oxide dropped from 80wt% to 10wt%. The platinum catalyst has been embedded in the porous oxide layer by wet impregnation. The production of alumina on the outermost layer of 3D-printed iso reticular foam structures led to a net increase in surface area. Direct anodization was found to reduce high-temperature fluctuations and increase mechanical resistance. Despite the catalyst's increased porosity, they found that there was less pressure drop. It should be noted that the rate of heat transfer is increased when the catalyst is in close proximity with an aluminum body. Nearly 50% conversion was achieved with very little catalyst (just 8% oxygen).

7.3.6. *Process intensification for esterification reaction*

In esterification reactions, process intensification entails maximizing the reaction conditions to attain greater selectivity and conversion rates, while using fewer resources and generating less waste. Numerous techniques, such as catalyst optimization, dynamic separation, microreactor technology, choosing a solvent and recycling, as well as process integration, can be used to achieve this. These techniques can be used to improve the kinetics of reactions, reduce processing times and render esterification processes safer and more effective overall. This not only makes ester synthesis more financially viable, but it also meets industry requirements for more environmentally and resource-conscious chemical processes.

Process intensification was carried out on the esterification reaction by Khudsange and Wasewar (2017) in order to generate propyl butyrate by pervaporation. In earlier times, esters were formed through the reaction of acids and alcohol using catalysts including HI, HCl, etc. They were made in a variety of reactors, such as microreactors and reactive distillation, resulting in high energy uses based on the system's vapor–liquid equilibria and azeotropic mixture. By integrating the esterification process with pervaporation, they accelerated the process that reduced energy usage, enabled operation beyond vapor–liquid equilibria, handled azeotrope and improved environmental friendliness. Thermodynamic equilibrium sets a limit on the reactant's conversion. Propanol and butyric acid were combined with the help of p-toluenesulfonic acid, which acts as a catalyst. A composite membrane made of polyvinyl alcohol (PVA) and polyethersulfone (PES) was used for pervaporation. It was discovered that the molar ratio and temperature had a direct correlation with the conversion of acid. The conversion of butyric acid rose quickly as well, from 71.61% to a maximum of 92.94% at 353 K, upon increasing the concentration of catalyst from 1 weight percent to 2.5 weight percent. The obliteration of water was the root cause of this rise in conversion. Because of their hydrophilic nature, PVA and PES continually eliminated water from the reaction mixture.

7.3.7. *Process intensification in pharmaceutical operations*

In the pharmaceutical industry, "process intensification" refers to the deployment of innovative innovations and methods to boost the productivity, sustainability and efficiency of medication manufacturing processes. It entails maximizing several phases of pharmaceutical manufacturing, including formulation, packaging, synthesis and purification, in order to maximize product quality, minimize environmental effect, lower costs and increase yields. Pharmaceutical operations frequently use solvent-free synthesis, ongoing production, equipment miniaturization and the implementation of sophisticated process control systems as methods for process intensification. The importance of process intensification techniques in pharmaceutical operations has been highlighted by recent research publications and reviews. These approaches help solve issues associated with traditional batch manufacturing processes, such as limited scalability, high prices and long development times. They explore cutting-edge techniques and instruments such as flow chemistry, modular processing units, continuous crystallization and microreactor systems, for optimizing the production of pharmaceuticals. The aforementioned research underscores the potential of process intensification in quickening the timeframes for drug development, expediting the transition from laboratory to production scale and improving the sustainability attributes of pharmaceutical production.

7.3.8. *Process intensification in desalination*

In desalination, process intensification pertains to the application of cutting-edge technology and techniques to improve the productivity, sustainability and efficiency of brackish or saltwater water treatment operations. Reverse osmosis (RO) and thermal distillation are two examples of traditional desalination techniques that frequently need a large energy input, and have downsides such as fouling, scaling and expensive operating costs. By improving various desalination process elements, such as membrane design, system setup and energy recovery techniques, process intensification seeks to address these issues. Increased water flux rates and reduced energy usage in RO systems are made possible by sophisticated membrane materials with enhanced selectivity and fouling resistance, as well as creative module designs and flow patterns. The environmentally friendly nature of desalination activities is further improved by the addition of renewable energy sources, such as wind or solar power, and the use of energy-efficient pumps and recovery equipment. Furthermore, by optimizing water recovery and reducing waste generation, hybrid desalination systems that combine various technologies – such as membrane distillation or reverse osmosis with forward osmosis – offer possibilities for further process intensification. All things considered, process intensification in desalination offers hope for resolving the problems associated with water scarcity by offering economical, energy-efficient and ecologically friendly methods of producing fresh water. For the purpose of achieving the goals of process intensification in the desalination industry, Drioli et al. (2017) studied the function of membrane engineering. The membrane's attributes included simplicity of integration with other processes, low cost, high safety, small footprints, excellent selectivity and permeability for the transportation of particular components. Conventional desalination's drawback was its growth-hindering pressure-driven method. In a different investigation, membrane crystallizers (MCR) were used in conjunction with RO to desalinate seawater. In order to produce NaCl, the saltwater was first treated using nanofiltration and RO, then the MCR approach to RO concentration. Along with salt recovery, freshwater recovery increased from 50% to 90%. Because of the temperature variance acting as a driving factor, the MCR does not encounter osmotic phenomena like RO does. Reverse osmosis (RO) was made up 60% of the desalination process. By integrating it with renewable energy sources such as wind or solar energy, they performed better and increased the process' economy. In the end, the desired "zero liquid discharge" was attained. Wind and solar power are combined with a traditional energy source, which may be a diesel generator, since they cannot run consistently without storage batteries. When building the process, many factors were taken into account, including productivity, adaptability, modularity, feed compositions, temperature variations and pressure variations.

7.3.9. *Biological product recovery and intensification process*

In order to recover biological products, techniques for isolating and purifying important biomolecules from challenging biological sources, such as proteins, enzymes and antibodies, have to be optimized and enhanced. This is known as process intensification. Since they require an abundance of chemicals and solvents, traditional downstream processing procedures can have low yields, high costs and environmental issues. By improving the bioproduct recovery processes' efficiency, sustainability and selectivity, process intensification solutions aim to address these issues. Developing cutting-edge separation technologies such as membrane filtration, chromatography and precipitation techniques – that offer better purity, higher throughput and lower solvent use than traditional procedures – is one strategy for process intensification. By integrating these technologies into multi-step purification platforms, recovery times can be reduced and the number of unit operations needed can be minimized. The intensification of biological product production and recovery has been examined by Vaghari et al. (2015). Bioprocesses aimed to be essential to biological reactions that needed a number of intricate steps and pieces of apparatus in order to manufacture various molecules. These chemicals were traditionally created using artificial chemical processes. There was limited industrial use for these bioprocesses because of the huge footprint and costly expense of the equipment. High purity is attained by the goods in a diluted environment. For example, separating the reaction products selectively in situ was achieved using membrane bioreactors, which enhanced mass transfer rates in addition to process selectivity and yield. They claimed that because immobilized cell systems permitted the use of distinct growth rate biological reactors and since immobilized cells were found to have stronger catalytic stability than free cells, immobilized cell bioreactors were superior to free cell bioreactors.

7.3.10. *Intensification for nickel recovery*

The process of optimizing and improving procedures to extract nickel from ores, tailings and waste from industry streams is referred to as intensification for nickel recovery. Nickel is a valuable metal and is used extensively in many industries, such as electronics, batteries and stainless-steel manufacturing. Conventional techniques for recovering nickel, such as smelting and hydrometallurgical procedures, often require a lot of energy, chemicals and trash. With the goal of overcoming these challenges, process intensification techniques work to increase the sustainability, efficiency and selectivity of nickel recovery procedures. In order to remove Ni (II) from water, Gabli et al. (2018) suggested a process intensification methodology that paired an ion-exchange process with electrodialysis. In their experiments, they used Amberjet 1200 H cation exchange resin. They found that process efficiency is increased by the applied electric field. By using the ED cell to some extent, they

have also been able to address the limitation of ion exchange resins, which is that they require constant activation. They extended the ion exchange resin's longevity, enabling it to filter water even in the presence of extremely low quantities of metal ion contaminants. Additionally, they looked at the impacts of several variables such as the concentration of Ni (II) ions at the input, the current density, the quantity of resin used, etc. Their findings showed that HNO_3>HCl>H_2SO_4>NaCl was the order in which the electrolyte was most efficiently regenerated. Efficacy in terms of concentration factor and rate of recovery was extremely poor in the case of ED without resin.

7.3.11. *Process intensification for colemanite leaching*

Enhancing the efficacy and efficiency of the leaching procedure used for eliminating boron from colemanite ores is known as process intensification for colemanite leaching. An excellent supplier of boron is colemanite, which is used in the manufacture of glass, ceramics and agriculture, as well as in other industries. Traditional colemanite leaching methods frequently have important reagent use, protracted processing periods and low extraction rates. With the goal of overcoming these barriers, process intensification solutions combine novel techniques and adjust critical parameters to enhance the overall leaching performance. To boost the recovery of the boric acid, Olufemi et al. (2016) enhanced the leaching of colemanite ($2CaO.3B_2O_3.5H_2O$). The most commonly used boron compound, boric acid, was prepared by adding sulfuric acid to colemanite to dissolve it. It was a secondary mineral that developed following the initial disintegration of other minerals. Since gypsum was a byproduct, it needed to be segregated. The colemanites were initially ground in a hammer mill and then crushed in a jaw crusher before being sieved. A diameter of 150 μm has been found to be the largest. It was found that the batch method outperformed the semi-batch method. Since acids dissolve easily, they were used in the leaching of metals that were heavy. They found that variables such as particle size, pH, time, lixiviant concentration and agitation speed influenced the rate of leaching. The procedure was described by the shrinking core model, which postulates that the reaction starts at the particle's outer skin and moves into the center of the solid particles, leaving behind a solid product layer referred to as ash. As a consequence, the solid reactant dissolved and the product solidified at the same time.

7.3.12. *Process intensification for mixing operations*

Optimizing and improving the mixing processes used in a variety of industries, such as food processing, pharmaceuticals, chemical manufacture and cosmetics, has been referred to as process intensification in mixing operations. To guarantee

product quality, optimize reaction speeds and accomplish uniform component distribution, effective mixing is important. Long mixing times, inconsistent mixing and too much consumption of energy are just a few of the disadvantages of traditional mixing techniques. In order to tackle these problems, process intensification methods work to increase mixing efficiency, shorten processing times and use less energy and resources. In order to accomplish a non-Newtonian fluid mixing process that uses less energy, Jegatheeswaran et al. (2018) enhanced mixing performance in a chaotic SMX static mixer. They performed a comparison analysis of the techniques of electrical resistance tomography (ERT) and computational fluid dynamics (CFD), focusing on the intensification of fluid deformation. They compared the experimental result with a number of parameter results, including pressure drop data, the CFD model's mixing index and the secondary fluid's concentration profile. They used a 0.5% xanthan gum solution by weight as the working fluid, and the secondary fluid was water, a Newtonian fluid with a constant viscosity. Diffusion, chaotic advection produced by the SMX static mixer element, bulk advection of the primary fluid and other mechanisms all contributed to the dispersion of the secondary fluid within the primary fluid. The shear-thinning primary fluid in the SMX static mixer was able to be deformed by the secondary fluid due to its high velocity and ability to deflect in many directions. A more consistent radial dispersion of the second fluid in the main fluid was achieved as fluid deformation was increased at a greater secondary-to-primary velocity ratio.

7.4. Conclusion and future prospects

In the upcoming years, process intensification (PI), which is at the cutting edge of technological advancement, holds an opportunity to completely alter production processes in an array of businesses. In light of the growing demand for cost-effectiveness, long-term viability and efficiency, PI offers a plethora of opportunities that may completely transform the context of industry. The study of sophisticated methods of production is one of the most promising opportunities. Through the implementation of cutting-edge methods such as modularization, microreactors and continuous processing, industries may achieve unprecedented levels of results while using fewer resources. For instance, ongoing processing minimizes downtime and streamlines processes while allowing continuous production. On the one hand, microreactors offer more exact control over chemical processes in small areas, resulting in purer and higher yielding chemicals. On the other hand, modularization makes it easier to construct process units that are additionally scalable and adjustable, and improves adaptability and flexibility in rapidly shifting markets. The emergence of Industry 4.0 and digitalization has further enhanced PI's potential. Industries may optimize processes in real time, while laying a basis for data-driven decision-making, autonomous operations, predictive maintenance and predictive maintenance by harnessing the power of technological advances, IoT and

sophisticated analytics. Proactive interventions are made feasible by continuous control and monitoring systems, which minimize interruptions and improve productivity. In addition, sophisticated analytics enable companies to derive valuable information from massive data sets, allowing them to get the most use out of resources, lower energy costs and improve overall performance. The starting point of opportunities for process intensification in the future is sustainability. PI presents a path towards more environmentally conscious and sustainable operations as demand on industries to reduce their environmental impact grows. By cutting down on the generation of waste, using less energy and switching hazardous substances with more secure options, PI helps businesses to comply with stringent laws and satisfy consumer demands for environmentally friendly products. The design of processes that put efficiency, safety and responsibility for the environment foremost is influenced by the principles of green chemistry, which spur innovation towards environmentally conscious solutions.

The foreseeable future of PI is especially bright in the fields of bioprocessing and medicines. The need for scalable and inexpensive production procedures is expanding due to the increasing need for biopharmaceuticals and customized therapies. Higher production, faster production cycles and more versatility can be achieved by integrating improved biological processing techniques including perfusion, continuous chromatography and in-line purification, made feasible by PI. These advances not only lower production costs, but also hasten the development and delivery of medicines that can save the lives of patients worldwide. Another frontier in process intensification will be represented by decentralized and modular systems in the future. Through the implementation of modular process units and decentralized manufacturing, industries can improve their resilience, scalability and flexibility. Production can be located closer to the point of use thanks to decentralization, which lowers transportation costs and lessens the environmental effects of lengthy supply chains. Production facilities may be quickly deployed and reconfigured thanks to modularization, which makes it possible to react quickly to shifting operational needs and demands from the market. In order to spur innovation and accelerate the use of PI technologies, cross-industry cooperation is expected to be essential. Through the utilization of knowledge and skills from other fields, industries can promote collaboration and jointly develop innovative solutions that have wider relevance. The widespread adoption of PI across industries is ultimately enabled by collaborative initiatives and partnerships, which enable the exchange of best practices, the pooling of resources and the exploration of fresh market prospects. In conclusion, creativity, sustainability and teamwork define the potential for process intensification in the future. With advancements in digitalization, sustainable manufacturing techniques and cross-disciplinary cooperation, PI offers the ability to help industries throughout the world achieve new levels of resilience, efficiency and competitiveness. Companies are going to benefit from a more

sustainable, adaptable and prosperous future if they seize these opportunities and go ahead with process intensification.

7.5. References

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8

Nanotechnology in Chemical Engineering

Nanoscience and nanotechnology significantly reshape various interdisciplinary fields, with a particularly transformative impact on chemical engineering. The rapid expansion of nanomaterial applications spans various industries, including agriculture, pharmaceuticals, chemicals, cosmetics, petrochemicals and automotive sectors. Within chemical engineering, nanotechnology's most prominent contribution is the development of nanocomposites. These materials, which incorporate nano-fillers ranging from 1 to 100 nanometers, are classified into zero-dimensional, one-dimensional, two-dimensional and three-dimensional structures. Each type of nanocomposite exhibits unique properties that markedly enhance the performance and functionality of chemical products and processes.

A deep understanding of these nanoscale materials' thermal and mechanical properties is crucial for designing high-quality, effective products. Nanocomposites' distinct characteristics, such as increased strength, flexibility and conductivity, enable advancements in various applications within the chemical industry. These properties facilitate the development of more robust and efficient materials, driving innovation in product design and manufacturing processes. Integrating nanotechnology into chemical engineering is poised to usher in substantial changes across several key areas. In materials development, nanotechnology promises to create substances with extraordinary properties. Innovations such as graphene and carbon nanotubes are expected to revolutionize manufacturing by producing smarter, more durable products. These advancements will open up new possibilities and applications across multiple industries.

This chapter highlights the crucial role of nanotechnology in chemical engineering, emphasizing its potential applications, future prospects and the challenges accompanying its implementation. By exploring these aspects, this chapter aims to provide a comprehensive overview of how nanotechnology is set to drive significant advancements and transform conventional practices in chemical engineering.

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8.1. Introduction to nanotechnology

Nanotechnology is the science and engineering of manipulating matter at the atomic and molecular scale, typically within the range of 1 to 100 nanometers. At these dimensions, materials often exhibit unique physical, chemical and biological properties that differ significantly from their bulk counterparts. This field encompasses a wide array of techniques and approaches to designing, producing and applying structures, devices and systems by controlling shape and size at the nanometer scale.

Nanotechnology, the science and engineering of materials at the nanoscale, represents one of the most significant advancements in modern science and technology. By manipulating matter at atomic and molecular levels, nanotechnology enables the creation of materials and devices with novel properties and unattainable functions at larger scales. This revolutionary field can transform many industries, including electronics, energy, aerospace, healthcare and materials science, by offering unprecedented capabilities and efficiencies. Figure 8.1 shows the interdisciplinary scope of multiple applications, and Figure 8.2 represents the generalized features and functions of nanosystems. Furthermore, nanotechnology has become a driving force reshaping multiple sectors. Continuous advancements in this field drive innovation, significantly influencing and transforming industries. The miniaturization of electronic equipment is one of the best examples of nanotechnology's impact, leading to the development of smaller, faster and more efficient components. It has contributed to more efficient energy storage and conversion systems in the energy sector. The aerospace industry leverages nanotechnology to create lighter, stronger and more durable materials, while in healthcare, it has opened new frontiers in diagnosis, treatment and drug delivery. Materials science has been profoundly impacted by creating materials with unique properties. By continually pushing the boundaries of what is possible, nanotechnology is paving the way for groundbreaking applications that could redefine our approach to solving complex problems and improving the quality of life (Varghese 2013; Vilos 2014; Ndikau et al. 2017; Mahmoud et al. 2019; Varghese et al. 2019; Tudó et al. 2020; Ahmed et al. 2021; Baggioli et al. 2021).

8.2. Role of nanotechnology in chemical engineering

In chemical engineering, nanotechnology heralds a new era of innovation by enabling the design and creation of materials with unprecedented properties. These advanced materials find extensive applications, particularly in pharmaceuticals, where nanotechnology facilitates the development of precise drug delivery systems. These systems can significantly enhance drug efficacy by ensuring that medications are delivered directly to the targeted cells or tissues. For example, nanoparticles can

be engineered to deliver chemotherapy drugs directly to cancer cells, minimizing side effects on healthy cells and improving overall treatment outcomes. Moreover, nanotechnology has a profound impact on catalysis. Engineered nanomaterials, such as metal nanoparticles and nanostructured catalysts, exhibit remarkable activity and selectivity in chemical reactions. These nanocatalysts can accelerate reaction rates and improve efficiency, leading to more sustainable and cost-effective industrial processes. For instance, in the petrochemical industry, nanocatalysts can enhance the conversion of raw materials into valuable products with higher yields and lower energy consumption. Nanocatalysts can break down pollutants and reduce emissions in environmental applications, contributing to cleaner and greener technologies.

The ability to manipulate materials at the nanoscale also opens up new possibilities in developing sensors and diagnostic tools. Nanotechnology enables the creation of susceptible and specific sensors which can detect trace amounts of chemicals or biological agents. These sensors are crucial in various fields, including environmental monitoring, food safety and medical diagnostics. For example, nanosensors can detect early signs of diseases by identifying specific biomarkers in bodily fluids, allowing for timely intervention and improved patient outcomes (Lee et al. 2010; Pagliaro 2015; Emeka et al. 2021; Iravani et al. 2023).

Furthermore, nanotechnology holds great promise for addressing critical environmental challenges. In particular, its role in water treatment and pollution remediation is effective and sustainable. Nanomaterials such as carbon nanotubes and graphene oxide can clean water more efficiently than traditional methods, offering a powerful solution to some of the most pressing environmental problems (Patra et al. 2018; Madamsetty et al. 2019; Yu et al. 2021).

The swift advancement of nanotechnology in chemical engineering focuses on manipulating and controlling materials at the nanoscale. This reveals its versatility across applications such as eco-friendly nanoparticle synthesis, advancements in disease diagnosis and transformative manufacturing processes. For example, nanosensors can detect diseases early, allowing for timely and effective treatment. Its profound implications underscore its potential to revolutionize industries, foster environmental sustainability and push the boundaries of scientific and engineering possibilities (Nouailhat 2006; Naidu et al. 2014; Peng et al. 2018; Bayda et al. 2019; Farjadian et al. 2019; Varghese et al. 2019; Baig et al. 2021; Lisa et al. 2021; Remya et al. 2022; Ojukwu and Nwaiwu 2023).

A pivotal role of nanotechnology lies in enabling green synthesis techniques for nanoparticles. This eco-conscious process harnesses natural elements such as bacteria, fungi and plants, avoiding toxic chemicals and harmful byproducts. For instance, gold nanoparticles can be synthesized using plant extracts, which are safer and more environmentally friendly than conventional chemical methods. By doing

so, it minimizes potential hazards associated with traditional methods, significantly reduces energy consumption and waste generation and aligns with sustainability and environmental friendliness (Nouailhat 2006; Peng et al. 2018; Varghese et al. 2019; Baig et al. 2021; Vishnu et al. 2022).

Green synthesis offers numerous advantages over traditional physical and chemical methods, rooted in sustainability, safety and efficiency. It guides responsible, eco-centric manufacturing practices in the expansive realm of nanotechnology. Creating nanoparticles using natural sources such as microorganisms and plants through green synthesis enables precise control over their size, shape and surface characteristics. For instance, fungi can generate silver nanoparticles with antibacterial properties, which have the potential to be used in the next generation of medical devices and intelligent medical systems. This approach facilitates the development of nanoparticles with specific functionalities, including antibacterial, antifungal, antiviral, antioxidant and anticancer properties. Green synthesis mitigates potential adverse effects on human health and the environment by avoiding toxic chemicals (Miu and Dinischiotu 2022; Ying et al. 2022; Kazemi et al. 2023).

Incorporating nanotechnology into chemical engineering has sparked a paradigm shift, introducing more efficient and sustainable synthesis and production methods. Its impact extends to enhancing the performance and efficiency of chemical processes, amplifying catalytic reactions, increasing surface area and enabling selective separation processes. For example, nanoporous materials may help to separate gaseous mixtures more efficiently in industrial processes. This integration has unlocked possibilities for sustainable and eco-conscious industrial practices by manipulating materials at the nanoscale. It promises to revolutionize healthcare, manufacturing and energy industries by offering improved material properties, heightened efficiency and reduced environmental impact (Aman and Jain 2019; Huston et al. 2021; Miu and Dinischiotu 2022; Kazemi et al. 2023). This eco-friendly approach facilitates the development of nanoparticles with specific functionalities, including antibacterial, antifungal, antiviral, antioxidant and anticancer properties. Green synthesis mitigates potential adverse effects on human health and the environment by avoiding toxic chemicals (Nouailhat 2006; Ruan et al. 2012; Elnashaie et al. 2015; Peng et al. 2018; Baig et al. 2021; Golan et al. 2021).

Integrating nanotechnology into chemical engineering can potentially drive a paradigm shift toward sustainable and environmentally friendly practices in material design, drug delivery, catalysis and sensor technology. Its potential to revolutionize various industries and facilitate innovative, efficient and eco-conscious advancements highlights its importance in shaping the future of manufacturing and industrial processes. The ongoing progress in nanotechnology is set to transform chemical engineering, leading to a future characterized by enhanced performance,

efficiency and sustainability. Its potential to revolutionize industries and pave the way for innovative, efficient and eco-conscious advancements underscores its significance in shaping the future of manufacturing and industrial processes.

8.3. Emerging trends in nanotechnology-based chemical engineering

Nanotechnology is at the forefront of transforming chemical engineering, driving significant advancements across various applications (Patra et al. 2018; Madamsetty et al. 2019; Tudó et al. 2020; Ahmed et al. 2021; Anjum et al. 2021; Yu et al. 2021; Remya et al. 2022; Haleem et al. 2023). As researchers and engineers continue to explore the potential of nanoscale materials and processes, several emerging trends are shaping the future of chemical engineering. Current trends in nanotechnology in chemical engineering focus on significantly enhancing the properties and functionalities of materials. These advancements are creating exciting opportunities for innovation across various sectors. The rapid emergence of nanotechnology in chemical engineering is also poised to revolutionize multiple industries, including healthcare, manufacturing and energy.

One of the most prominent trends is the development of advanced nanocomposites. By incorporating nanoparticles into polymer matrices, researchers create materials with enhanced properties, such as increased strength, flexibility and thermal stability (Castro et al. 2015; Baig et al. 2021). These nanocomposites are finding applications in a range of industries, from aerospace to automotive, where their superior performance is essential. For example, the integration of carbon nanotubes or graphene into polymers can produce materials that are lighter, stronger and more resistant to environmental degradation (Gamage et al. 2022; Remya et al. 2022). This advancement improves the material's mechanical properties and opens up new possibilities for innovative applications and designs.

Another significant trend is the application of nanotechnology to drug delivery systems. Nanotechnology is revolutionizing drug delivery systems by enabling targeted and controlled release of therapeutic agents. Nanoparticles can be engineered to deliver drugs directly to specific cells or tissues, such as cancer cells, thereby enhancing treatment efficacy and reducing side effects (Vilos 2014; Patra et al. 2018; Anjum et al. 2021; Haleem et al. 2023). This precision medicine approach is transforming the pharmaceutical industry, offering new possibilities for personalized treatments. For instance, nanoparticles coated with targeting ligands can navigate the body and release their payload only at the disease site, providing a more effective and less invasive treatment option (Vilos 2014; Patra et al. 2018).

In chemical manufacturing, nanomaterials and nanoparticles are used to design more efficient catalysts. These advanced catalysts can accelerate chemical reactions

with excellent selectivity and efficiency, reducing waste and energy consumption. For example, nanocatalysts (Peng et al. 2018) can facilitate more effective conversion of raw materials into valuable products, improving the overall sustainability of chemical processes. Using nanomaterials in catalysis is another critical trend driving innovation in chemical engineering. Nanocatalysts, with their high surface area and tunable properties, enhance the efficiency and selectivity of chemical reactions. This advancement is crucial for various industrial processes, including petrochemical refining and green chemistry. For example, nano-sized catalysts can accelerate reactions and improve yields while minimizing waste and energy consumption. Their ability to facilitate more sustainable chemical processes contributes to a shift toward greener manufacturing practices (Parveen et al. 2016; Ndikau et al. 2017; Aman and Jain 2019; Huston et al. 2021; Khanzada et al. 2021; Miu and Dinischiotu 2022; Ying et al. 2022; Azad et al. 2023; Gupta et al. 2023; Kazemi et al. 2023).

Nanotechnology significantly advances sustainable and eco-friendly chemical engineering practices by developing green synthesis methods. These methods harness natural resources, such as microorganisms and plants, to produce nanoparticles with minimal environmental impact. By reducing dependence on toxic chemicals and cutting down on waste (Nouailhat 2006; Peng et al. 2018; Fardood et al. 2020), green synthesis provides a safer and more sustainable alternative to traditional chemical processes (Parveen et al. 2016; Ndikau et al. 2017; Aman and Jain 2019; Huston et al. 2021; Khanzada et al. 2021; Miu and Dinischiotu 2022; Ying et al. 2022; Azad et al. 2023; Gupta et al. 2023; Kazemi et al. 2023). For instance, silver nanoparticles can be synthesized using plant extracts, offering a more environmentally friendly option than conventional chemical methods. These advancements align with global sustainability goals and promote environmentally conscious manufacturing practices. Nanotechnology is leading the charge in developing sustainable processes by focusing on reducing environmental impact, optimizing resource use and minimizing waste. Techniques such as green synthesis highlight this shift toward eco-friendly approaches, underscoring nanotechnology's crucial role in achieving broader sustainability and environmental stewardship objectives (Nouailhat 2006; Peng et al. 2018; Remya et al. 2022).

Nanotechnology is enhancing the development of sensors and diagnostic tools with unprecedented sensitivity and specificity. Nanomaterials are being used to create sensors that can detect trace amounts of chemicals or biological agents, offering applications in environmental monitoring, food safety and medical diagnostics. For instance, nanoscale sensors can identify early biomarkers of diseases, enabling timely intervention and improving patient outcomes (Nouailhat 2006; Peng et al. 2018; Remya et al. 2022). This capability transforms how we monitor and respond to various health and environmental challenges.

Integrating nanotechnology into energy applications is driving advancements in energy storage, conversion and efficiency (Lisa et al. 2021). Nanomaterials are used in solar cells, batteries and fuel cells to enhance performance and extend lifespans. For example, quantum dots in photovoltaic cells can improve light absorption and conversion efficiency, while nanostructured materials in batteries can increase storage capacity and reduce charging times. These advancements contribute to more efficient and sustainable energy solutions, addressing critical needs in energy production and consumption (Alarfaj et al. 2018; Lisa et al. 2021; Vishnu et al. 2022).

In tissue engineering, nanotechnology facilitates the creation of scaffolds and structures that mimic the natural extracellular matrix. These nanostructured scaffolds promote tissue regeneration and repair by providing a supportive cell growth and development environment. This approach holds promise for advancing regenerative medicine and developing new treatments for tissue damage and loss (Patra et al. 2018; Madamsetty et al. 2019; Yu et al. 2021).

The emerging trends in nanotechnology-based chemical engineering are redefining the boundaries of what is possible in the field. From advanced nanocomposites and innovative drug delivery systems to efficient catalysis and sustainable practices, these trends drive significant improvements in material performance, process efficiency and environmental sustainability. As research and development continue to advance, nanotechnology is set to play an increasingly pivotal role in shaping the future of chemical engineering and addressing global challenges across various industries (Nouailhat 2006; Peng et al. 2018; Ojukwu and Nwaiwu 2023).

8.4. Challenges and solutions in nanotechnology for chemical engineers

Chemical engineers pioneering nanotechnology face several intricate challenges critical to advancing and applying this emerging field. One major challenge is the precise design and control of nanomaterial synthesis to achieve specific, tailored properties. Due to the unique demands of working at the nanoscale, this task demands sophisticated techniques and a profound understanding of material science.

Another significant challenge is ensuring the safe handling and disposal of nanomaterials. Given their small size and distinctive properties, nanomaterials can pose potential risks to human health and the environment. Chemical engineers must develop and enforce robust protocols to manage these materials safely throughout their lifecycle, from production to disposal (Lee et al. 2010; Gamage et al. 2022).

Ethical considerations also play a crucial role in the development and application of nanotechnology. The potential impacts of nanomaterials on human health and the environment necessitate scrutiny. Chemical engineers are responsible for addressing these ethical issues to ensure that advancements in nanotechnology do not compromise safety or environmental protection (Nouailhat 2006; Ruan et al. 2012; Elnashaie et al. 2015; Peng et al. 2018; Ojukwu and Nwaiwu 2023). In addition to these overarching challenges, several specific issues must be addressed:

– *Scale-up and manufacturing*: transitioning from laboratory scale to commercial manufacturing poses significant challenges. Issues with uniformity, reproducibility and cost-effectiveness often arise. Chemical engineers are developing advanced manufacturing techniques, such as microreactor technology, continuous flow synthesis and automation, to achieve consistent results on a larger scale while managing costs (Farjadian et al. 2019; Pandey and Jain 2020).

– *Environmental and health safety*: the potential risks associated with nanomaterials, including their impact on human health and the environment, are not fully understood. Rigorous research and regulatory frameworks are necessary to assess and mitigate these risks. Chemical engineers play a key role in developing safer nanomaterials and processes, implementing risk assessments and establishing standardized safety protocols (Lee et al. 2010; Anjum et al. 2021; Remya et al. 2022).

– *Standardization and characterization*: the small size and diverse properties of nanomaterials make characterization and standardization complex. Variations in size, shape and surface characteristics can affect performance and behavior (Ruan et al. 2012; Aman and Jain 2019; Baig et al. 2021). Advancements in characterization techniques, such as high-resolution microscopy and spectroscopy, are essential. Establishing industry-wide standards and protocols and collaboration between researchers, regulatory bodies and industry stakeholders is crucial for consistency and reliability (Farjadian et al. 2019).

– *Integration with existing technologies*: integrating nanotechnology with existing chemical engineering technologies can be challenging due to differences in scale and operational conditions. Developing hybrid technologies that combine nanotechnology with traditional practices can facilitate this integration (Lisa et al. 2021). Chemical engineers can explore ways to enhance existing processes with nanomaterials and use pilot projects to ensure seamless integration (Elnashaie et al. 2015; Peng et al. 2018; Lisa et al. 2021).

– *Economic feasibility*: the high cost of developing and producing nanomaterials can limit their widespread adoption. Reducing production costs through process optimization, efficient resource use and economies of scale is essential. Chemical engineers should focus on cost-effective synthesis methods and demonstrate the

long-term economic benefits of nanotechnology to justify investment (Farjadian et al. 2019; Pandey and Jain 2020; Lisa et al. 2021).

– *Intellectual property and regulatory issues*: the rapid advancement of nanotechnology raises concerns about intellectual property rights and regulatory compliance. Engaging with intellectual property experts and staying informed about evolving regulations can help navigate these challenges. Collaborative efforts between industry, academia and regulatory agencies can also promote the responsible development and commercialization of nanotechnology (Elnashaie et al. 2015; Peng et al. 2018; Farjadian et al. 2019; Lisa et al. 2021).

By addressing these challenges through innovative solutions and interdisciplinary collaboration, chemical engineers can fully harness the potential of nanotechnology. This approach will drive advancements in the field, leading to impactful solutions across various industries while ensuring safety, efficiency and ethical considerations are met.

8.5. Impact of nanotechnology on the future of chemical engineering

The anticipated impact of nanotechnology on the future of chemical engineering is profound, as it stands to revolutionize the field across multiple dimensions (Seeman 2003; Peng et al. 2018; Varghese et al. 2019; Baig et al. 2021; Lisa et al. 2021; Jagessar 2024). Nanotechnology involves manipulating and controlling matter at the nanoscale – one billionth of a meter – enabling unprecedented precision in designing and producing materials with enhanced properties and functionalities (Peng et al. 2018; Varghese et al. 2019; Baig et al. 2021; Lisa et al. 2021). This innovation promises to substantially boost the efficiency and sustainability of chemical processes, creating advanced materials with diverse and transformative industrial applications.

8.5.1. *Enhanced material properties*

Nanotechnology facilitates the manipulation of materials at the atomic and molecular levels, allowing for the creation of substances with extraordinary attributes. Nanomaterials, such as carbon nanotubes, quantum dots and nanowires, exhibit unique properties such as increased strength, reduced weight and enhanced thermal and electrical conductivity (Lisa et al. 2021). These advancements will significantly impact various industries:

– *Construction:* enhanced materials will develop more assertive, more durable building materials that can withstand extreme conditions, potentially revolutionizing

the construction industry (Elnashaie et al. 2015; Sudha et al. 2018; Bayda et al. 2020; Vishnu et al. 2022).

– *Electronics:* nanotechnology will enable the creation of smaller, faster and more efficient electronic devices, paving the way for advancements in consumer electronics, computing and telecommunications (Peng et al. 2018; Bayda et al. 2020).

– *Manufacturing:* superior materials will improve the performance and longevity of manufacturing components, resulting in increased efficiency and reduced maintenance costs.

8.5.2. *Smart materials*

The combination of nanotechnology and innovative materials represents a particularly transformative development. Nanotechnology involves manipulating matter at the atomic and molecular levels, allowing precise control over material properties. Nanotechnology enhances its performance and functionality when integrated with smart materials by providing superior strength, flexibility, responsiveness and efficiency.

This integration results in materials with improved thermal and electrical conductivity, making them more effective in diverse applications. Nanotechnology boosts the sensitivity and responsiveness of smart materials, incorporating nanoscale elements such as carbon nanotubes or quantum dots into sensors and actuators for higher sensitivity and faster response times. This advancement is crucial for medical diagnostics, environmental monitoring and advanced manufacturing.

The ability to tailor innovative materials' properties is another advantage of combining them with nanotechnology. By controlling the size, shape and distribution of nanoparticles, smart materials can be customized to respond to specific stimuli. This customization is valuable in aerospace, defense and healthcare fields, where materials must exhibit precise behaviors under varying conditions.

In medical devices, the fusion of nanotechnology and smart materials leads to innovations such as advanced drug delivery systems that target specific cells or tissues, improving treatment effectiveness while minimizing side effects. In addition, smart materials used in tissue engineering and regenerative medicine benefit from enhanced functionality and performance through nanotechnology.

Environmental monitoring also benefits from this synergy, as nano-sized sensors can detect low concentrations of pollutants or ecological changes with high

precision, enabling better management of environmental issues. Integrating nanotechnology with smart materials in consumer electronics results in more advanced devices, improving the performance of touchscreens, displays and sensors.

Energy storage and conversion technologies also see improvements through this integration. Nanomaterials enhance the performance of batteries, supercapacitors and fuel cells, making energy solutions more efficient and sustainable. Innovations in nano-engineered materials for solar cells further enhance energy conversion and storage, supporting the transition to renewable energy sources.

8.5.3. *Advanced drug delivery systems*

Nanotechnology will enhance drug delivery systems in pharmaceuticals by allowing for targeted and controlled release of medications. Nanoparticles can be engineered to deliver drugs precisely to specific cells or tissues, thereby improving efficacy and minimizing side effects. This advancement will be particularly transformative for treating complex diseases, such as cancer, where nanoparticles can be tailored to target and destroy cancer cells while sparing healthy ones.

8.5.4. *Improved catalysis*

Nanotechnology will significantly advance catalytic processes within chemical engineering. Engineered nanomaterials can serve as highly effective catalysts, improving reaction rates and selectivity. This will lead to more efficient chemical processes, reduced energy consumption and lower waste production.

For example, nanocatalysts could enhance the efficiency of petrochemical processes or expedite reactions in green chemistry, fostering more sustainable industrial practices.

8.5.5. *Sustainable and eco-friendly processes*

A significant advantage of nanotechnology is its ability to drive sustainable practices in chemical engineering. Green synthesis methods, which use natural sources such as microorganisms and plant extracts to produce nanoparticles, reduce environmental impact by minimizing toxic chemicals and cutting down waste.

Nanotechnology will support the development of eco-friendly processes and materials, aligning with global sustainability goals and promoting environmentally responsible manufacturing.

8.5.6. *Innovations in sensor technology*

Nanotechnology will advance sensor technology by enabling the creation of susceptible and specific sensors. These nanosensors can detect minute quantities of chemicals or biological agents with unprecedented precision. Applications include environmental monitoring, food safety and medical diagnostics. For instance, nanosensors could identify early disease biomarkers, allowing for timely and accurate diagnosis.

8.5.7. *Breakthroughs in energy storage and conversion*

Nanotechnology is set to revolutionize energy storage and conversion technologies. Nanomaterials can enhance the performance of batteries and supercapacitors, resulting in higher energy density and faster charge/discharge rates. Innovations in nano-engineered materials for solar and fuel cells will also improve energy efficiency and sustainability, aiding the transition to renewable energy sources.

8.5.8. *Development of new manufacturing techniques*

The integration of nanotechnology into chemical engineering will lead to the creation of novel manufacturing techniques. Methods such as nano-fabrication and self-assembly will enable the production of intricate structures with high precision. This will impact various industries, including electronics, by facilitating the development of more advanced and compact electronic devices.

8.6. Case studies on the application of nanotechnology in chemical engineering

8.6.1. *Case study 1: nanoparticles as catalysts in chemical reactions*

Nanoparticles exhibit unique physical and chemical properties due to their high surface area-to-volume ratio. This characteristic makes them highly effective as catalysts in chemical reactions. The increased surface area allows more reactants to interact with the catalyst, enhancing the overall reaction rate and selectivity. These improvements can lead to more efficient, cost-effective and environmentally friendly industrial processes (Madan et al. 2015; Karakaş 2021; Lisa et al. 2021).

A significant application of nanocatalysts is in the hydrogenation of olefins using platinum nanoparticles. Hydrogenation is a vital process in the chemical industry,

converting unsaturated hydrocarbons (olefins) into saturated hydrocarbons (alkanes) by adding hydrogen. Traditionally, platinum catalysts are used for this process, but when platinum particles are reduced to the nanoscale, their catalytic activity increases significantly (Madan et al. 2015; Karakaş 2021). The nanoparticles' larger surface area offers more active sites for the hydrogenation reaction. Research has shown platinum nanoparticles exhibit much higher catalytic activity than bulk platinum, leading to faster reaction rates and higher product yields. Moreover, nanoparticles can offer improved selectivity, ensuring that the desired product is formed preferentially over unwanted byproducts (Sudha et al. 2018; Bayda et al. 2020).

The use of platinum nanoparticles in catalysis has several notable impacts. Firstly, nanoparticles enhance reaction rates due to their high surface area, allowing more reactant molecules to interact with the catalyst simultaneously (Karakaş 2021). This increased efficiency can result in shorter reaction times and higher throughput in industrial processes. Secondly, the heightened activity of nanoparticles means that smaller amounts of catalyst are needed to achieve the same or better performance compared to bulk catalysts (Madan et al. 2015; Karakaş 2021). This reduction in catalyst usage can lead to substantial cost savings, especially when using expensive materials such as platinum. Thirdly, nanoparticles contribute to more sustainable chemical processes (Sudha et al. 2018). Their efficiency reduces the energy required for reactions, and their selectivity minimizes the production of unwanted byproducts, reducing waste and the need for additional purification steps. The potential for lower catalyst consumption also means that fewer raw materials are needed, reducing the environmental impact associated with mining and refining these materials. Finally, the unique properties of nanoparticles open new possibilities for designing catalysts tailored for specific reactions, leading to the development of novel catalytic processes that were not feasible with traditional catalysts (Madan et al. 2015; Karakaş 2021).

Hence, using nanoparticles as catalysts in chemical engineering represents a significant advancement in the field. By harnessing their unique properties, industries can enhance efficiency, reduce costs and adopt more sustainable practices, thus fostering innovation and growth.

8.6.2. *Case study 2: nanotechnology in water purification and treatment*

Nanotechnology is making significant strides in water treatment, offering promising advancements for purifying and managing water resources. This technology is transforming water purification and wastewater treatment by using the unique properties of nanomaterials, such as their increased surface area and reactivity. The application of nanotechnology introduces highly efficient,

precision-targeted methods for eliminating contaminants, setting new benchmarks in water treatment practices (Karakaş 2021).

A key development in this field is the creation of *nanofiltration (NF) membranes* (Elnashaie et al. 2015; Remya et al. 2022; Ojukwu and Nwaiwu 2023). These membranes, engineered with nanoscale pores, effectively filter out a broad range of contaminants, including salts, organic molecules and microorganisms. In practice, NF membranes are used in desalination to remove salts from seawater or brackish water, making it suitable for drinking and irrigation and treating industrial wastewater by removing organic compounds and pollutants. The benefits of NF include high efficiency in contaminant removal, reduced energy consumption compared to reverse osmosis, and improved water quality and safety (Karakaş 2021).

Nanoparticles also play a crucial role in water purification through various mechanisms such as *adsorption, photocatalysis* and *catalytic reactions*. For example, nanoparticles such as activated carbon or metal oxides can adsorb pollutants such as heavy metals, dyes and pesticides. Photocatalytic nanoparticles, such as titanium dioxide (TiO_2), can degrade organic pollutants under UV light, converting them into harmless byproducts (Peng et al. 2018; Karakaş 2021). In addition, nanocatalysts facilitate reactions that detoxify or neutralize harmful substances in water. These methods effectively remove a wide range of contaminants, offer rapid purification and are suitable for treating surface and groundwater (Karakaş 2021; Ojukwu and Nwaiwu 2023).

Nanotechnology further enhances water treatment systems by developing *advanced coatings and filters* (Karakaş 2021; Vishnu et al. 2022). Nanostructured coatings with antimicrobial properties prevent bacterial growth and biofilm formation on filtration membranes and equipment. Self-cleaning filters made from nanostructured materials reduce fouling and extend the lifespan of these systems. These innovations result in improved performance, reduced maintenance and operational costs, and enhanced safety and hygiene (Lee et al. 2010).

Nanosensors are also instrumental in monitoring water quality with high sensitivity and accuracy. They provide real-time data on parameters such as pH, turbidity and contaminant levels and can detect even low concentrations of pollutants (Lee et al. 2010; Karakaş 2021). This capability allows for early intervention and better management of water quality issues, leading to more informed decision-making.

In wastewater treatment, nanotechnology improves conventional processes and supports resource recovery. Nanoreactors enhance biological and chemical treatment processes in wastewater plants, while nanomaterials facilitate the recovery of

valuable metals and other resources, contributing to recycling and sustainability (Lee et al. 2010; Varghese et al. 2019; Remya et al. 2022). These advancements result in more efficient treatment processes, potential resource recovery, lower environmental impact and operational costs.

Overall, nanotechnology delivers advanced solutions for water treatment, enhancing filtration, purification, monitoring and resource recovery. These innovations promise better water quality, increased efficiency and more sustainable practices, marking a major leap forward and establishing meticulous and effective contaminant removal as a standard practice.

8.6.3. *Case study 3: nanotechnology in soil pollution remediation*

Nanotechnology has revolutionized soil pollution remediation, offering sophisticated methods for addressing contamination that traditionally demands significant resources and effort. Among the leading applications of nanotechnology in this field is the use of nanoparticles for effectively removing or transforming pollutants in the soil (Seeman 2003; Karakaş 2021; Gamage et al. 2022).

Nanoparticle-based contaminant removal represents a pivotal technique. For instance, nanoparticles such as zero-valent iron (ZVI) and magnetite are used to address heavy metal contamination. These nanoparticles interact with metals such as lead, arsenic and chromium to either neutralize their toxicity or immobilize them, preventing their spread (Seeman 2003). Their reactive properties enable them to convert hazardous metals into less harmful forms or secure them in a stable state.

In addition, *organic pollutant degradation* is achieved through nanoparticles such as TiO_2 and zinc oxide (ZnO). These nanoparticles serve as catalysts in breaking down organic contaminants such as pesticides, pharmaceuticals and industrial chemicals (Palithya et al. 2021; Vishnu et al. 2022).

Under specific conditions, such as exposure to light, these nanoparticles facilitate the breakdown of these pollutants into less harmful byproducts, thus mitigating their environmental impact.

Another innovative approach is the use of nanocapsules for *contaminant transport*. These nanocapsules can be designed to deliver reactive agents directly to specific contaminated areas within the soil (Palithya et al. 2021; Ojukwu and Nwaiwu 2023). This targeted delivery enhances the remediation process by ensuring that the reactive agents are precisely applied to the pollutants, thereby improving the overall effectiveness of the cleanup.

Enhanced *soil washing* is another area where nanotechnology proves beneficial. Integrating nanomaterials into soil-washing solutions mobilizes contaminants more effectively (Palithya et al. 2021). Nanomaterials aid in breaking down or dispersing pollutants, which facilitates their removal from the soil. This advancement enhances traditional soil washing methods, leading to more efficient remediation of contaminated sites.

The advantages of applying nanotechnology to soil pollution remediation are significant. It provides high efficiency in addressing a wide range of contaminants, including heavy metals and organic pollutants (Ruan et al. 2012; Elnashaie et al. 2015). Nanotechnology enables in situ treatment, reducing the need for excavation and minimizing disruption to the surrounding environment. This results in a more streamlined and sustainable remediation process, showcasing the potential of nanomaterials to offer effective and environmentally friendly solutions to soil pollution challenges.

8.6.4. *Case study 4: nanotechnology in air pollution remediation*

Nanotechnology has revolutionized the approach to air pollution control, offering cutting-edge solutions for particulate matter and gaseous pollutants. This technology has introduced several advanced methods that significantly enhance air quality and address environmental and health concerns.

Nanocatalysts for air purification are at the forefront of this innovation. These catalysts are incorporated into air filters to accelerate the breakdown of pollutants (Karakaş 2021; Gamage et al. 2022). For instance, nanocatalysts effectively decompose volatile organic compounds (VOCs) and nitrogen oxides (NOx), which are prevalent in emissions from industrial processes and vehicles (Elnashaie et al. 2015; Peng et al. 2018; Gamage et al. 2022). Nanocatalysts play a crucial role in reducing air pollution and improving air quality by facilitating chemical reactions that convert these harmful substances into less toxic byproducts.

Nanostructured filters represent another significant advancement. These filters use nanomaterials, such as carbon nanotubes or nanofibers, to capture fine particulate matter and harmful gases more efficiently than traditional filters (Vishnu et al. 2022). The unique properties of nanostructured filters – such as their large surface area and small pore size – enhance their ability to remove airborne pollutants, resulting in cleaner and healthier air (Gamage et al. 2022).

Photocatalytic air purifiers use nanoparticles such as TiO_2 to degrade airborne pollutants when exposed to ultraviolet (UV) light (Karakaş 2021). This photocatalytic process breaks down harmful substances into non-toxic byproducts,

effectively purifying the air. This technology is particularly effective for improving indoor air quality and reducing hazardous pollutants.

The benefits of nanotechnology in air pollution control are substantial. It offers improved air quality through more effective pollutant removal, vital for safeguarding public health and the environment (Gamage et al. 2022; Remya et al. 2022). In addition, nanotechnology has the potential to lower emissions from industrial sources and vehicles, helping to meet stringent air quality standards. These advancements represent a significant leap forward in environmental technology, providing more effective and sustainable solutions for managing air pollution (Gamage et al. 2022).

Ultimately, nanotechnology represents a significant advancement in soil and air pollution remediation. By harnessing the unique properties of nanomaterials, it offers targeted and highly effective solutions for contaminant removal and air purification. In soil remediation, nanotechnology enhances the efficiency of contaminant extraction, reduces environmental disruption and introduces advanced cleanup techniques. Air pollution control improves the capture and breakdown of pollutants, leading to better air quality and supporting sustainable practices. These technological innovations mark a new era in environmental remediation, providing more efficient, effective and sustainable methods for protecting natural resources and public health.

8.6.5. *Case study 5: nanoremediation of oil spills*

Oil spills represent a severe environmental hazard, and nanotechnology provides novel solutions to manage these incidents more effectively. One significant application is the use of *nanomaterial-based absorbents* for the remediation of oil spills in large water bodies (Elnashaie et al. 2015; Peng et al. 2018; Gamage et al. 2022). These materials, such as carbon nanotubes and nanofibers, have unique properties that allow them to absorb and efficiently contain oil spills (Gamage et al. 2022). Their nanostructured nature gives them an exceptionally high surface area, which enhances their ability to capture and hold oil. This capability makes the process of removing oil from water surfaces faster and more effective, compared to traditional absorbents such as booms and pads, which often struggle to manage large spills or recover the oil (Elnashaie et al. 2015; Peng et al. 2018; Lisa et al. 2021).

Another key advancement is the deployment of nanocatalysts for oil degradation (Ruan et al. 2012; Elnashaie et al. 2015; Peng et al. 2018; Pandey and Jain 2020; Lisa et al. 2021; Gamage et al. 2022). Nanocatalysts are designed to accelerate the breakdown of hydrocarbons found in oil spills (Karakaş 2021; Gamage et al. 2022). These catalysts speed up chemical reactions that break down oil into less harmful

substances, thus facilitating a more rapid natural degradation process. By boosting the rate at which oil is broken down, nanocatalysts improve the speed and efficiency of spill response efforts (Pandey and Jain 2020; Gamage et al. 2022). This approach not only helps mitigate the spill's immediate effects but also contributes to long-term environmental recovery.

The benefits of applying nanotechnology to oil spill remediation are considerable. The methods developed offer enhanced efficiency in absorbing and degrading oil contaminants, significantly reducing the environmental impact of spills. They also improve response times compared to conventional methods, enabling quicker mitigation of damage. In addition, recovering valuable hydrocarbons from spills presents economic advantages, as it helps offset some of the costs associated with cleanup operations and reduces waste.

8.6.6. *Case study 6: nanotechnology for groundwater remediation*

In groundwater remediation, nanotechnology offers cutting-edge solutions for cleaning water tainted by a range of pollutants, including organic chemicals and heavy metals. *Nanoparticle injection* is one key technique (Karakaş 2021; Gamage et al. 2022; Remya et al. 2022). This process involves injecting nanoparticles into contaminated groundwater to assist in removing or transforming pollutants (Gamage et al. 2022). The nanoparticles engage in chemical reactions such as reduction or oxidation, which help break down pollutants or convert them into less harmful forms. For example, these nanoparticles can interact with heavy metals to stabilize them, stopping their spread and reducing toxicity. This method proves highly effective even at low contaminant concentrations, making it crucial for addressing widespread groundwater pollution.

Another critical application is using *nanostructured filters* for groundwater remediation (Gamage et al. 2022; Vishnu et al. 2022). These filters, which incorporate nanomaterials, capture and remove contaminants from groundwater. The unique properties of nanomaterials, including their small size and large surface area, enhance the filter's ability to trap pollutants more effectively than conventional filtration systems. This capability includes capturing contaminants that traditional filters might miss at very low concentrations. As a result, nanostructured filters are invaluable for both industrial and environmental groundwater treatment.

There are substantial benefits to applying nanotechnology to groundwater remediation. This technology effectively treats complex contaminant mixtures, handles pollution at low concentrations and enables real-time monitoring and adjustment of remediation efforts. These innovations lead to notable improvements in the efficiency and effectiveness of groundwater cleanup, ultimately supporting

better management of contaminated water resources and protecting public health and the environment.

8.6.7. *Case study 7: nanotechnology in drug delivery*

Nanotechnology has dramatically transformed the field of drug delivery, offering sophisticated solutions for transporting therapeutic agents with remarkable precision. This advancement enhances treatment effectiveness and reduces side effects by leveraging the unique properties of nanomaterials (Vilos 2014; Patra et al. 2018; Ahmed et al. 2021; Mitchell et al. 2021; Vishnu et al. 2022).

One of the key breakthroughs is *targeted drug delivery*. By using nanocarriers such as liposomes, dendrimers and polymeric nanoparticles, drugs can be directed specifically to diseased cells or tissues (Patra et al. 2018; Khanzada et al. 2021; Mitchell et al. 2021). These nanocarriers can be engineered to bind selectively to receptors on target cells, ensuring that therapeutic agents are delivered precisely where they are needed. Surface modifications with ligands or antibodies further enhance this targeting, concentrating the drug's effects on the affected areas while minimizing exposure to healthy cells (Khanzada et al. 2021).

Controlled release systems are another significant advancement made possible by nanotechnology. Nanocarriers designed for controlled release can gradually dispense their drug payload over extended periods. This approach helps maintain therapeutic drug levels, reducing dosing frequency and improving patient adherence. In addition, some nanocarriers are engineered to release their contents in response to specific environmental triggers, such as changes in pH or temperature, which ensures that the drug is activated only in the intended conditions (Moshed et al. 2017; Anjum et al. 2021; Khanzada et al. 2021; Mitchell et al. 2021; Haleem et al. 2023).

Nanotechnology also addresses issues of poor *bioavailability*, which is often associated with certain drugs. Nanocrystals can significantly improve solubility and dissolution rates by reducing drug particles to the nanoscale. Nanostructured carriers can protect drugs from degradation and facilitate their transport across biological barriers, such as the blood–brain barrier, which many drugs struggle to penetrate (Anjum et al. 2021; Haleem et al. 2023).

Moreover, nanotechnology integrates diagnostic and imaging capabilities with drug delivery, creating a field known as theranostics. Theranostic nanocarriers combine therapeutic and diagnostic functions, enabling real-time drug distribution and effectiveness monitoring. This integration allows for more personalized and adaptive therapies, as the movement and impact of drugs within the body can be

tracked and assessed with precision (Moshed et al. 2017; Anjum et al. 2021; Haleem et al. 2023).

Hence, nanotechnology has fundamentally changed drug delivery by introducing precise, controlled and efficient methods for administering therapeutic agents. The reported Figure 8.3 shows the process of drug target to the specified application. The creation of sophisticated nanocarriers has advanced drug targeting, optimized controlled release, improved bioavailability and integrated diagnostic features. These innovations result in more effective treatments, reduced side effects and enhanced patient outcomes. These developments represent a significant progression in medical science, opening up new opportunities for personalized and effective therapeutic options.

8.7. Future prospects of nanotechnology in chemical engineering

Integrating nanotechnology into chemical engineering is poised to bring transformative changes across various fields. Nanotechnology is redefining conventional practices and driving innovation by advancing areas such as materials science, precision chemical processes, drug delivery, environmental remediation, water treatment and energy solutions. The synergy between nanotechnology and other advanced technologies, such as artificial intelligence (AI), promises to deliver more effective, sustainable and innovative solutions. This collaboration is shaping the future of chemical engineering and contributing to the progress of numerous industries. The following points highlight some of these advancements in detail.

8.7.1. *Advanced materials development*

The future of advanced materials development is set to be revolutionized by nanotechnology, which offers the ability to create materials with exceptional performance characteristics. Researchers can enhance properties such as strength, flexibility and conductivity by manipulating substances at the nanoscale. Upcoming advancements in nanotechnology will lead to the development of smarter, more durable materials with unprecedented capabilities, transforming industries ranging from electronics to manufacturing and opening new possibilities for innovation and application.

– *Enhanced properties:* nanotechnology is advancing materials science by facilitating the creation of materials with remarkable attributes. Nanomaterials such as graphene and carbon nanotubes are distinguished by their unparalleled strength, flexibility and electrical conductivity (Lisa et al. 2021; Vishnu et al. 2022). These properties significantly surpass traditional materials, promising to drive progress in diverse sectors including electronics, aerospace and construction.

– *Smart materials:* the development of smart materials represents a major leap forward, as these materials are designed to respond dynamically to environmental changes such as temperature, pressure or pH. By adjusting their properties in reaction to external stimuli, smart materials enable innovative applications such as self-healing structures, adaptive coatings and responsive textiles (Vishnu et al. 2022; Lisa et al. 2021). These advancements will enhance functionality and performance, offering customized solutions to meet a wide range of industrial needs.

8.7.2. *Precision chemical processes*

The future of precision chemical processes is set to be revolutionized by nanotechnology, offering unmatched control and efficiency in chemical reactions (Ruan et al. 2012; Elnashaie et al. 2015; Peng et al. 2018; Lisa et al. 2021). By manipulating materials at the nanoscale, researchers can precisely adjust reaction conditions, boost catalyst performance and reduce waste. These advancements are expected to create more sustainable and cost-effective manufacturing methods, enhance resource utilization and elevate the efficiency of chemical processes, ultimately fostering innovation across diverse industries.

– *Controlled reactions*: nanotechnology introduces a new dimension of precision by allowing for the manipulation of materials at the nanoscale (Vishnu et al. 2022). This capability enables the optimization of catalyst performance and reaction efficiency while reducing the production of byproducts (Sudha et al. 2018; Bayda et al. 2020; Golan et al. 2021). The result is more controlled and effective chemical reactions, leading to substantial advancements in manufacturing processes.

– *Sustainable manufacturing*: the precision enabled by nanotechnology fosters more sustainable manufacturing practices. By cutting down on resource use and waste generation, nanotechnology streamlines production processes and lessens the environmental impact (Shi and Plata 2018; Vishnu et al. 2022). This aligns with the broader objective of achieving chemical engineering and manufacturing sustainability.

8.7.3. *Innovations in drug delivery*

The future of innovations in drug delivery is on the brink of a major breakthrough, driven by advancements in nanotechnology (Vilos 2014; Moshed et al. 2017; Patra et al. 2018; Ahmed et al. 2021; Anjum et al. 2021; Mitchell et al. 2021; Vishnu et al. 2022; Haleem et al. 2023). Emerging technologies promise to enhance the precision, effectiveness and efficiency of delivering therapeutic agents. Researchers use sophisticated nanocarriers to achieve targeted delivery to specific cells or tissues, improve controlled release mechanisms and minimize side effects.

These innovations are set to transform treatment paradigms, offering more personalized and effective therapeutic options for a wide range of medical conditions (Anjum et al. 2021; Mitchell et al. 2021; Haleem et al. 2023).

– *Targeted therapies*: nanotechnology will transform drug delivery systems by developing advanced nanocarriers that can deliver therapeutic agents directly to specific cells or tissues. These targeted therapies will enhance the effectiveness of treatments, particularly for diseases that require precise targeting, such as cancer (Khanzada et al. 2021; Mitchell et al. 2021). Focusing the drug's action on diseased cells will minimize side effects on healthy tissues, leading to improved patient outcomes.

– *Controlled release*: nanocarriers with controlled release capabilities will allow for the gradual release of drugs over extended periods. This innovation will facilitate the management of chronic conditions by maintaining therapeutic levels of medication and reducing dosing frequency (Anjum et al. 2021; Khanzada et al. 2021; Mitchell et al. 2021; Haleem et al. 2023). In addition, some nanocarriers can be engineered to release drugs in response to specific physiological triggers, further enhancing treatment precision (Khanzada et al. 2021; Vishnu et al. 2022).

8.7.4. *Sustainable environmental remediation*

The future of sustainable environmental remediation is being transformed by advancements in nanotechnology. These breakthroughs can potentially revolutionize soil, water and air pollutant management. By leveraging the unique properties of nanomaterials, future techniques will improve contaminant removal efficiency, facilitate real-time monitoring and promote eco-friendly practices (Shi and Plata 2018; Gamage et al. 2022; Remya et al. 2022). This evolution aims to tackle environmental challenges more effectively, aligning with broader sustainability and conservation goals to foster cleaner and healthier ecosystems.

– *Pollutant cleanup*: nanotechnology enhances environmental remediation by optimizing techniques for removing pollutants from soil, water and air. Specialized nanomaterials can be designed to target and break down contaminants more effectively, providing solutions for complex pollution problems (Gamage et al. 2022; Vishnu et al. 2022). Integration of real-time monitoring technologies with nanomaterials offers immediate data on pollution levels, aiding in proactive environmental management (Gamage et al. 2022).

– *Sustainable practices*: innovations driven by nanotechnology contribute to sustainable environmental management by developing effective pollution control methods and conserving resources (Lisa et al. 2021; Vishnu et al. 2022). These advancements tackle pressing environmental challenges such as soil degradation and water contamination while fostering overall ecosystem health.

8.7.5. *Water treatment advancements*

The future of water treatment is poised for transformation through nanotechnology, which promises to revolutionize purification methods and enhance filtration systems (Karakaş 2021; Gamage et al. 2022). By leveraging nanomaterials with unique properties, future advancements will enable more efficient removal of contaminants, including microorganisms and chemicals, ensuring cleaner and safer water sources.

Nanotechnology's ability to target and eliminate pollutants at the molecular level will lead to breakthroughs in water treatment processes, paving the way for innovative solutions and improved water quality (Karakaş 2021; Gamage et al. 2022; Remya et al. 2022).

– *Enhanced filtration*: nanotechnology will lead to the development of advanced filtration systems capable of removing a wide range of contaminants, including microorganisms, chemicals and heavy metals. Nanomaterial-based filters will offer higher efficiency and longer lifespans compared to traditional filtration methods, ensuring safer and cleaner water sources (Karakaş 2021; Vishnu et al. 2022).

– *Novel purification methods*: future advancements will focus on developing innovative purification techniques that improve water treatment processes. Nanotechnology will enable the creation of highly effective purification systems that address emerging contaminants and adapt to varying water quality challenges, contributing to more reliable and sustainable water treatment solutions (Karakaş 2021; Gamage et al. 2022; Remya et al. 2022).

8.7.6. *Energy solutions*

The future of energy solutions is set to be dramatically influenced by advances in nanotechnology. Emerging innovations in nanomaterials promise to enhance the performance and efficiency of energy storage and conversion systems. For instance, advancements in nanotechnology are expected to lead to the development of more effective batteries, fuel cells and solar cells, contributing to more sustainable and efficient energy technologies. By improving energy storage capabilities and conversion efficiency, these breakthroughs aim to address the growing demand for cleaner and more reliable energy sources, paving the way for a more sustainable energy future (Alarfaj et al. 2018; Shi and Plata 2018; Vishnu et al. 2022).

– *Improved storage and conversion*: nanotechnology will enhance energy storage and conversion systems by improving the performance of batteries, fuel cells and solar cells (Shi and Plata 2018; Golan et al. 2021). Nanomaterials will increase energy density, faster charging times and higher efficiency, driving the development

of more sustainable energy technologies. These advancements will support the transition to cleaner and more efficient energy sources.

– *Energy efficiency*: integrating nanotechnology will boost energy efficiency by optimizing energy storage and conversion processes (Pandey and Jain 2020; Golan et al. 2021). Enhanced materials and technologies will contribute to developing next-generation energy solutions, supporting efforts to reduce energy consumption and greenhouse gas emissions.

8.7.7. *Integration with AI and automation*

The future of chemical engineering will be increasingly shaped by integrating nanotechnology with AI and automation. This convergence promises to elevate precision and efficiency in chemical processes by leveraging AI to optimize reaction conditions, predict material behaviors and automate complex tasks (Ananikov 2024).

The synergy of nanotechnology with AI and automation will enable smarter, more adaptive chemical engineering systems, enhancing both the speed and accuracy of manufacturing processes (Nandipati et al. 2024; Naik and Jagtap 2024). As these technologies advance, they will drive innovation, streamline operations and contribute to more sustainable and efficient industrial practices.

– *Smarter processes*: combining nanotechnology with AI and automation will lead to smarter chemical engineering processes. AI-driven applications will optimize reaction conditions, predict material behavior and automate complex tasks, enhancing the efficiency and precision of chemical engineering operations (Ur Rehman et al. 2024).

– *Increased efficiency*: the integration of AI and automation with nanotechnology will drive further advancements in efficiency and precision (Egorov et al. 2021). This synergy will enable more innovative and effective solutions, setting the stage for a future where chemical engineering processes are optimized for performance, sustainability and scalability (Habeeb et al. 2023).

8.8. Conclusion

The future of chemical engineering is poised for a profound transformation with the integration of nanotechnology. This revolutionary innovation is set to advance numerous key areas significantly. In advanced materials development, nanotechnology will facilitate the creation of materials with exceptional properties, such as enhanced strength, flexibility and conductivity. Breakthroughs such as graphene and carbon

nanotubes will usher in smarter, more durable products, revolutionizing manufacturing and opening new possibilities across various industries. In precision chemical processes, nanotechnology will provide unparalleled control over chemical reactions. By optimizing catalyst performance, enhancing reaction efficiency and minimizing waste, this technology will foster more sustainable and cost-effective manufacturing practices, driving innovation and refining industrial processes.

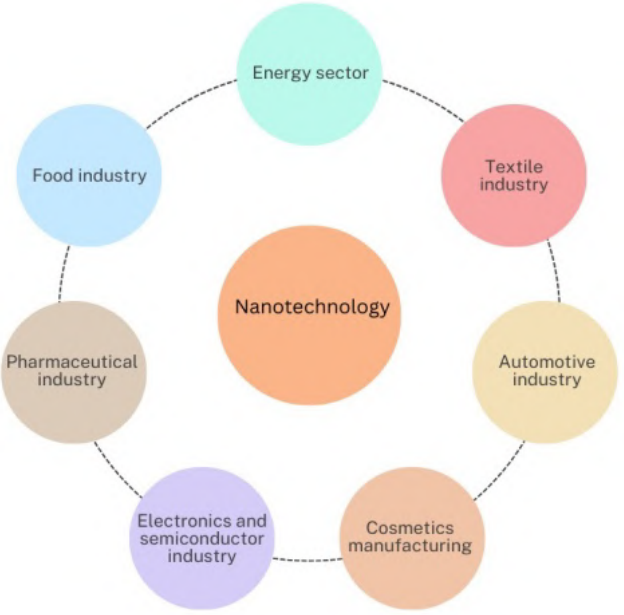


Figure 8.1. *Nanotechnology in various interdisciplinary applications. For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

The realm of drug delivery will see transformative improvements through nanotechnology. Advanced nanocarriers will enable more precise targeting of therapies and controlled release, significantly boosting treatment efficacy, reducing side effects and advancing personalized medicine. Sustainable environmental remediation will greatly benefit from nanotechnology, improving methods for cleaning soil, water and air pollutants. Innovations will enhance contaminant removal, support real-time monitoring and align with broader sustainability and environmental stewardship goals. Water treatment will advance with nanotechnology, leading to more efficient filtration and purification methods. These advancements will ensure cleaner and safer water sources, addressing critical needs in water management. In energy solutions, nanotechnology will enhance the

performance of storage and conversion systems, leading to more efficient and sustainable energy technologies. Improvements in batteries, fuel cells and solar cells will drive progress in this vital sector. Finally, the integration of nanotechnology with AI and automation will revolutionize chemical engineering processes. AI-driven applications will optimize reaction conditions, predict material behavior and automate complex tasks, significantly advancing efficiency and precision.

Overall, nanotechnology represents a transformative force in chemical engineering, poised to redefine traditional practices and drive innovation across multiple domains. By leveraging the unique properties of nanomaterials and combining them with cutting-edge technologies, we are on the cusp of achieving more effective, sustainable and groundbreaking solutions that will benefit both industry and society.

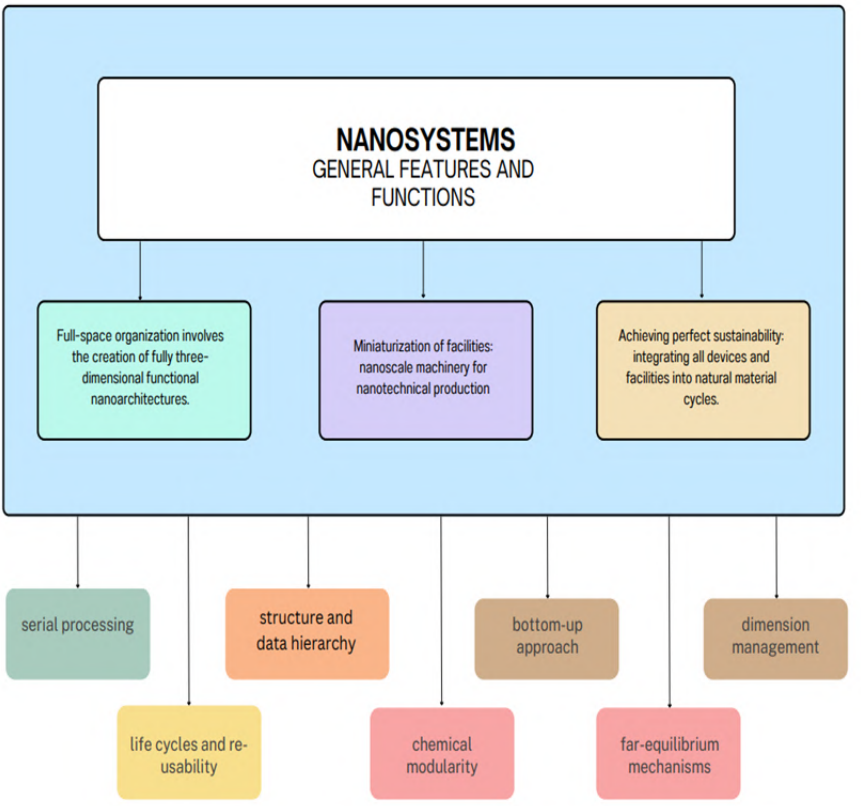


Figure 8.2. *General features and functions of nanosystems. For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

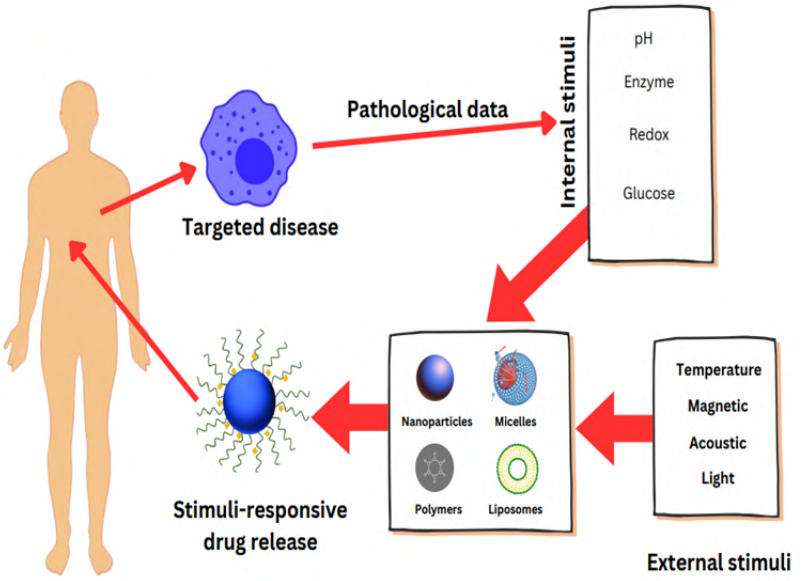


Figure 8.3. *Nanotechnology in targeted drug delivery systems. For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

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PART 3

Sustainability and Safety

9

Green Chemistry and Sustainable Processes

This study delves into the innovative field of “green chemistry”, which focuses on minimizing the environmental and health impacts of traditional chemical processes. It explores core principles such as atom economy, pollution prevention and the use of safer chemicals. The chapter highlights the practical applications of green chemistry in various industries, including pharmaceuticals, agriculture, materials science, energy production, manufacturing and environmental remediation. Emphasis is placed on its role in developing safer, more efficient and eco-friendly products and processes.

Despite its significant potential for sustainability, green chemistry faces challenges such as economic feasibility, regulatory barriers, public awareness, and the need for education and training. The chapter also examines the integration of green chemistry with sustainable processes, which go beyond chemical reactions to include recycling, waste reduction, energy efficiency, water conservation, renewable resources and the circular economy. It stresses the importance of these practices in tackling environmental challenges and fostering a more balanced relationship between science and the environment.

This comprehensive analysis underscores the necessity of adopting greener and more sustainable practices within chemistry and across various industries. The synergy between green chemistry and sustainable processes promotes resource efficiency, reduces carbon emissions, conserves water and decreases reliance on fossil fuels, supporting a resilient and sustainable economy.

Chapter written by Amit PARASHAR, Anurag TEWARI, Prahalad PRASAD PAROHA, Shikha GOVIL, Rajeev Kumar SINGH, Shailendra BADAL and Pastor ARGULLES.

9.1. Introduction

Green chemistry is a revolutionary discipline that has emerged as a response to the environmental and health concerns associated with conventional chemical processes. It focuses on designing products and processes that minimize or eliminate the use and generation of hazardous substances. This study delves into the principles, practices and applications of green chemistry, as well as its integral connection with sustainable processes (Horváth and Anastas 2007).

Green chemistry seeks to transform the chemical industry by promoting sustainable practices that minimize environmental impact and enhance efficiency. Key principles include designing less hazardous syntheses to reduce toxic by-products and improving energy efficiency in chemical processes. For instance, replacing traditional solvents with water or ionic liquids can reduce chemical hazards and energy consumption. Using renewable feedstocks, such as plant-based materials, decreases dependence on fossil fuels and promotes sustainability. Designing chemicals for degradation ensures that they break down into harmless substances post-use, mitigating long-term environmental effects. Real-time analysis techniques enable immediate monitoring and control, preventing pollution at the source (Erythropel et al. 2018).

In agriculture, green chemistry applications such as bio-pesticides and organic fertilizers reduce harmful runoff and soil contamination. Energy production benefits from innovations such as more efficient solar cells and biofuels. Environmental remediation uses biodegradable materials to clean up pollutants effectively. Despite its promise, green chemistry faces challenges, including economic feasibility and technological limitations. Sustainable processes are essential for overcoming these barriers (Poliakoff 2002).

Green chemistry represents a pivotal approach in modern chemistry aimed at mitigating the environmental and health impacts associated with traditional chemical practices. Green chemistry finds application across diverse sectors, illustrating its versatility and impact. In pharmaceuticals, innovations such as solvent-free reactions and catalytic processes have revolutionized drug manufacturing, making it safer and more sustainable. In agriculture, green chemistry promotes the development of safer pesticides and precision farming techniques that optimize resource use and minimize environmental impact (Anastas and Eghbali 2009).

Similarly, in materials science, the green chemistry focuses on creating biodegradable plastics and eco-friendly coatings that reduce reliance on fossil fuels and minimize waste. Energy production benefits from green chemistry through advancements in renewable fuels, fuel cells and solar energy technologies, which enhance efficiency and reduce greenhouse gas emissions. The manufacturing sector

integrates green chemistry to achieve lean and green manufacturing processes, emphasizing waste reduction, energy efficiency and sustainable product design (Pollard 2006).

Despite its promise, green chemistry encounters several challenges. Economic viability often presents a barrier, as initial investments in research, development and infrastructure for greener technologies can be prohibitive for some industries. Regulatory frameworks, originally designed for conventional practices, may not adequately accommodate or incentivize green chemistry innovations, slowing their adoption. Public awareness and education about the benefits of green chemistry are essential for fostering demand and acceptance among consumers and businesses. In addition, there is a need for comprehensive education and training programs to equip current and future chemists/scientists with the skills and knowledge to implement green chemistry practices effectively (Keith et al. 2007).

9.2. The principles of green chemistry

Green chemistry principles guide chemists and industries towards developing processes that inherently reduce waste generation, minimize energy consumption and eliminate or reduce the use of toxic substances. Several industries have adopted green chemistry principles to streamline drug/product synthesis, reducing the environmental footprint and enhancing safety (Anastas and Eghbali 2009).

Green chemistry, the practice of designing chemical products and processes that reduce or eliminate hazardous substances, has shown significant potential through various case studies. One notable example is the development of bio-based plastics. Companies such as Nature Works LLC have pioneered the production of polylactic acid (PLA) from renewable resources such as corn starch. With a lower carbon footprint and less environmental impact than conventional plastics derived from petroleum, this biodegradable plastic provides a sustainable substitute (Ganesh et al. 2021).

In the pharmaceutical industry, Pfizer's development of a greener synthesis route for the drug sildenafil (Viagra) exemplifies the application of green chemistry principles. By optimizing the reaction conditions and using safer solvents, Pfizer significantly reduced waste and improved overall process efficiency. Another compelling case study involves the textile industry, where traditional dyeing processes are notorious for their environmental impact. The adoption of supercritical carbon dioxide ($scCO_2$) as a solvent for dyeing fabrics eliminates the need for water and reduces the use of harmful chemicals. Companies such as Dye Coo have commercialized this technology, demonstrating its feasibility and environmental benefits (da Silva 2024).

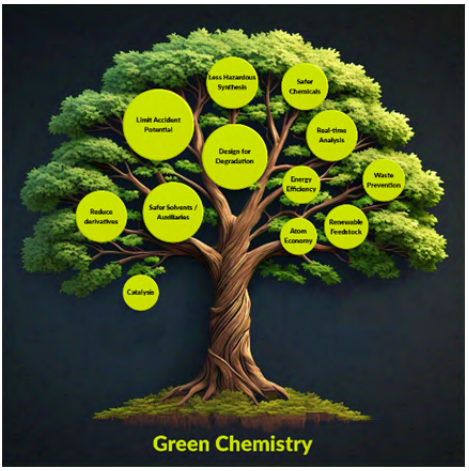


Figure 9.1. *Principle of green chemistry. For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

In agriculture, the use of biopesticides derived from natural sources such as neem oil provides an eco-friendly alternative to synthetic pesticides. These biopesticides are biodegradable and pose minimal risk to nontarget organisms and the environment. Environmental remediation has also benefited from green chemistry. The use of nano-iron particles for cleaning up groundwater contaminated with chlorinated solvents is a prime example. These particles effectively degrade pollutants into nontoxic compounds, offering a sustainable solution for environmental clean-up. Through examples of innovations that support sustainability, lessen their impact on the environment and increase efficiency, these case studies demonstrate the revolutionary potential of green chemistry in a variety of sectors (Yıldız et al. 2024).

9.2.1. *Prevention*

The avoidance of pollution at its source is the fundamental tenet of green chemistry. Green chemistry encourages the design of processes that do not produce waste in the first place, as opposed to dealing with trash and emissions after they are formed. Chemists are encouraged by this idea to take proactive steps to lessen their influence on the environment. By adopting prevention strategies, the chemical industry can significantly reduce the release of harmful substances into the environment. This involves designing chemical reactions that are inherently cleaner, using fewer or nontoxic reagents and minimizing the generation of hazardous by-products. A classic example is the replacement of a solvent-based reaction with a

solvent-free one, thereby eliminating the need for solvent recovery and reducing waste (Garrigues et al. 2019).

Preventing pollution at its source is the foundational idea of green chemistry. This principle underscores the importance of designing chemical processes that inherently avoid the creation of waste, rather than dealing with waste and emissions after they are generated. Prevention in green chemistry is a proactive approach that seeks to minimize the environmental footprint of chemical manufacturing from the outset. The rationale behind the prevention principle is rooted in both environmental and economic benefits. Environmentally, by preventing pollution at its source, we can reduce the release of harmful substances into the air, water and soil, thereby protecting ecosystems and human health. Economically, preventing waste reduces the costs associated with waste management and disposal and can improve the efficiency of chemical processes, leading to cost savings for the industry (Wang 2024).

For example, in traditional chemical processes, significant resources are often allocated to treat and dispose of waste. By designing processes that minimize or eliminate waste production, these resources can be redirected towards more productive uses.

Furthermore, these designs frequently lead to procedures that lower the likelihood of accidents and make workers safer, which can further save expenses and improve overall safety. A classic example of prevention in action is the replacement of solvent-based reactions with solvent-free alternatives. Solvents are often volatile organic compounds (VOCs) that can contribute to air pollution and pose health risks. By eliminating the use of solvents, not only is the need for solvent recovery and disposal eliminated, but also the overall environmental impact of the reaction is significantly reduced. This shift not only aligns with green chemistry principles but also demonstrates the potential for innovation in developing cleaner, more sustainable chemical processes (Horváth and Anastas 2007; Tregnago 2024).

9.2.2. *Atom economy*

Atom economy is a fundamental concept in green chemistry. It is based on the idea that chemical reactions should be designed to maximize the use of all atoms in the reactants, ensuring that the majority of the atoms end up in the desired product rather than as waste. An efficient atom economy is essential for resource conservation and waste reduction. For example, in the synthesis of pharmaceuticals, designing routes with a high atom economy can minimize the amount of waste generated, which is particularly important when producing expensive or complex molecules (Trost 1991).

The principle of atom economy is crucial for several reasons, both environmentally and economically. Efficient atom economy directly correlates with resource conservation and waste reduction. In traditional chemical processes, a significant portion of the atoms from reactants can end up as by-products or waste, which not only necessitates additional steps for waste management but also involves the loss of valuable raw materials. Chemists may create more effective methods that maximize atom economy, better use raw resources, cut waste and reduce the negative environmental effects of chemical manufacture (Trost 1995). The following lists a few instances of atomic economies:

– *Ibuprofen synthesis*: traditional synthesis of ibuprofen involved six steps with a significant amount of waste at each stage. In contrast, the Boots Company developed a more efficient three-step synthesis with a much higher atom economy. This newer method reduced the generation of waste significantly and improved the overall efficiency of the production process.

– *Green oxidation reactions*: traditional oxidation reactions often use stoichiometric amounts of reagents that generate substantial waste. An example of improving atom economy is the use of catalytic oxidants, such as using hydrogen peroxide (H_2O_2) instead of permanganate (MnO_4^-) for oxidation reactions. H_2O_2 decomposes into water and oxygen, which are benign, while MnO_4^- produces manganese dioxide (MnO_2), which requires disposal (Shapiro and Caspi 1998).

9.2.3. *Less hazardous chemical syntheses*

A key goal of green chemistry is to use and produce chemicals that are less hazardous to human health and the environment. This principle entails avoiding or minimizing the use of toxic substances in chemical processes. It encourages the development of safer alternatives and the replacement of hazardous reagents with less harmful ones. In practice, it involves the use of green solvents, nontoxic catalysts and the development of methods that reduce or eliminate the need for harmful reagents. The application of less hazardous chemical syntheses is particularly evident in industries such as pharmaceuticals, where drug development processes have become significantly safer through the adoption of green chemistry principles. It encourages the development of safer alternatives and the replacement of hazardous reagents with less harmful ones (Arias-Andres 2018).

By focusing on less hazardous syntheses, chemists can reduce these risks, making chemical processes safer for workers, consumers and the environment, reducing the use of hazardous substances also aligns with regulatory trends that increasingly demand safer chemicals and processes. Companies that adopt these practices can avoid the costs and liabilities associated with hazardous waste management and regulatory compliance (Sanghi and Singh 2012). In addition, safer

chemicals and processes can lead to better consumer acceptance and marketability of products which are given as follows:

– *Pharmaceutical industry*: in drug development, the use of less hazardous syntheses has led to significant improvements. For example, the traditional synthesis of the anti-inflammatory drug ibuprofen involved the use of large quantities of hazardous solvents and reagents. A greener synthesis developed by BHC Company (now part of BASF) uses a catalytic process that significantly reduces the use of hazardous substances and minimizes waste production.

– *Green solvents*: the replacement of traditional organic solvents with greener alternatives is a common practice. For example, $scCO_2$ and water are increasingly used as solvents in chemical reactions. Having less of an effect on the environment, these solvents are nontoxic. An example is the use of $scCO_2$ in the extraction of natural products and in polymerizations.

– *Nontoxic catalysts*: traditional catalysts often involve heavy metals that can be toxic and difficult to dispose of safely. Green chemistry promotes the use of nontoxic catalysts, such as enzymes, which are biodegradable and can operate under mild conditions. For example, the use of enzyme catalysis in the production of biodiesel from vegetable oils is a safer alternative to conventional methods that use sodium methoxide, a hazardous substance.

– *Biodegradable polymers*: the development of biodegradable polymers, such as PLA derived from renewable resources such as corn starch, offers a less hazardous alternative to traditional petroleum-based plastics. These polymers decompose more easily and reduce the environmental impact associated with plastic waste.

– *Safer pesticides*: in agriculture, the development of biopesticides derived from natural sources, such as neem oil or beneficial microorganisms, offers a safer alternative to synthetic chemical pesticides. These biopesticides are less toxic to nontarget organisms, including humans, and are more environmentally friendly (Gajewski et al. 2017; Tucker et al. 2010).

9.2.4. *Design for energy efficiency*

One essential component of sustainable chemistry is energy usage. The field of green chemistry aims to decrease the overall energy consumption and enhance the efficiency of chemical processes through design. By reducing energy usage and related greenhouse gas emissions, this approach seeks to lessen the environmental impact of chemical processes. Strategies for achieving energy efficiency include optimizing reaction conditions, reducing the number of synthetic steps and using catalysts that lower the energy barriers of reactions. The development of cleaner and

more efficient energy sources, such as renewable energy, also aligns with this principle (Ramchuran 2023).

Chemical process energy efficiency is critical for both cost reduction and environmental impact mitigation. Frequently, burning fossil fuels releases greenhouse gases such as carbon dioxide (CO_2) into the atmosphere during the energy generation process. We can drastically cut these emissions and slow down climate change by developing energy-efficient procedures. Optimizing energy use also enhances the overall sustainability of chemical manufacturing. Energy-intensive processes can be costly and resource-draining. By lowering energy requirements, industries can achieve more sustainable operations, reduce dependency on nonrenewable energy sources and improve their economic viability. This approach aligns with global sustainability goals and regulatory trends pushing towards carbon neutrality (Green 2016):

– *Microwave-assisted organic synthesis (MAOS)*: traditional heating methods in chemical reactions often lead to significant energy loss. Microwave-assisted synthesis offers a more energy-efficient alternative by directly heating the reactants, thus reducing the reaction time and energy consumption. For example, the synthesis of pharmaceuticals using microwave irradiation has been shown to be faster and more efficient compared to conventional heating methods.

– *Flow chemistry*: flow chemistry involves conducting reactions in a continuous flow rather than in batch processes. This method improves heat and mass transfer, leading to better control over reaction conditions and higher energy efficiency. An example is the continuous flow synthesis of active pharmaceutical ingredients (APIs), which can significantly reduce energy usage compared to traditional batch processing.

– *Catalysis*: catalysts are crucial for lowering the activation energy of reactions, allowing them to proceed under milder conditions and with less energy input. For instance, the use of transition metal catalysts in hydrogenation reactions can achieve high conversion rates at lower temperatures and pressures, thereby saving energy.

– *Renewable energy integration*: integrating renewable energy sources, such as solar and wind, into chemical processes can further enhance energy efficiency. For example, solar energy can be used to drive photochemical reactions, reducing the reliance on fossil fuels and decreasing greenhouse gas emissions.

– *Optimized reaction conditions*: fine-tuning reaction parameters, such as temperature, pressure and solvent choice, can lead to significant energy savings. For instance, conducting reactions at room temperature and atmospheric pressure, when possible, avoids the energy costs associated with heating and pressurizing the system (Argyropoulos 2007).

9.2.5. *Use of renewable feedstocks*

Green chemistry emphasizes the importance of using renewable and sustainable feedstocks. This principle encourages the chemical industry to move away from relying solely on nonrenewable resources and to explore alternative, eco-friendly sources of raw materials. By incorporating renewable feedstocks, such as biomass, into chemical processes, we reduce our reliance on fossil fuels and finite resources. This has positive implications for resource conservation and reduces the carbon footprint associated with chemical production (Gandini 2008).

Renewable feedstocks often have a lower environmental impact. Biomass, for instance, can be sourced from agricultural residues, forestry by-products and other waste materials, making it a more sustainable option. The use of such materials can also help in managing waste and reducing the overall carbon footprint of chemical production. Renewable feedstocks typically result in lower net CO_2 emissions, as the carbon they contain is part of the natural carbon cycle, unlike the carbon from fossil fuels which adds to atmospheric CO_2 levels when burned (Peralta-Yahya 2012):

– *PLA* is derived from renewable resources such as corn starch or sugarcane. It is used in a variety of applications, from packaging materials to medical devices. The production of PLA from renewable biomass not only reduces dependency on petroleum-based plastics but also minimizes environmental pollution, as PLA decomposes into nontoxic by-products under industrial composting conditions.

– *Bio-based succinic acid* traditionally, succinic acid, an important chemical used in food, pharmaceuticals, and as a precursor to various polymers, is produced from petroleum-based feedstocks. However, advancements in biotechnology have enabled the production of bio-based succinic acid from renewable biomass, such as agricultural residues and lignocellulosic feedstocks. This bio-based process reduces greenhouse gas emissions and promotes a circular economy by using renewable resources (Che and Yang 2022).

9.2.6. *Reduction of derivatives*

The principle of reducing derivatives promotes the idea of simplifying chemical processes. It encourages chemists to minimize the use of unnecessary reagents, protective groups and intermediates. The reduction of derivatives not only simplifies synthesis but also reduces waste generation. A classic example is the reduction of protecting groups in organic synthesis. By designing reactions that do not require the installation and removal of protecting groups, the number of synthetic steps and waste generated can be substantially reduced (Lopez and Montalvo 2012).

The principle of reducing derivatives in green chemistry advocates for simplifying chemical processes by minimizing the use of unnecessary reagents, protective groups and intermediates. This approach not only streamlines synthesis but also reduces waste generation and improves overall efficiency. In organic synthesis, the use of protecting groups is common to shield reactive functional groups from unwanted reactions during transformations. However, the installation and removal of these groups typically require additional reagents and steps, leading to increased waste and lower overall yield (Mohamed et al. 2012). By developing methodologies that avoid the need for protecting groups or use more selective reactions, chemists can significantly reduce the environmental impact of chemical processes by adopting the following syntheses.

– *Oligosaccharide synthesis*: traditional methods for synthesizing complex oligosaccharides often involve the use of multiple protecting groups to control regioselectivity and stereochemistry. Modern approaches, such as one-pot or sequential reactions that minimize the need for protecting groups, have been developed to streamline the synthesis process and reduce waste generation.

– *Peptide synthesis*: in peptide chemistry, the use of orthogonal protecting groups is essential to control the selective coupling of amino acids. However, advancements in solid-phase peptide synthesis and peptide ligation strategies have reduced the dependency on protecting groups, leading to more efficient and environmentally friendly synthetic routes.

– *Metal-catalyzed reactions*: transition metal-catalyzed reactions, such as cross-coupling reactions and C-H activation, often proceed with high selectivity and do not require the use of protecting groups. These reactions enable direct functionalization of molecules, minimizing synthetic steps and waste production compared to traditional methods (Brentner 2012).

9.2.7. *Catalysis*

Catalysis is a central concept in green chemistry. It involves using catalysts to facilitate chemical reactions, typically under milder conditions and with lower energy requirements. Catalysts can enhance reaction rates, selectivity and efficiency, all of which contribute to greener processes. Catalysis reduces the number of reactants required, which in turn minimizes waste generation. In addition, catalysts often enable the use of less hazardous reagents, further aligning with the principle of less hazardous chemical syntheses (Sheldon 2008).

Catalysis is pivotal in green chemistry for its ability to accelerate chemical reactions under milder conditions, thereby reducing energy consumption and minimizing environmental impact. Catalysts work by lowering the activation energy barrier of reactions, allowing them to proceed at lower temperatures and pressures.

This efficiency not only improves reaction rates and selectivity but also conserves resources by reducing the number of reactants needed. By promoting more efficient use of raw materials, catalysis reduces waste generation and enhances the overall sustainability of chemical processes. Moreover, catalysts often enable the substitution of more hazardous reagents with safer alternatives, aligning with the principle of less hazardous chemical syntheses (Kilty and Sachtler 1974; Stuart and Fagnou 2007):

– *Transition metal catalysts*: palladium, platinum and other transition metals are commonly used as catalysts in various organic transformations, such as cross-coupling reactions and hydrogenations. These catalysts enable efficient bond formation and functionalization of molecules under mild conditions, reducing the need for harsh reagents.

– *Enzymatic catalysis*: enzymes are biocatalysts that facilitate biochemical reactions with high specificity and efficiency. They operate under mild conditions (ambient temperature and pH), reducing energy requirements and waste generation compared to traditional chemical processes.

– *Homogeneous catalysis*: homogeneous catalysts, such as organometallic complexes, dissolve in the same phase as reactants and facilitate reactions with high selectivity. These catalysts are effective in promoting green chemistry principles by minimizing by-products and enabling the use of renewable feedstocks (Ravikumar and Singh 2012).

9.2.8. *Design for degradation*

It is important to consider the end of life of chemical products throughout their design. In order to lessen a product's environmental persistence, green chemistry advocates producing goods that can break down into nontoxic materials. Reduced plastic waste is a result of biodegradable polymers, which are made to organically decompose in the environment. A fundamental part of this idea is the creation of items that can be recycled or broken down effectively and securely. In green chemistry, designing products with degradation in mind is crucial for reducing environmental impact. This principle advocates for developing chemical products that can break down into nontoxic substances after use, thereby minimizing persistence in the environment and potential harm to ecosystems. By ensuring products degrade safely, green chemistry aims to mitigate pollution and promote sustainability (Anderson and Gonzalez 2012). Few examples have been shown to explain design degradation:

– *PLA*: PLA is a biodegradable polymer derived from renewable resources such as corn starch or sugarcane. It is used in packaging materials and biomedical applications and degrades into nontoxic compounds under composting conditions.

– *Green surfactants*: compared to persistent conventional surfactants, environmentally friendly surfactants are made to break down easily into nontoxic chemicals after usage, reducing their influence on aquatic ecosystems.

– *Bio-based lubricants*: biodegradable lubricants synthesized from vegetable oils or other renewable sources decompose efficiently, reducing environmental contamination from used lubricants (Veleva and Cue 2019).

9.2.9. *Real-time analysis*

Real-time analysis involves the use of advanced monitoring and control techniques during chemical processes. This allows for immediate adjustments, increasing efficiency, minimizing waste and enhancing safety. Modern analytical tools, such as in-line spectroscopy and process mass spectrometry, enable real-time analysis and process optimization. By implementing these technologies, industries can reduce the need for rework and minimize environmental impacts (Zhang et al. 2018). Real-time analysis is integral part of green chemistry as it uses advanced monitoring and control techniques during chemical processes which are given as follows:

– *Pharmaceutical manufacturing*: real-time monitoring in pharmaceutical synthesis allows for immediate adjustments to optimize reaction conditions, ensuring consistent product quality and reducing production costs.

– *Chemical process control*: in chemical synthesis, in-line spectroscopy and process mass spectrometry enable real-time detection of intermediates and impurities, facilitating prompt corrective actions to maintain process efficiency and purity.

– *Environmental monitoring*: real-time analysis is used in environmental monitoring to detect pollutants in air, water and soil, enabling timely interventions to mitigate environmental impacts (Kümmerer and Clark 2016).

9.3. Applications of green chemistry

9.3.1. *Pharmaceuticals*

The pharmaceutical industry has greatly benefited from the principles of green chemistry. Precise control over critical parameters such as temperature and pressure leads to higher yields and reduced energy usage. In chemical production, continuous monitoring helps in adjusting catalyst concentrations or reaction times to minimize the formation of unwanted by-products. Implementing green chemistry in pharmaceuticals not only aligns with regulatory pressures and corporate

sustainability goals but also enhances operational efficiency and reduces costs in the long term. By adopting safer synthesis routes, selecting greener solvents, using efficient catalysis, designing eco-friendly formulations and using sustainable analytical techniques, pharmaceutical companies can improve their environmental footprint while maintaining high standards of product safety and efficacy by adopting the following processes (Li and Trost 2008).

– *Green synthesis of artemisinin*: artemisinin, an antimalarial drug, is now synthesized using a more efficient and eco-friendly process involving biocatalysis, which reduces waste and improves yield.

– *Ionic liquids in drug formulations*: ionic liquids are being explored as solvents in pharmaceutical formulations due to their low toxicity and recyclability, replacing traditional organic solvents.

– *Catalytic hydrogenation in API synthesis*: transition metal catalysts such as palladium are used in the hydrogenation of APIs, reducing environmental impact and improving process efficiency (Shapiro and Caspi 1998).

9.3.2. *Agriculture*

Implementing green chemistry principles in agriculture addresses environmental concerns while improving productivity and sustainability. By reducing chemical inputs, minimizing environmental pollution and promoting eco-friendly alternatives, green chemistry supports long-term agricultural viability and global food security. Agriculture depends on a variety of chemical inputs, including safer pesticides, fertilizers, pesticides, precision agriculture, biodegradable packaging, natural pest control, sustainable crop protection and herbicides (Gajewski et al. 2017). Green chemistry is transforming this industry by the following inputs.

– *Biopesticides*: *Bacillus thuringiensis* (Bt) formulations are used as biopesticides to control insect pests while posing minimal risk to beneficial organisms and the environment.

– *Precision agriculture technologies*: soil sensors and satellite imagery are used in precision agriculture to optimize fertilizer application and irrigation, reducing nutrient runoff and conserving water resources.

– *Biodegradable mulches*: mulching films made from biodegradable polymers such as PLA are used to suppress weeds and conserve soil moisture without contributing to plastic pollution (Sheldon 2005).

9.3.3. *Materials science*

Green chemistry is instrumental in the development of sustainable materials and products with reduced environmental impact. Integrating green chemistry principles into materials science enhances sustainability by reducing energy consumption, minimizing waste generation and mitigating environmental impacts associated with traditional materials production by focusing on biodegradability, eco-friendly formulations, reduced toxicity and recyclability (Clark and Macquarrie 2007).

– *Biodegradable plastics*: green chemistry facilitates the development of biodegradable plastics derived from renewable resources such as PLA and polyhydroxyalkanoates (PHAs). These materials offer alternatives to traditional plastics, reducing waste accumulation in landfills and oceans.

– *Eco-friendly coatings and adhesives*: green chemistry innovations result in environmentally friendly adhesives and coatings that release less VOCs and are less harmful to the environment and public health. For example, water-based paints and adhesives reduce air pollution and enhance interior air quality.

– *Green nanomaterials*: green chemistry promotes the synthesis of nanomaterials with reduced environmental impact and toxicity. Applications in electronics, energy storage (e.g. lithium-ion batteries) and sensors benefit from nanomaterials that are safer to manufacture and use.

– *Recyclable materials*: designing materials with recyclability in mind supports a circular economy by reducing the consumption of virgin resources. Examples include recyclable polymers and composites that maintain performance properties through multiple cycles of use and recycling (Sanderson 2011).

The creation of materials that contribute to a more sustainable future is encouraged by green chemistry. Key application domains include the following:

– *Water-based coatings*: water-based paints and coatings replace solvent-based alternatives, reducing VOC emissions and improving indoor air quality.

– *Green nanomaterials*: silver nanoparticles synthesized using green chemistry principles exhibit lower toxicity and environmental impact compared to conventional methods, suitable for antibacterial applications (DeSimone 2002).

9.3.4. *Energy production*

The energy sector benefits from green chemistry in various ways, as it seeks to reduce environmental impact and transition to renewable sources of energy.

Integrating green chemistry in energy production promotes sustainability by reducing carbon footprint, enhancing energy efficiency and fostering the transition to renewable energy sources.

By advancing renewable fuels, fuel cell technologies, solar energy solutions and carbon capture methods, green chemistry contributes to a cleaner and more sustainable energy future with the development of the following (Poliakoff and Licence 2007).

– *Renewable fuels*: green chemistry principles are instrumental in developing biofuels derived from biomass and hydrogen fuel produced via sustainable methods such as electrolysis. These fuels offer alternatives to fossil fuels, reducing greenhouse gas emissions and dependence on finite resources.

– *Fuel cells*: green chemistry advancements enhance fuel cell technology, improving efficiency and reducing emissions in transportation and stationary applications. For instance, proton exchange membrane fuel cells (PEMFCs) use platinum-based catalysts synthesized using greener methods, enhancing performance and durability.

– *Solar energy*: green chemistry innovations focus on improving the efficiency and sustainability of solar cells through materials such as perovskites and organic photovoltaics. These technologies enable cost-effective solar energy production with reduced environmental footprint compared to conventional silicon-based cells.

– *Carbon capture*: developing carbon capture and storage (CCS) technologies involves green chemistry approaches to capture and mitigate carbon emissions from fossil fuel combustion, contributing to climate change mitigation efforts (Constable 2002).

Green chemistry plays a pivotal role in transforming the energy sector towards sustainability by fostering innovations in renewable energy sources and reducing environmental impact, which includes:

– *Biofuels*: ethanol produced from corn or cellulosic biomass using enzymatic hydrolysis exemplifies green chemistry's application in renewable fuels, reducing greenhouse gas emissions compared to conventional gasoline.

– *Hydrogen fuel cells*: PEMFCs use platinum-based catalysts synthesized through green methods such as electrochemical deposition, enhancing efficiency and durability in hydrogen fuel cell vehicles.

– *Perovskite solar cells*: perovskite materials, synthesized using eco-friendly solvents and methods, exhibit high efficiency and potential for low-cost solar energy generation compared to traditional silicon-based photovoltaics (Tang 2005).

9.3.5. *Manufacturing*

Green chemistry principles are widely applicable in manufacturing industries, where efficiency and sustainability are paramount. This includes:

– *Lean and green manufacturing*: by integrating lean manufacturing practices with green chemistry, industries minimize waste generation, reduce energy consumption and optimize resource utilization. For example, Toyota's adoption of lean principles in automobile manufacturing has significantly reduced waste while improving efficiency.

– *Green engineering*: green engineering strategies focus on designing processes and products that minimize environmental impact. This includes optimizing chemical reactions to reduce solvent and energy use, as seen in the development of eco-friendly detergents using enzymatic reactions instead of harsh chemicals.

– *Recycling in manufacturing*: incorporating recycling and reuse practices in manufacturing processes helps minimize resource depletion and waste generation. For instance, recycling aluminum in beverage can manufacturing reduces energy consumption by up to 95% compared to producing aluminum from raw materials.

– *Safer cleaning products*: green chemistry drives the formulation of safer and environmentally friendly cleaning products, such as biodegradable surfactants and enzymes, reducing harmful chemical discharge into water bodies and ecosystems.

– *Sustainable packaging*: designing eco-friendly packaging materials such as bioplastics and compostable packaging reduces plastic waste and environmental footprint. For instance, Coca Cola's Plant Bottle™ uses plant-derived plastics for packaging, reducing dependence on fossil fuels.

Green chemistry in manufacturing sector enhances sustainability by reducing environmental impact, optimizing resource efficiency and meeting regulatory requirements. Industries may save a lot of money and practice environmental stewardship at the same time by using lean and green manufacturing techniques, including green engineering ideas, encouraging recycling, creating safer cleaning products and creating sustainable packaging (Dömling 2006; Trakhtenberg and Warner 2007):

– *Toyota production system (TPS)*: TPS integrates lean principles with environmental sustainability, minimizing waste generation and optimizing resource efficiency in automotive manufacturing.

– *Enzymatic detergents*: enzymatic detergents use biocatalysts in place of traditional harsh chemicals, reducing water pollution and improving biodegradability.

– *Aluminum can recycling*: the aluminum can industry recycles nearly 70% of used cans globally, conserving resources and reducing energy consumption significantly (Bashkin et al. 1999).

9.3.6. *Environmental remediation*

Green chemistry is not only about preventing pollution but also about cleaning up existing pollution in an environmentally friendly manner. It contributes to environmental remediation in several ways: *bioremediation, phytoremediation, green remediation and natural resource restoration.* Green chemistry plays a crucial role in environmental remediation by offering sustainable and eco-friendly approaches to clean up polluted sites and restore natural environments. Green chemistry in environmental remediation offers cost-effective and sustainable solutions to mitigate pollution and restore ecosystems (Lancaster 2016). By leveraging bioremediation, phytoremediation, green remediation practices and natural resource restoration, green chemistry contributes to long-term environmental health and resilience by the following inputs.

– *Exxon Valdez oil spill*: bioremediation using *Pseudomonas* species effectively reduced oil contamination in Prince William Sound, Alaska, after the Exxon Valdez oil spill.

– *Phytoremediation of heavy metals*: *Populus* trees were used to remediate heavy metal-contaminated soils in mining sites, reducing soil toxicity and improving ecosystem health.

– *Green remediation guidelines*: the U.S. Environmental Protection Agency (EPA) promotes green remediation practices that minimize environmental impacts during cleanup activities, ensuring sustainable site management (Varma 1999).

9.4. Challenges and barriers

While green chemistry offers immense potential for sustainability, several challenges and barriers need to be addressed.

9.4.1. *Economic viability*

Transitioning to green chemistry involves upfront costs for R&D and process changes, which can be prohibitive for smaller companies. Developing cost-effective green alternatives is crucial to overcoming this barrier. For example, the development of enzymatic processes to replace traditional chemical synthesis has shown promise in reducing costs and waste generation (Sheldon and Woodley 2018).

9.4.2. *Regulatory hurdles*

Existing regulations are often tailored to conventional chemical processes, posing challenges for the adoption of green chemistry innovations. Collaborative efforts between industry, government agencies and scientific communities are essential to revise regulations and streamline approval processes. Case studies include the European Union's REACH regulation, which encourages the use of safer chemicals through a comprehensive evaluation process.

9.4.3. *Public awareness*

Many consumers and businesses lack awareness of green chemistry's benefits. Public education campaigns, such as those by NGOs and industry associations, play a crucial role in raising awareness. For instance, the Green Chemistry Institute's outreach programs highlight the environmental and health advantages of sustainable chemistry, driving consumer demand for greener products.

9.4.4. *Education and training*

There is a significant gap in education and training programs focused on green chemistry principles. Collaborative initiatives between universities, research institutions and industry associations are needed to develop comprehensive training programs and certifications. Case studies include academic programs that integrate green chemistry into curricula, preparing future chemists and engineers to implement sustainable practices effectively (Raj et al. 2022).

Addressing these challenges is crucial for accelerating the adoption of green chemistry, which promises not only environmental benefits but also economic advantages through innovation and efficiency gains. By focusing on economic viability, regulatory adaptation, public awareness and education, stakeholders can create an enabling environment for sustainable chemistry practices, which are given as follows:

– *Enzymatic synthesis*: Novozymes' development of enzymatic processes for producing biofuels has reduced production costs and environmental impact compared to conventional methods.

– *REACH regulation*: the EU's Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) regulation promotes safer chemical alternatives through rigorous evaluation and authorization processes.

– *Green Chemistry Institute*: the American Chemical Society's Green Chemistry Institute promotes education and awareness of green chemistry principles

through conferences, workshops and educational resources (Smith et al. 2005; López-Porfiri et al. 2023).

9.5. Sustainable processes

Green chemistry is closely linked to sustainable processes, which extend beyond the scope of chemical reactions and encompass a broader range of industrial and societal practices. Some of the key aspects of sustainable processes are explained in the following subsections.

9.5.1. *Recycling*

Recycling plays a pivotal role in sustainable processes by reducing the consumption of raw materials, energy use and waste generation. For instance, recycling paper, plastics and metals conserves resources and lowers greenhouse gas emissions compared to producing new materials. Case studies include the recycling of PET plastics into new bottles, which reduces landfill waste and energy consumption (Nimkar 2018).

9.5.2. *Waste reduction*

Sustainable processes focus on minimizing waste throughout production and consumption cycles. This involves designing products with minimal packaging, optimizing manufacturing to reduce scrap and adopting circular economy principles where products are reused or recycled. Examples include companies using closed-loop manufacturing to recycle production waste back into their processes (Bisschops and Spanjers 2003).

9.5.3. *Energy efficiency*

Efficient energy use is critical for sustainability, promoting the adoption of renewable energy sources and energy-efficient technologies. Industries implement strategies such as combined heat and power (CHP) systems and smart grids to optimize energy consumption and reduce carbon emissions (Wang et al. 2019).

9.5.4. *Water conservation*

Sustainable processes emphasize water conservation through practices such as reducing water use in manufacturing, recycling wastewater and using water-saving

technologies in agriculture and industry. Technologies such as drip irrigation and grey water reuse contribute to water conservation efforts (Roy Choudhury 2013).

9.5.5. *Renewable resources*

Prioritizing renewable resources over nonrenewable ones in production processes reduces environmental impacts and supports the transition to a circular economy. This includes using renewable raw materials and bio-based fuels, contributing to sustainability goals (Gladysz 2005).

9.5.6. *Circular economy*

Sustainable processes promote a circular economy where products are designed for longevity, easy disassembly and material recovery. This approach minimizes waste, promotes resource reuse and fosters a more efficient economic system. By integrating these sustainable practices, industries can reduce their ecological footprint, enhance resource efficiency and meet growing consumer demands for environmentally friendly products (Barla et al. 2018). These projects support long-term economic viability and resilience in addition to the environment. The shared advantages are enumerated as follows:

– *Closed-loop manufacturing*: interface, a carpet manufacturer, implements a closed-loop recycling system where old carpets are collected, recycled into new materials and reused in production processes.

– *Drip irrigation systems*: drip irrigation is a practical example of water conservation in agriculture as it uses devices to distribute water directly to plant roots, reducing waste and increasing crop yields.

– *Renewable energy adoption*: Tesla's Gigafactory in Nevada incorporates solar panels and energy-efficient practices, reducing reliance on fossil fuels and demonstrating energy efficiency in manufacturing (To et al. 2019).

9.6. Case study: green chemistry in the textile industry

The textile industry is notorious for its significant environmental footprint due to its water and chemical-intensive processes. Green chemistry principles offer a solution to mitigate these impacts. Here is a case study on how green chemistry is transforming the textile industry: incorporating green chemistry techniques into the textile sector not only mitigates environmental contamination but also fulfils customer preferences for eco-friendly merchandise (Labinger and Bercaw 2002). By adopting eco-friendly dyes, biodegradable textiles, water recycling and reducing

chemical usage, textile manufacturers can enhance their environmental credentials and operational efficiency. Some examples of the process and case studies are provided in the following sections.

9.6.1. *Dyeing processes*

Traditionally, dyeing fabrics involve copious amounts of water, energy and the use of toxic dyes. Green chemistry has led to the development of eco-friendly dyes that require less water and energy and do not produce harmful by-products. Some dyes even use bio-based materials, reducing the environmental impact of dye production. One significant advancement in green chemistry in the textile industry involves the use of natural dyes and waterless dyeing technologies. Traditional dyeing processes are water-intensive and often involve toxic chemicals. Companies such as Dye Coo have developed waterless dyeing technologies that use CO_2 instead of water, reducing energy consumption and eliminating the need for chemicals such as surfactants and fixing agents (Amin and Blackburn 2015; Biranje et al. 2024).

9.6.2. *Biodegradable textiles*

The textile industry is moving towards the production of biodegradable and compostable textiles. These textiles are designed to break down naturally after their useful life, reducing the burden of textile waste in landfills and oceans. The development of biodegradable textiles and sustainable fibers is another area where green chemistry is making strides. For instance, Lenzing AG has pioneered the production of TENCEL™ fibers, which are derived from sustainably sourced wood pulp and produced using an environmentally responsible closed-loop process that minimizes waste and emissions (Christie 2007).

9.6.3. *Water recycling*

Sustainable textile manufacturers are implementing water recycling systems. In order to minimize freshwater use and water body contamination, these systems clean and repurpose effluent from dyeing and finishing operations. Water recycling and closed-loop systems are increasingly adopted to minimize water use and pollution in textile manufacturing.

Patagonia has implemented advanced wastewater treatment and recycling systems in their facilities, reducing freshwater consumption and ensuring that treated water meets stringent environmental standards before being reused (Clark 1999; De Smet et al. 2020).

9.6.4. *Reduced chemical use*

Green chemistry principles encourage the reduction of chemical use in textile production. This involves substituting toxic chemicals with safer alternatives, as well as designing processes that require fewer chemicals overall. Archroma's approach exemplifies green chemistry principles by promoting the use of renewable resources, reducing hazardous chemical inputs and optimizing resource efficiency throughout the dyeing process (Shirvan et al. 2018). These innovations not only address environmental concerns but also respond to increasing consumer demand for sustainable and eco-friendly textiles. Archroma, a global leader in specialty chemicals, has developed an innovative approach to textile dyeing known as Advanced Denim. This process uses eco-friendly dyeing technologies that significantly reduce water consumption, energy use and chemical inputs compared to traditional methods. For instance, their EarthColors® range of dyes uses natural waste materials such as almond shells, saw palmetto and rosemary leaves to produce a wide spectrum of colors without the need for synthetic chemicals (Petersen and Pai 1981; Whittaker and Heine 2018).

9.7. Conclusion

Green chemistry and sustainable processes are integral to addressing the environmental challenges of the 21st century. It is possible to build a more sustainable future if we reconsider how we handle chemical processes, goods and industrial activities. Many industries have developed safer and more environmentally friendly products and processes as a result of the application of these concepts.

While challenges exist, the benefits of green chemistry and sustainable processes are clear: a healthier environment, resource conservation and a more sustainable economy. The continued integration of these principles into our daily lives is essential for a greener and more sustainable world. The future of chemistry lies in the hands of those who embrace and implement these principles, fostering a harmonious relationship between science and the environment.

In agriculture, the adoption of precision farming techniques reduces the environmental footprint by optimizing the use of fertilizers, pesticides and water. Similarly, the automotive industry has made strides with the development of lightweight, recyclable materials that improve fuel efficiency and reduce emissions.

Despite the benefits, challenges remain, including economic viability, regulatory adaptation and public awareness. Economic considerations often deter companies from investing in green chemistry innovations initially, despite potential long-term

savings. Regulatory frameworks designed around traditional practices can impede the adoption of greener alternatives. Furthermore, public awareness and education about the benefits of green chemistry are crucial for fostering widespread adoption.

Nevertheless, the advantages of green chemistry are compelling. They include a cleaner environment, reduced resource depletion and the promotion of sustainable economic growth. Continued integration of these principles is vital for mitigating climate change impacts and achieving global sustainability goals.

The advancement and application of green chemistry concepts will determine the direction that green chemistry takes in the future. A greener and more sustainable world may be achieved by cultivating a symbiotic link between scientific advancement and environmental management.

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10

Waste Minimization and Resource Recovery

Nowadays, waste generation is a global concern that faces major challenges concerning its minimization and management. Improper waste management is leading to significant environmental pollution hazards. Waste minimization is one of the possible solutions for this major world problem. It is one of the cleaner technologies that uses technical interventions leading to pollution-free industrial operations. This chapter mainly deals with the concept of waste minimization, the advantages of waste minimization, and various techniques. Various chemical engineering processes that can be enhanced through waste minimization are also discussed. An integral part of waste minimization is the resource recovery process, in which certain materials from waste are separated and recycled into new products. The major challenge in waste minimization is how to sustain the process. The waste minimization process should be incorporated with the ultimate commitment and prevalence of production at any cost, and it should always be the prime priority. The measures should be implemented properly to achieve the desired goal.

10.1. Introduction

Nowadays, industrial waste is a great cause of concern, affecting the environment on a large scale. Waste minimization is a technique for reducing waste materials to a level as low as reasonably achievable (Bureau of Energy Efficiency 2015). The goal is achieved through recycling, reuse and treatment, considering equally primary and secondary wastes produced by reprocessing and clean-up operations in industries (Nokele and Sebola-Samanyanga 2022). It is an approach for managing waste that emphasizes reducing the concentration and harmfulness of the toxic waste generated. It should be followed by conventional treatment solutions, as waste minimization is not an easy task to perform. Reduction of waste production

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at the origin can be the most suitable process for implementing waste minimization (O'Leary and Walsh 1995). Afterwards, focus should be given to the recycling of waste inside the organization. Finally, products can be modified to achieve the goal of minimum waste generation.

Various types of industrial wastes include liquid waste, solid waste and some specific chemical wastes. Liquid waste production is mainly from domestic and industrial operations (Ahmed et al. 2021). Water is used in large amounts in industries, and when hazardous materials such as radioactive chemicals, bad water, organic liquids, washing liquids, etc. enter various water bodies such as oceans, rivers, ponds, lakes, etc., it ultimately leads to environmental pollution (Al Yaqout 2003). Solid waste from industries includes various materials such as plastics, wood, packages, etc. Although some options can be considered for using the waste as feedstock for other processes, it can also be recycled. With the help of recycling, the load on clearing the waste becomes economically low and by using appropriate disposal practices, it can be ensured that managing waste and its treatment is environmentally friendly and economically beneficial (Bennett 1997). One of the other wastes that is largely generated in industries is chemical wastes that contain highly corrosive, toxic and explosive materials (CPHEEO 2000). Disposing of this type of waste requires great care because it can cause great damage to the ecosystem. Government authorities have established specific standards for proper disposal because failure to do so could pose a threat to human life and other environmental species.

Consequently, it is necessary that each industry and manufacturer follow the rules and regulations of the government for each type of industrial waste. The standards that are set for the effluent help reduce the impact of waste on the environment. There are various ways to minimize waste, namely source reduction of waste, recycling and proper treatment of waste. Among waste minimizing techniques, reducing waste at the source itself is the most effective and impactful method, which reduces damage to the environment. The above technique targets the elimination of the waste from its starting point. Furthermore, the recycling technique is adapted for waste reduction, in which the waste is applied for another process or reused in the same process (Krishna and Pavan 2019). The other minimizing method is treatment of the waste, which mainly involves chemical, physical and biological methods (Srebrenkoska et al. 2014).

Moreover, chemical engineering is the field that provides different innovations to convert waste into important and valued products. Chemical engineers have applied the current techniques to produce energy from waste, which has led to a reduction in the dependency of individuals on nonrenewable sources (Crittenden and Kolaczkowski 1992). Waste materials can be recycled chemically, in which the waste is brought down to smaller pieces to be converted back to their original form, and novel

creations are achieved (Halim and Srinivasan 2006). Chemical engineering plays a crucial role in developing technologies that extract value from different waste streams, promote resource recovery, and minimize environmental degradation. Chemical engineering solutions offer tremendous potential in transforming waste into valuable resources, addressing the global waste crisis and moving towards a more sustainable future. By embracing waste-to-energy technologies, chemical recycling, resource recovery and sustainability assessments, we can minimize waste generation, conserve resources and reduce environmental impact. With the perception of sustainability in managing waste, an appropriate approach to preparing policies can be developed, which also includes all of the investors in a society. This approach can explain the progress, assessment and execution of the waste management policy.

10.2. Types of wastes and various waste minimization techniques

For developing countries, development is a necessity for nation-building and increasing the growth of a country. Consequently, the severe threat of contamination to the environment has increased, and waste can be considered as an inevitable part of development. In addition to this, with the increasing requirement for feedstock in industries, the nonrenewable sources are decreasing at a rapid rate.

There are various forms of industrial waste, including solid, liquid, and some toxic chemical waste. Various industries, including iron and steel mills, thermal power generation plants, pulp and paper industries, and other agricultural products-based industries, contribute to the generation of large amounts of solid waste, which leads to environmental pollution. One possible solution for this problem is the application of the generated waste as feedstock in the industry itself. In the present day, various regions of the world are successfully applying this approach. Several countries have implied various policies that restrict industries from generating huge amounts of waste. This has imparted motivation to investigators to look for possible methods for reusing industrial by-products. In addition to this, social and economic conditions are also varying, so ecologically practicing waste management is a new challenge. The chief contributors to solid waste are the thermal power generation factories generating fly ash, blast furnace slag, steel slag, etc. Some metal-based industries produce wastes like red mud, sugar industries generate press mud, paper factories generate lime, and ultimately, fertilizer plants produce gypsum.

Typically, a thousand-megawatt station applying coal of 3,500 kcal/kg and ash content of approximately 40% would need about 500 hectares for disposing fly ash for about 30 years of operation (Alam and Akhtar 2011). Hence, fly ash waste must

be used to reduce ecosystem damage. Henceforth, it should be a mandatory thing to reuse fly ash in the most possible way to save environment from getting depreciated. Iron and steel industries also contribute to waste generation in the form of slag and other types of waste that are dumped into nearby land, including agricultural fields (Behera 2010). However, slag produced from blast furnaces can be used in the cement industry after being converted into granular form, but this demands a lot of effort (CPHEEO 2000). Another waste is red mud waste generated from aluminum and copper factories, which is discarded into nearby water bodies and is becoming a cause for concern. However, red mud is appreciably used for making ridged sheets in some countries, and this practice should be highly encouraged (Reddy et al. 2021). Also, lime mud waste is one of the types of waste that is produced from paper and pulp factories and dumped on nearby lands. Ultimately, this leads to serious soil pollution.

Because of the high silica content, it is difficult to recover the calcium oxide content from the sludge.

Another type of waste is liquid waste, which is also contributed by manufacturing industries. All of the wastewater coming out as effluent from industries is very lethal to human life because it contains highly toxic chemicals (Sathya et al. 2022). Wastewater coming from industries contaminates water bodies and aquatic species and ultimately pollutes groundwater. There are numerous techniques to treat these industrial effluents, which must be adapted so that the waste causes no harm to the environment. Wastewater coming out as effluent from industries is comprised of dyes, heavy metals, pesticides, medicinal waste, etc. (Afzaal et al. 2022). Specifically, the main components in industrial wastewater include Cr, Zn, Pb, Cu, Fe, Cd, Ni, Ar, Hg and phenols. Phenolic chemicals are mainly contributed by oil refineries, and petrochemical factories generate waste containing hydrocarbons, sulfides, anilines, olefins, and benzene compounds (Srebrenkoska et al. 2014; Singh and Tripathi 2020).

Waste minimization can be achieved primarily through source reduction, recycling and treatment. Source reduction, also known as waste prevention or pollution prevention, is the elimination of waste before it is created. This involves the design, manufacture, purchase or use of materials and products to reduce the amount or toxicity of what is thrown away. Source reduction means stopping waste before it occurs. The practice of source reduction benefits the environment by reducing energy consumption and pollution, conserving natural resources, and extending valuable landfill space. It can also have economic benefits by reducing the costs of transporting, disposing or recycling waste. In addition, source reduction can

save us money every day. It is a rational strategy for reducing the quantity of the product and therefore all of the dangerous consequences related to its disposal. Source reduction includes subtracting the quantity of feedstock and aiming to manufacture a certain product that is highly durable in the long term, repairable, less toxic, reusable and highly proficient. It also focuses on effective application by consumers so that waste is reduced. Consequently, this achieves a generous and significant cost reduction. In addition, source reduction can also be achieved by changing the input material, making modifications in the machine operating instructions, making equipment modifications and also bringing a significant change in the existing technology. In addition, source reduction is cost-efficient as it reduces the cost of pollution control, purchase, use and regulatory compliance.

Furthermore, recycling is also a waste minimization technique adopted by industries. This can be achieved by reusing waste materials in the same process or for another useful application within the industry, as well as by modifying the waste generation process to convert the waste material into a material that can be reused for another application within or outside the company. Currently, hundreds of millions of tons of nonhazardous industrial waste materials are not being reused and recycled, at a substantial cost to both the company that generates the waste and the companies that produce new goods, requiring the purchase of more expensive raw materials as recycled materials are not available. Recycling reduces the costs we would otherwise incur from disposing of unused materials and by-products. It can provide us with a steady, reliable stream. Recycling can help a company reach its environmental goals and improve its standing with local governments and the community at large.

Finally, one of the waste minimization techniques includes treatment method. This technique involves treating different types of waste, including solid or liquid waste, using different techniques. Significant contributors of wastewater are power generation plants, food processing factories, iron and steel industries, nuclear sectors, pulp and paper, etc. (Singh and Tripathi 2020). Seventy million cars are manufactured around the world annually, which contributes to the generation of thirty-four trillion liters of wastewater. This wastewater severely affects aquatic life. To solve the problem related to these types of waste, there are mainly three stages of treatment: primary, secondary and tertiary. In the primary stage, various filtering tools are used, which aim to eliminate the larger wastes that comprise half of the percentage of suspended particles. The part of the waste that passes through the filter is called primary sludge, which is sent to secondary treatment. In the secondary treatment, biological species are used to separate contaminants from wastewater. The treated water is then sent to a tertiary treatment, in which chemical methods are used for treatment.

10.3. Advantages of waste minimization

In order to achieve the goal of sustainability, waste minimization that targets zero discharge is considered a powerful technique. However, this task requires much effort in terms of manpower, time and money. One emerging technique to achieve zero discharge in a chemical process is an automation system that targets the synthesis of waste-minimizing processes. The application of an automation system enables a variety of design innovations and operating parameter alterations in a process plant, as well as the evaluation of parameters.

10.4. Process enhancement through waste minimization in chemical engineering

Chemical engineering plays an important role in understanding the concept of chemical processes that help minimize process waste and in assessing waste minimization (Douglas 1992; Shadiya et al. 2012). Here, various ways in which chemical engineering is revolutionizing waste management and creating a sustainable future are discussed. Some main methods include the following:

– *Pyrolysis*: this technique is performed at elevated temperatures and under regulated conditions to convert plastic waste into useful products. This technique is also helpful in generating heat and power from the plastic waste (Korevaar 2004).

– *Anaerobic digestion*: this process is performed in the absence of oxygen in which organic waste is broken down to produce biogas, mainly methane. This nonconventional fuel can be used to generate electricity, heat and transport.

Chemical recycling is an emerging field that focuses on breaking down waste materials into their basic chemical building blocks to enable the creation of new products. Unlike mechanical recycling, which degrades quality and limits recycled products, chemical recycling offers numerous advantages.

– *Polymer upcycling*: chemical engineering processes enable the conversion of plastic waste, such as PET bottles, into their original monomers (Akehata 1991). These monomers can then be used to produce high-quality virgin plastics, reducing the need for new fossil fuel-based plastics.

– *Precious metal recovery*: electronic waste containing valuable metals such as gold, silver and platinum can be efficiently processed using chemical recycling methods. This enables the recovery of these precious metals, reducing the demand for mining and minimizing environmental impact (Khor et al. 2007).

Rees (2021) conducted experiments to achieve the waste minimization goal using the source reduction methodology (Abu Reesh 2021). The investigations

mainly focused on the backmixing of the reactor and operating parameters and their effects on the environment. The experiments were designed using two modeling procedures to simulate the product based on the process technique. During the process, two highly toxic products were generated, including acetonitrile and hydrogen cyanide. The production of acetonitrile and hydrogen cyanide was reduced by eliminating the backmixing of the reactor and reducing the residence time and temperature.

Shadiya et al. (2012) also adopted a simultaneous approach to maximize profits while minimizing waste through source reduction with the implementation of multi-objective optimization with process simulation, which is presented in this paper (Shadiya et al. 2012). This method mainly consists of four steps, including creating and analyzing the process model, identifying the substitutes for the process, and finally selecting the substitutes and applying the optimized technique focused on multiple objectives. ASPEN PLUS^{TM} 12.1 was used to model and evaluate the process. According to the results, it was found that the plug flow reactor scheme was more suitable compared to the continuous stirred tank reactor scheme. Due to the optimization and modification, the process showed an increase of 69%, compared to the previous one, and a decrease of 38% in waste production.

10.5. Resource recovery as an efficient way to minimize waste

Chemical engineering plays a crucial role in developing technologies that extract value from different waste streams, promote resource recovery and minimize environmental degradation. Examples of resource recovery techniques are shown below.

– *Phosphorus recovery*: phosphorus is an essential element in fertilizers, but is becoming depleted from natural sources. Chemical engineers are pioneering methods to recover phosphorus from wastewater and organic waste to reduce its scarcity and pollution in water bodies (Witek-Krowiak et al. 2022).

– *Metal extraction:* valuable metals such as copper and aluminum can be efficiently extracted from industrial and electronic waste using chemical processes. This not only conserves natural resources but also reduces the energy-intensive mining processes associated with the extraction of these metals (Kaya 2016).

There are serious technical challenges for internal waste reduction and recovery, which only increase when moving from solids to liquids to gases. Reduction in generated waste typically occurs through changes to manufacturing equipment and practices. Recovery of process waste provides the easiest, most near-term and greatest opportunities for efficiency improvements. These waste streams already exist on the industrial site, and their recovery can be capitalized on by using existing

capital assets and knowledge. The recovery of downstream waste requires additional technological advances due to the further processing they have undergone. However, in many cases, existing capital assets can reuse the recovered material. The recovery of downstream waste also has other logistical, economic and technological obstacles due to its relative novelty. Various options for resource recovery in chemical process industries are as follows.

a) *Gaseous effluent resource recovery*: scrubbing, adsorption and thermal systems currently use gaseous effluents to remove unwanted contaminants before atmospheric discharge. The opportunities lie in recovering useful products or energy from these streams. There are a variety of technologies applicable to gaseous streams, including adsorption scrubbers, low-temperature separations for product recovery and reaction technologies for energy recovery (Gao and Zheng 2023). Additional resource recovery processes, scale and economic challenges arise when applying these technologies more broadly because the valuable components (products or fuels) subsist at dilute concentrations in large volumetric streams. Bioreactors, biofilters and scrubbers show potential as they use organisms to process volatile emissions and have a more "earth-friendly" benefit than traditional treatment because the final disposed material can serve as commercial compost or mulch.

b) *Liquid effluent resource recovery*: process water and solvents have a natural affinity to retain products and by-products at very dilute concentrations. Concentrating the components of aqueous streams into useful/recovered products typically requires costly and energy-intensive separation and/or reprocessing technologies. Such recovery will require technologies capable of high selectivity and high flux, handling a wide variety of components, and equipment comprising robust materials to avoid fouling or corrosion (Mandal and Kulkarni 2011). Depending on the type of separation and timing, reintegrating the recovered materials into the processes can increase yield and overall productivity. Separating the components of aqueous streams facilitates the treatment of the recovered water and can make it usable again as input water. Furthermore, the sale or reuse of recovered products is more practical in concentrated form. Examples of the research needed in this area include the integration of reaction and separation systems such as reactive distillation, membrane reactors and supercritical fluid systems.

c) *Solid waste resource recovery*: typical solid wastes such as process sludge and residues, process consumables (e.g. filter media, adsorbents and catalysts), off-specification products and low-value by-products vary greatly in their potential value and utility. The chemical industry is good at recovering solid wastes on-site (Sen 2023). However, resource recovery techniques can further optimize the value of these wastes and either recycle them on-site or convert the waste into a commercially useful material (i.e. input to another industry as fuel or raw material).

On-site reuse reduces raw material and transportation costs and makes more efficient and economical use of existing capital assets.

d) *Production optimization*: optimizing or changing the process to generate less waste, as opposed to capturing and reusing the waste, will enhance sustainability. Operational optimization can be achieved through the implementation of equipment and operational and control optimization technologies. Process optimization, the most important method due to the large amounts and inherent high value of waste streams in the chemical industry, consists of multiple, dependent processing steps. Further research needs to identify new, more material- and energy-efficient replacement products, new chemical pathways, more efficient processing steps, and cheaper, more effective catalysts so that the overall processes will have a smaller waste footprint and/or more valuable by-products as a result of the new waste stream configurations.

e) *Downstream waste recovery*: nearly all nonconsumable products from the chemical industries have recovery potential through downstream recycling (Voss et al. 2022). This recycling targets manufacturers who use the raw or processed output from the chemical industries to produce finished consumer products. Recycling has long focused on paper, plastics and oils because the recovered waste often requires less energy to process into the final product than other raw streams. The chemical industry can take a similar approach and reprocess waste or scrap material from downstream manufacturers into new raw materials.

f) *Immense challenges to downstream waste recovery undoubtedly remain*. The technologies and processes for effectively collecting, sorting and processing the waste streams for many products require comprehensive research in the areas of identification and sorting, operational and handling methods, and the chemical and preprocessing steps necessary to make the recycled waste viable for reuse.

10.6. Sustaining waste minimization

Because of the increasing importance of sustainable development of humankind, government authorities and all concerned industrialists are seeking strategies to reduce waste and the associated costs. Industrial waste is gaining much attention because of its harmful effects on the ecosystem. Consequently, various sectors can benefit from the application of waste management techniques (Okedu et al. 2022).

Waste minimization should mainly aim to develop a model to use waste efficiently in a circular economy (Ugwu et al. 2021). This economy is focused on returning waste to the manufacturing process as feedstock, energy or new products. Ultimately, it will reduce greenhouse gas discharges, thereby reducing the cost related to carbon footprint and preserving natural resources. In addition, it will promote energy efficacy and a reduction in solid waste per year.

To achieve the goal of waste-to-energy conversion, nonrecyclable waste can be processed through combustion via electricity or steam instead of dumping it in landfills. Therefore, this technique will contribute to the generation of clean energy, the extenuation of gases and the reduction of climate change impacts because there is no emission of methane gas (Yang et al. 2018). Emerging techniques are more focused on regaining the value of waste following the clean energy recovery approach and adapting tools with very low emissions.

There is one more emerging approach that targets developing renewable sources of energy and ultimately leading to a bio-based economy. Therefore, this approach focuses on the development of eco-friendly processes for biomass conversion.

Chemical engineers also play a vital role in evaluating the environmental impact of waste management processes and optimizing them for maximum sustainability. Important benefits can be achieved through life cycle assessments and process optimization, including the following:

– *Reduced carbon footprint* can be achieved by assessing the environmental impact of different waste management options. Chemical engineers help identify alternatives with lower carbon footprints, thereby reducing greenhouse gas emissions. Energy efficiency can be achieved by optimizing waste treatment processes to ensure minimum energy consumption and maximum energy recovery, resulting in improved overall energy efficiency.

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11

Safety Management: Hazard Identification and Risk Assessment at the Workplace

A secure work environment requires prioritizing safety management, identifying potential hazards and conducting thorough risk assessments. A comprehensive safety management system is essential, which defines workplace safety policies, procedures and roles. Hazard identification is crucial, and tools such as job safety analysis and safety data sheets are used to identify potential risks. Risk assessment involves thoroughly evaluating severity, likelihood and potential consequences of each hazard. Addressing potential risks involves implementing appropriate measures, maintaining records, providing employee training, preparing for emergencies, and monitoring and enhancing control measures. Ensuring strict compliance with safety regulations and standards is crucial, and monitoring and improving safety measures is imperative. Studying and gaining insights from incidents is paramount, and employee participation is encouraged. Regular evaluation of the safety management system and risk assessment processes ensures efficiency. By implementing these measures as part of a comprehensive safety management system, companies can develop a proactive approach to identifying, assessing and mitigating workplace hazards, thereby promoting a safer work environment for all employees. In this study, we delved into the concept of risk. Various techniques can be used to identify potential dangers in the work environment. Additionally, various potential outcomes related to this risk assessment should be considered. We will also cover probabilistic risk assessment, quantitative risk analysis and hazard identification strategies.

11.1. Introduction

Risk in the chemical industry refers to the likelihood of an adverse event or incident and the potential consequences or impacts. It involves the possibility of

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hazardous events such as chemical spills, leaks, fires, explosions and other unexpected occurrences. The implications of these events can range from causalities and property damage to environmental contamination. These risks are often associated with chemical hazards such as toxicity, flammability, reactivity and corrosivity. In risk assessment, prospective risks are systematically identified, evaluated and prioritized. Risk management involves implementing measures to control, minimize or eliminate these risks. Regulatory compliance is essential for risk management. Unfortunately, the awareness of hazards often only arises after an incident occurs. Recognizing potential hazards and implementing preventive measures is crucial to avoid unfortunate incidents. Every process in a chemical plant requires (Taylor et al. 2023) meticulous deliberation of the following:

1) What are the possible risks involved?

2) What are the possible dangers, and how could they appear?

3) What are the chances?

4) What are the consequences?

The initial inquiry focuses on identifying potential hazards. Evaluating risks entails identifying possible accidents, assessing the probability of these incidents and contemplating their potential consequences (Stefana et al. 2022). Possible outcomes could include harm to individuals, environmental damage, or adverse effects on production and equipment (Reason 1995). Identifying possible dangers and evaluating associated risks are commonly categorized as hazard evaluation (Ericson 2015). Risk assessment is often referred to as hazard analysis (Basu 2016). A method that evaluates potential dangers by calculating probabilities is commonly known as a probabilistic risk assessment (Apostolakis 1978).

In contrast, a method that considers both likelihood and consequences is called quantitative risk analysis (QRA) (Rider et al. 2000). Figure 11.1 shows the typical process of using hazard identification and risk assessment. Once the process is described, the potential hazards and possible accidents are identified. This is followed by a simultaneous examination of both the likelihood and the impact of an incident. This information is compiled into a final risk assessment (Haimes 2005).

Once the risk is deemed acceptable, the study is considered complete, and the process can be implemented (Fischhoff 1981). If the level of risk is deemed unacceptable, then adjustments must be made to the system and the procedure is initiated again (Aven 2015). The method outlined in Figure 11.1 is often shortened depending on the situation.

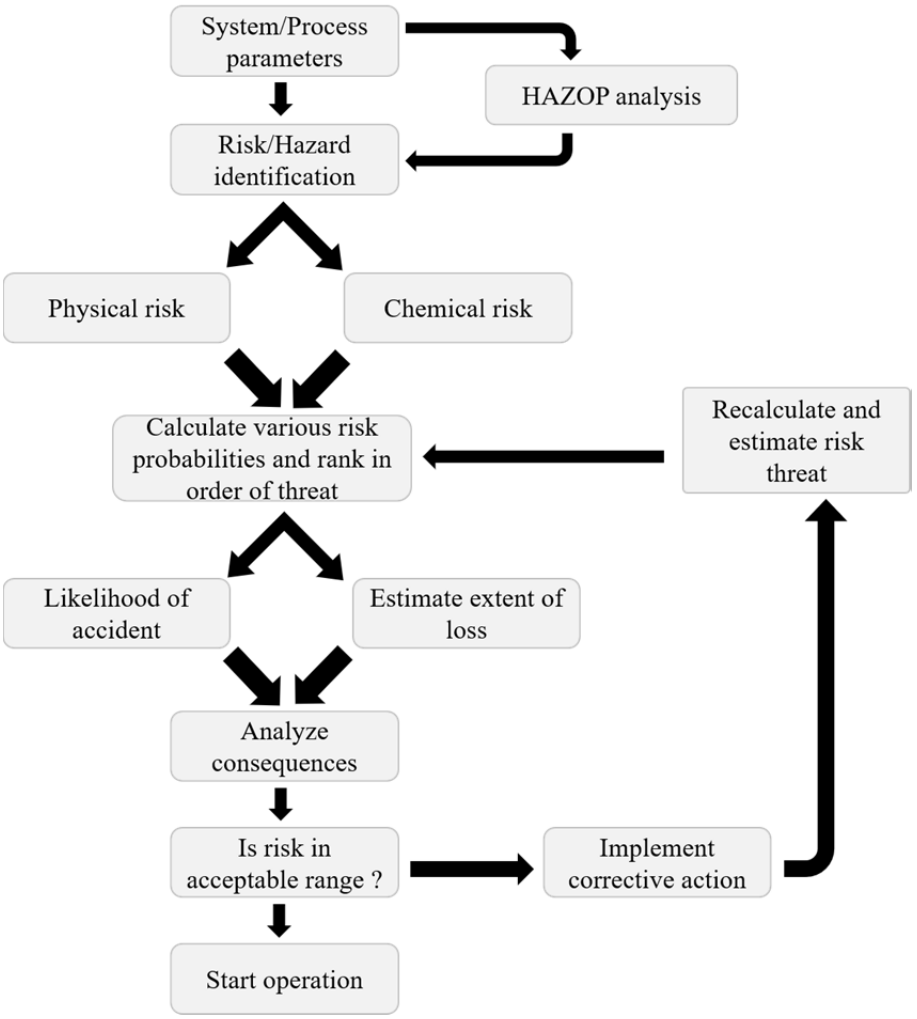


Figure 11.1. *Hazard identification and risk assessment process flow (prepared for this work)*

Without access to failure rate data for the relevant equipment, it is not possible to fully implement risk assessment procedures (Bahr 2014). Many plant sites (and even subunits within a plant) adapt the method to suit their specific situation. Risk identification and assessment studies are crucial at any process stage, whether during the initial design or ongoing operations (Cameron et al. 2017). If the study uses the initial design, it is advisable to complete it promptly. It allows for easy integration of modifications into the final design. Potential hazards can be separately identified

from assessing the associated risks (Rout and Sikdar 2017). However, optimal results are achieved when these tasks are performed in conjunction. One result is that potential risks with low likelihood and minimal impact are identified and dealt with, leading to an overly cautious approach. This implies that safety measures and equipment that may not be essential or cost-effective are implemented (McNay et al. 2019). What is the likelihood of their occurrence, and what actions should be taken in response? Most facilities have minimal likelihood of these hazards occurring, so no specific preventive measures are necessary (Modarre 2006).

Similarly, risks that have a low likelihood of occurrence but which have minimal impact are often overlooked. Every organization implementing these procedures should have appropriate criteria in place. There are numerous approaches to conduct hazard identification and risk assessment (CCPS 1992).

Here, we will discuss only some of the commonly used methods. There is no one-size-fits-all approach that is perfect for every application. Choosing the most effective approach requires a wealth of expertise. Many companies adopt these methods or make adjustments to suit their specific operation. The hazard identification methods outlined in this chapter include the following.

1) Process hazards checklists: this checklist contains a comprehensive list of items and potential issues that need to be thoroughly examined in the process (Hyatt 2018).

2) Safety assessments: this can range from a basic list of potentially dangerous substances to a comprehensive analysis similar to the Dow indices (Etowa et al. 2002). The Dow indices are a type of structured rating that, like an income tax, assigns points for safe practices and deductions for risks (Lele 2012).

3) Hazards and Operability (HAZOP) studies: these offer an organized yet creative setting for investigating possible hazards and operational concerns (Hyatt 2018). Participants are asked to go through many situations involving a certain piece of equipment and evaluate the possibility and potential risks of each event.

4) Safety review: this is an extremely effective, less formal method of conducting a HAZOP investigation. The expertise and collaboration of the group reviewing the process have a significant impact on the result (Crawley and Tyler 2015).

Furthermore, we will discuss hazard identification approaches, including certain aspects of risk assessment. Additionally, we will explore the ideas behind Layer of Protection Analysis (LOPA) and emphasize how QRA and LOPA relate to one another. Our primary goal is to evaluate and analyze the likelihood of various

accident situations. The last two sections show how frequencies are applied in research using both QRA and LOPA, where LOPA is a condensed form of QRA. The study offers valuable insights that can be quickly put into practice, leading to significant improvements in the design and operation of the chemical industry.

11.2. Hazard identification

Identifying risks in the chemical industry is an essential step in safeguarding the well-being of individuals, the surrounding community and the natural environment. Chemical hazards can arise from various sources, including the materials used, the manufacturing, storage and transportation processes, and waste disposal. Here is a systematic strategy to identify possible hazards in the chemical industry.

1) Inventory management: maintain a detailed and current record of all chemicals used or stored at the site. Provide information about the features, possible hazards and quantities of each substance.

2) Familiarize yourself with the material safety data sheet (LOPA) for a comprehensive understanding of all chemicals. Identify the potential risks of each material, including its physical, chemical and toxicological properties.

3) Conduct a comprehensive analysis of each chemical process. Identify potential areas of concern, such as issues with equipment, leaks or unexpected reactions.

4) Inspect and evaluate all equipment and machinery involved in handling substances. Identify potential areas of concern that could lead to failure, corrosion, leaks or other hazards.

5) Evaluate chemical storage facilities to ensure they meet safety standards. Pay attention to potential issues related to compatibility, segregation or inadequate containment measures.

6) Analyze and assess routes for the safe and efficient transportation of substances. Identify possible dangers related to incidents during transportation, leaks or spills.

7) Identify potential sources of ignition and explosive atmospheres, which is of utmost importance in maintaining fire and explosion safety. Ensure proper safety measures are in place to minimize the risk of fire and explosions, such as using specialized equipment that can effectively prevent explosions.

8) Identify potential sources of toxic releases during regular operations or in the event of accidents, which is crucial. Implement strategies to reduce the likelihood of encountering potential dangers.

9) Evaluate emergency preparedness: evaluate the plans and procedures for emergency response. Assess potential hazards and analyze the effectiveness of preventive measures.

10) Factors to consider: take into account a range of factors that can potentially contribute to hazards, such as fatigue, training and communication issues. Implement measures to address human factors and promote a strong safety culture, which is paramount.

11) Assess environmental impacts: examine the potential environmental effects of processes and emissions. Implement specific measures to minimize environmental damage, such as creating plans to contain and respond to spills.

12) Meet regulatory standards: ensure compliance with all applicable safety regulations at the local, regional and national levels. Ensure that procedures are regularly updated to keep up with changing regulatory requirements.

13) Ongoing evaluation: continuously assess and update hazard assessments to accommodate process, equipment or regulation changes.

14) Promote active involvement from employees in identifying possible dangers. Encourage reporting of potential hazards and near misses.

15) Training and education: it is crucial to provide employees with comprehensive training on the potential hazards associated with various substances, as well as the correct procedures for handling them safely. Additionally, it is essential to equip them with the knowledge and skills to effectively respond to emergencies.

By conducting a comprehensive examination and assessment of possible hazards, the chemical industry can effectively establish strategies to prevent accidents and ensure the well-being of employees, local residents and the surroundings (Crowl and Louvar 2001). Regular audits, reviews and updates to safety procedures are essential for maintaining a robust safety management system in the industry.

11.3. Process hazards checklist

A process hazards checklist is a thorough inventory of potential issues and areas that need careful examination. The list provides a helpful reminder for the reviewer or operator to stay vigilant about possible problem areas (Nolan 2014). A checklist is an essential tool that can be used during the design of a process to identify any potential hazards, or it can also be used before the operation of the process. However, here is a general example of a process safety checklist. Note that this is a

standard template and may need to be tailored to meet the specific needs of your industry and processes.

a) Process overview:

– explaining the procedure;

– identifying essential equipment and units.

b) Identifying potential hazards:

– identifying the possible risks that may occur during the process;

– identifying substances that may pose a risk to health or the environment.

c) Evaluating the process:

– reviewing the process design documents;

– ensuring adherence to design standards and codes.

d) Procedures for operation:

– accessing and evaluating standard operating procedures (SOPs);

– assessing the clarity and effectiveness of SOPs.

e) Education and skills:

– verifying staff training records;

– assessing the skill level of operators.

f) Ensuring equipment integrity:

– performing comprehensive inspections of critical equipment;

– verifying maintenance records and schedules.

g) Preparedness for emergencies:

– assessing measures in place to handle potential emergencies;

– assessing the availability and efficiency of emergency equipment.

h) Process control:

– evaluating process control systems;

– testing and validating alarm systems and interlocks.

Safety instrumented systems (SIS) play a crucial role in ensuring the safety and reliability of industrial processes (Innal et al. 2015). These systems are essential for

identifying and reducing potential dangers and ensuring the safety of both individuals and machinery (Rausand 2014). By using cutting-edge technologies and strictly adhering to safety measures, industries can effectively mitigate the potential for accidents and uphold a secure working environment (Thomson 2015). SIS are designed and engineered to meet stringent safety standards, ensuring reliable security measures and guaranteeing the precision and dependability of SIS testing and maintenance.

i) Pressure relief systems:

– conducting comprehensive inspections of pressure relief devices;

– verifying relief system design.

ii) Exploring an incident:

– reviewing past incident reports;

– verifying the steps taken to resolve the problem.

iii) Evaluating the process of managing change:

– assessing the effectiveness of the change management process;

– reviewing and verifying documentation for process modifications.

iv) Reviewing and examining processes:

– assessing internal and external audit findings;

– ensuring strict compliance with regulatory inspections.

v) Considering environmental factors:

– assessing the potential impact on the environment;

– promoting compliance with environmental regulations.

vi) Managing essential documents and records:

– examining safety documentation;

– maintaining meticulous record-keeping practices.

vii) Examining near misses:

– evaluating incidents that narrowly averted significant outcomes;

– verifying the steps taken to resolve the problem.

viii) Evaluating procedures:

– assessing the process for managing facility modifications;

– ensuring the precision and reliability of documentation and acquiring the required approvals for any modifications.

ix) Monitoring and assessing process performance:

– assessing process monitoring systems;

– evaluating crucial performance metrics.

x) Prioritizing contractor safety:

– prioritizing the strict adherence to contractors' safety practices;

– assessing the training and supervision offered by contractors.

xi) Maintaining compliance with regulations:

– prioritizing safety by strictly following all relevant regulations;

– ensuring proper documentation of permits and regulatory approvals.

This checklist is a valuable tool that can be tailored to suit the specific needs and complexities of industries and operations. Additionally, it is crucial to involve relevant stakeholders, including process operators, safety professionals and management, in developing and implementing the checklist. Regular reviews and updates are essential for ensuring ongoing process safety.

11.4. Hazard survey

A hazard survey can vary in complexity, from a simple inventory of potentially hazardous substances in a facility to more advanced procedures such as the Dow fire and explosion index (F&EI) and the Dow chemical exposure index (CEI). These methods are widely recognized and used to conduct thorough hazard surveys. These methods are structured and use a rating form similar to an income tax form. The final rating number reflects the comparative ranking of the hazard.

The F&EI also provides a way to calculate the financial consequences of an accident. The Dow F&EI is a valuable tool for evaluating the potential hazards associated with storing, handling and processing materials with a high risk of explosions and fires. The main goal of this procedure is to provide a highly structured approach based on objective factors for evaluating the relative severity of flammable hazards in a chemical plant. The primary forms used for the calculations are shown in Figures 11.2 and 11.3.

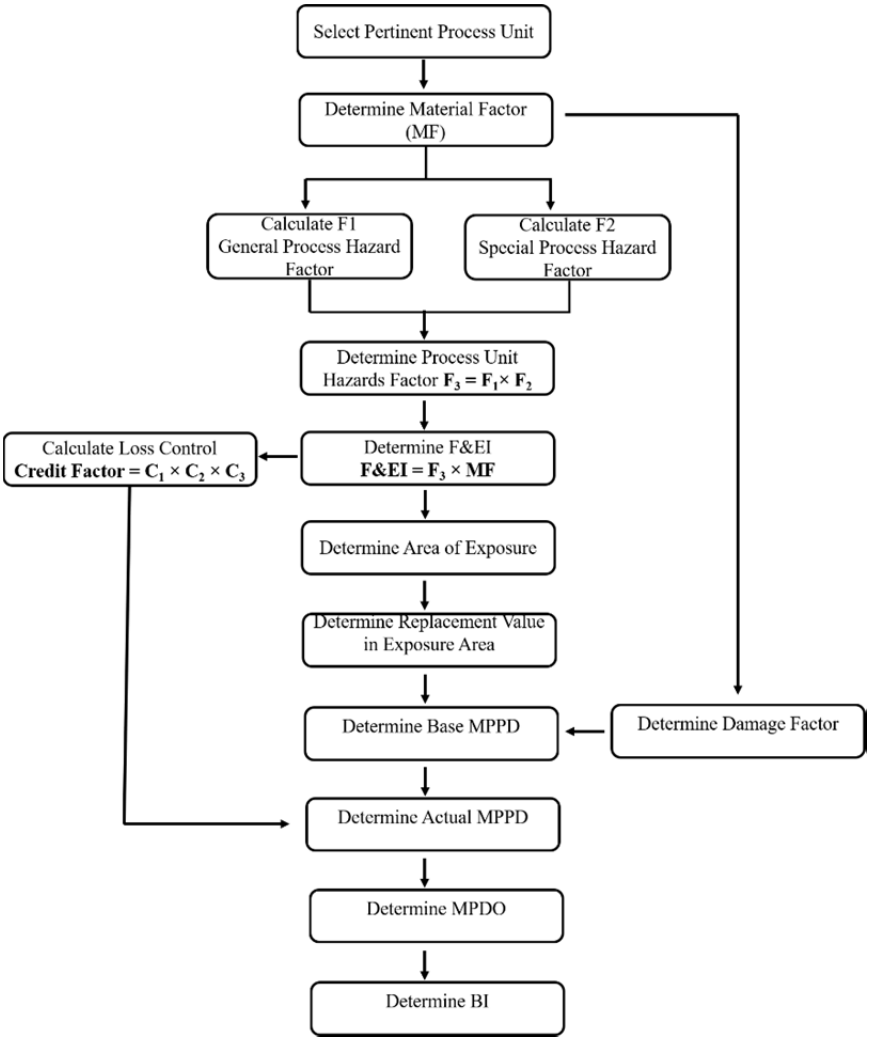


Figure 11.2. *Process for determining risk analysis data, including the fire and explosion index (prepared for this work)*

The process begins with a material factor that solely depends on the type of chemical(s) used. This factor is modified to account for various process hazards, both familiar and unique (Dimian et al. 2014). These adjustments or penalties are determined by multiple factors, including storage conditions, reaction types and fired heaters (Khan and Abbasi 1998a). After determining the F&EI, several safety methods and procedures are used to assess the possible repercussions of the danger (Heikkilä 1999).

Compound	Molecular weight (g/mol)	Material factor	Melting point (°C)	Boiling point (°C)	Flash point (°C)	Density (kg/m^3)
Acetone (CH_3COCH_3)	58.08	16	– 94.888	56.07	– 18	784
Acetylene (C_2H_2)	26.038	29	– 80.8	– 84.7	– 18.15	1.1
Benzene (C_6H_6)	78.114	16	5.5	80.1	– 11	876
Bromine (Br_2)	79.90	1	– 7.2	58.8	–	3119 (25°C)
Butadiene (C_4H_6)	54.09	24	– 108.9	– 4.4	– 76.11	615
Butane (C_4H_{10})	58.12	21	– 138	– 0.5	– 60	579
Calcium carbide (CaC_2)	64.09	24	2160	2300	–	2,220
Carbon monoxide (CO)	28.01	21	– 211.6	– 191.52	– 191	1.15
Chlorine (Cl_2)	35.4	1	– 101	– 34	–	2.96
Cyclohexane (C_6H_{12})	84.16	16	4–7	80.7	– 20	779 (25°C)
Diesel fuel	150 to – 250	10	–	157.2	37.7 to 148.8	800 to 880
Ethane (C_2H_6)	30.07	21	– 182.8	– 89	– 104	1.26
Ethylene (C_2H_4)	30.02	24	– 169	– 104	– 136	1.18
Methane (CH_4)	20.07	21	– 183	– 161	– 188	0.657
Methanol (CH_3OH)	32.04	16	– 98	64.7	9.7	791 (25°C)
Mineral oil	23.99	4	285	> 200	> 160	840 to 880 (20°C)
Octane $CH_3(CH_2)_6CH_3$	114.23	16	– 57	125–127	13	703
Pentane (C_5H_{12})	72.15	21	– 130	36.1	– 49	626
Petroleum (crude)	–	16	–	– 47.77 to 593.33	– 6.66 to 32.22	–
Propylene (C_3H_6)	42.08	21	– 185	– 47.7	– 108	1.76
Styrene (C_8H_8)	104.2	24	– 31	145	31	906
Toluene (C_7H_8)	92.14	16	– 95	110.6	4.4	870 (20°C)
Vinyl chloride (C_2H_3Cl)	62.5	24	– 153.8	– 13.4	– 62	911
Xylene (C_8H_{10})	106.17	16	– 7.4	138.5	30	864
Ethylbenzene ($C_6H_5CH_2CH_3$)	106.2	16	– 94.9	136.1	23	870 (20°C)

Table 11.1. *Selected data on various chemical compounds for the Dow F&EI*

The first phase of the approach entails mentally partitioning the process into separate process units. A processing unit generally comprises a solitary pump, reactor or storage tank (Hessel et al. 2004). An extensive procedure produces a multitude of distinct entities. Using the F&EI for all of these units is not feasible (Baker et al. 2012). The conventional method is to select the units that have been demonstrated to be most susceptible to threats (Khan and Abbasi 1998b). A process safety checklist or risk survey is commonly used to identify the units with the most significant level of risk for further examination. We now determine the material factor (MF) using the flowchart shown in Figure 11.2.

Table 11.1 presents data on molecular formulas for various important chemicals. This list also presents data on the material factor as well as flash, melting and boiling point temperatures. The additional information is also used in calculating the Dow F&EI.

Generally, materials with a higher MF value are more susceptible to flammability and/or explosiveness (Roy et al. 2016). The MF is determined by considering the qualities of the mixture when multiple materials are used together. We advise choosing the maximum value of the MF throughout all operating situations. Subsequently, it is imperative to ascertain the overall procedural risks. Sanctions are imposed for the following criteria:

1) Reactions that release heat and can cause self-heating.

2) Reactions that cannot take place without some kind of energetic stimulus, such as fire.

3) Pumping and connecting transfer lines are part of material handling and transfer.

4) Process units with lids to contain volatile vapors and keep them from escaping.

5) Limited passage for rescue devices.

6) Inadequate removal of combustible substances from the processing unit.

7) Penalties for unique process hazards are subsequently determined.

8) Hazardous substances that may hinder firefighting efforts.

9) Operating at a pressure lower than atmospheric pressure, posing a risk of outside air infiltration.

10) Operating inside or in close proximity to the flammable range.

11) Hazards associated with dust explosions.

12) Operating above atmospheric pressure.

13) Operating at low temperatures that may cause carbon steel containers to become brittle.

14) Amount of combustible substance.

15) Deterioration and wear of process unit structures.

16) Seepage occurring at the connections and seals.

17) Use of fired heaters that offer a readily available ignition source.

18) Hot oil heat exchange systems operating at temperatures above the ignition threshold of the oil.

19) Sizeable rotating machinery such as pumps and compressors.

The comprehensive Dow F&EI has explicit guidelines and associations for identifying both general and specific process hazards. To obtain the unit hazard factor (F3), we multiply the general process hazard factor (F1) and the particular process hazard factor (F2) (Sadeghi et al. 2020). After multiplying the unit hazard factor by the multiplication factor, the Dow F&EI is calculated. Table 11.2 presents the level of danger determined by the index value. The Dow F&EI can be used to assess the impact of an accident. This includes the highest estimated amount of property damage (MPPD) and the longest estimated duration of power outage (MPDO) (Sadiq and Amyotte 2003).

Dow F&EI	Degree of hazard
1–60	Light
61–96	Moderate
97–127	Intermediate
128–158	Heavy
159 and above	Severe

Table 11.2. *Degree of hazard measured by Dow F&EI*

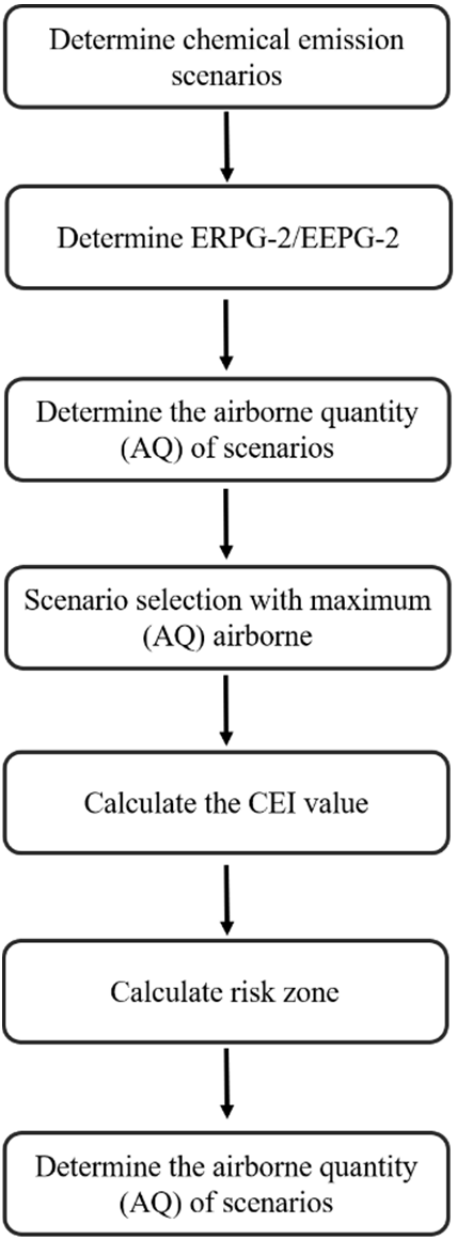


Figure 11.3. *Steps involved in the implementation of the DOW chemical exposure index (CEI) (prepared for this work)*

The scope of the damage is first assessed using a documented correlation in the complete Dow index, which is based on the previously established F&EI. The value of the equipment within this radius is then calculated. A damage factor is then applied to the portion of the equipment affected by the explosion or fire based on a provided correlation. Ultimately, a credit factor is factored in, considering the effectiveness of safety systems. The MPPD value represents the final amount in dollars. This value is used to estimate the MPDO through a correlation. Information about the procedure can be found in the comprehensive Dow reference. The Dow indices provide valuable insights into equipment spacing requirements. The F&EI uses an empirical correlation to determine the radius of exposure from the F&EI value. Anything beyond this distance would be safe from explosions or fires. Figure 11.3 shows how the CEI uses the ERPG (Emergency Response Planning Guidelines) values specific to the discharged substance to determine the hazard distance for probable chemical exposure. The Dow CEI provides a straightforward approach to assessing the potential health risks posed to individuals in nearby facilities or communities due to potential incidents involving the release of chemicals.

To use the CEI, the following are required: an accurate plant and surrounding area plan; a simplified process flowsheet outlining the containment vessels, main pipes and chemical inventories; and comprehensive data on the physical and chemical properties of the materials under investigation.

Here is a general outline of the information that is typically considered in exposure assessments, which can be adapted based on the specific details provided in the guide. Note that this guide is intended to provide general information and may not align precisely with the Dow CEI Guide in terms of format or content.

The Dow CEI assessment form includes the following:

1) Information about chemicals:

– name and structure of the chemical;

– properties related to the physical and chemical nature (e.g. melting point, boiling point, flash point, density, vapor pressure);

– data on toxicity (e.g. LD50, LC50, permissible exposure limits).

2) Process information:

– name/description of the process;

– process location;

– date of evaluation.

3) Ways of exposure:

– breathing in the chemicals;

– contacting the chemicals with the skin;

– swallowing the chemicals.

4) Exposure scenarios:

– under typical operating conditions;

– unsettling or urgent circumstances;

– activities related to maintenance and shutdown.

5) Occupational exposure limits:

– limits set by regulations;

– exposure limits specific to the company;

– mention of industry standards and guidelines.

6) Results of workplace exposure monitoring:

– selecting sampling sites and sampling frequencies;

– ensuring the accuracy and consistency of data.

7) Explanation of personal protective equipment (PPE):

– evaluating the efficacy of PPE in minimizing exposure;

– suggestions for enhanced PPE.

8) Engineering controls:

– using ventilation systems;

– structures and obstacles;

– designing equipment to minimize emissions is crucial for environmental sustainability.

9) Calculation of the exposure index:

– method for determining the exposure index;

– elements considered in the computation;

– understanding exposure index values.

10) Evaluation of potential risks:

– assessing overall risk;

– classifying exposure hazards (low, medium or high);

– identifying critical scenarios.

11) Measures to address the issue:

– current safety systems and controls;

– suggestions for further controls;

– plans for responding to emergencies and evacuating.

12) Documentation and references:

– supporting documents (e.g. exposure monitoring reports, safety data sheets, etc.);

– applicable codes and standards;

– mention of tools or models used for analysis.

13) Review and approval:

– names and signatures of individuals conducting the assessment;

– date of review and approval.

It is important to always refer to the specific guidelines and templates provided by Dow or other recognized sources for accurate and detailed information.

A flowchart of the procedure is shown in Figure 11.3. The process begins by establishing the potential occurrence of release incidents. This involves discharging substances from various sources such as pipes, hoses, pressure relief devices, vessels, and accidental spills and overflows from tanks. To estimate the rate of material release, the occurrences are used in conjunction with various simplified source models supplied in the Dow handbook. Using ERPGs and a simplified dispersion model, the CEI value and potential downwind hazard distances from a release can be determined.

Risk assessments effectively identify potential dangers related to equipment design, layout, material storage and other relevant factors. They are not effective in identifying hazards that may arise from incorrect operations or unexpected situations.

On the other hand, this method is highly systematic, requires minimal expertise, is straightforward to implement and yields rapid outcomes.

11.5. Hazards and operability (HAZOP) studies

A rigorous approach to identifying dangers in a chemical process that could lead to severe accidents is the HAZOP research. The procedure is highly efficient in identifying potential hazards and has gained widespread acceptance in the industry. The fundamental concept is to allow the mind to freely explore within a structured framework to thoroughly analyze potential processes and operational failures. Before initiating the HAZOP investigation, it is crucial to have thorough information about the specific process. This entails the use of current process flow diagrams, process and instrumentation diagrams, comprehensive equipment specifications, materials of construction, and mass and energy balances.

An extensive HAZOP investigation requires the participation of a heterogeneous team of experienced professionals from several domains such as plant operations, laboratory, technical and safety specialists. An individual must have expertise in leading HAZOP assessments and act as the chair of the committee. This individual takes charge of the discussion and should have expertise in the HAZOP procedure and the specific chemical process being evaluated. It is important to designate someone to record the results, although there are software options available from various vendors to help with this on a personal computer. The committee convenes regularly and dedicates a few hours to each meeting. The meeting should be kept concise to maintain the engagement and active participation of all committee members. A complex project of this magnitude typically requires several months of biweekly meetings to conduct the HAZOP study. Undoubtedly, conducting a comprehensive HAZOP study demands a significant commitment of time and effort, but the outcome's worth justifies the endeavor.

The HAZOP procedure involves a series of steps to conduct a thorough analysis:

1) Set up a detailed flow chart as a first step. Separate the various process units in the flow sheet. Thus, the reactor and storage tank could be considered two distinct entities, although they function as one.

2) Pick out a node (vessel, line, operational instruction) for analysis.

3) Explain the reasoning behind the design of the research node.

4) Select a process parameter from the following: state (solid, liquid or gas), agitation, volume, reaction, sample, component, start, stop, stability, power, inert, temperature, pressure, concentration, pH and viscosity.

5) Look for possible changes to the process parameter using a guiding word.

6) Identify any potential causes for the deviation and note any protective measures in place.

7) Assess the potential outcomes of the deviation, if any.

8) Suggest a course of action (what needs to be done, who should do it and when should it be done?).

9) Make sure to document all relevant details.

10) Ensure that steps 5 to 9 are performed until all pertinent guidelines have been used for the chosen process parameter.

11) Proceed with steps 4 to 10 repeatedly until all pertinent process parameters have been considered for the designated study node.

12) Proceed with steps 2 to 11 repeatedly until all research nodes have been assessed for the segment, and then proceed to the next area in the flow sheet.

Comprehending and using guiding words such as “AS WELL AS”, “PART OF” and “OTHER THAN” can occasionally pose difficulties. In addition to the intended design intent, the term “as well as” indicates that something else occurs. Various scenarios can occur, such as the liquid reaching its boiling point, the addition of another component, or the unexpected movement of a fluid. In this scenario, it indicates that a component is absent or that the stream is selectively directed to only a portion of the process. In some cases, a different substance may be used instead of the anticipated substance, relocated to another location, or solidified and become immovable. The terms “sooner than”, “later than” and “where else” can be applied to batch processing. Efficient record-keeping and use of the findings are crucial aspects of the HAZOP procedure. There are various techniques to achieve this, and most companies tailor their approach to suit their unique way of operation. One benefit of this approach is that it offers a comprehensive understanding of potential dangers, including details on how hazards can arise from operational procedures and disruptions in the process. Companies that conduct thorough HAZOP studies experience enhanced process performance, reduced downtime, improved product quality, decreased waste generation and increased employee confidence in process safety. There are some drawbacks to consider when using the HAZOP approach. It can be a time-consuming process that requires a significant amount of human resources. Additionally, it is worth noting that it may identify hazards that are not necessarily related to the overall risk.

11.6. Safety review

Another commonly used method for identifying safety issues in laboratory and process areas and finding solutions is safety reviews (Guldenmund 2000). There are two different classifications of safety reviews: informal and formal. The informal safety review is commonly used for minor alterations to existing procedures and

small-scale tests carried out in the laboratory or on a workbench (Stefanick 2014). The informal safety review procedure typically includes only a small group of individuals. It involves the person in charge of the process and a couple of others who are knowledgeable about safety protocols, even if they are not directly involved in the process (Crowl and Louvar 2001). The goal is to foster an engaging discussion where ideas can be shared and enhancements in safety can be devised. The reviewers gather casually to inspect the process equipment and operating procedures, providing suggestions to enhance the safety of the process (National Research Council 2014; Ménard and Trant 2020). It is essential to document any notable advancements in a memo for future reference by others. The enhancements should be put into effect before carrying out the procedure. The formal safety review is performed for new processes, significant alterations to existing methods and procedures that necessitate an updated evaluation. The formal safety review consists of a three-step procedure (Crowl and Louvar 2001). This entails the development of a thorough safety assessment report, followed by a committee's examination and inspection of the report and the process, subsequently implementing the recommendations (Reese 2018). The safety review report consists of the following sections.

Section I. Introduction:

a) Overview or summary: provides a concise overview of the outcomes of the formal safety assessment.

b) Assessment: this step is completed once the formal safety review is finalized.

c) Overview of the process: offers a concise overview of the procedure with a focus on the significant risks involved in the operation.

d) Reactions and stoichiometry: presents the equations for chemical reactions and their stoichiometry.

e) Engineering data: presents operating temperatures, pressures and pertinent physical information about the properties of the materials used.

Section II. Raw materials and products:

a) Discusses the potential hazards and challenges related to handling raw materials and products.

b) Explores methods to reduce these risks.

Section III. Setting up the equipment:

a) Equipment description: provides an overview of the equipment's configuration. Drawings of the equipment are provided.

b) Specifications for the equipment: uses the name and model number of the manufacturer to identify the device. It provides industrial machinery with related physical data and design information.

Section IV. Steps to follow:

a) Operating procedures: explains how the process is operated.

b) Safety procedures: describes the specific considerations related to the equipment, materials and procedures used to minimize potential risks. Here are some of the things that are included:

– Emergency shutdown: explains the process of safely stopping the equipment in the event of an emergency. This involves significant leaks, reactor instability and loss.

– Procedures for ensuring safety: examine the possible results of utility outages, including power outages, water shortages, air pressure, steam and inert padding. Detail the procedures to follow to guarantee a safe system failure by considering each possible scenario.

– Procedures for major releases: outlines the necessary steps to be taken in the event of a significant spill of hazardous or potentially combustible substances.

c) Waste disposal procedures: outlines the process for handling and managing materials that may pose a risk to health or the environment.

d) Cleanup procedures: outlines the steps for cleaning the process after use.

Section V. Safety checklist:

a) Presents a comprehensive safety checklist for the operator to fulfill before completing their tasks.

b) Running the process smoothly: this checklist is used before each startup.

Section VI. Material safety data sheets are provided for every hazardous material used.

11.7. Other methods

There are other methods that can be used to identify hazards:

1) Hypothetical analysis: this less formal method of identifying hazards involves using the phrase “what if” to explore various areas of investigation. For example, we could ask, what happens if the flow comes to a halt? The analysis team then

evaluates the potential consequences and devises solutions to any issues that may arise (Dwyer et al. 2004; Cox Jr. 2012).

2) Analysis of human error: this method is used to identify the components and steps of a process that are more prone to human error than usual (Kirwan 1998a). Control panel layout is a prime candidate for human error analysis due to potential design flaws that can lead to mistakes (Kirwan 1998b).

3) FMECA (Failure Modes, Effects and Criticality Analysis): this approach involves creating a comprehensive list of equipment in the process and identifying all potential failure modes for each item. The impact of a specific failure is analyzed in relation to the process (Catelani et al. 2021).

11.8. Risk assessment

This encompasses the process of identifying incidents and analyzing their potential consequences (Haimes 2005). Incident identification is the process of determining the cause and circumstances of an accident (Giannopoulos et al. 2012). This often involves an examination of the likelihood. Consequence analysis provides an assessment of the anticipated harm or destruction. This includes fatalities, damage to the ecosystem or physical assets, and the duration of operational disruption (Borghesi and Gaudenzi 2012).

The Dow F&EI incorporates an assessment of the MPPD and the MPDO. This type of analysis focuses on examining the outcomes or results of a specific action or event.

Nevertheless, these figures are derived by relatively simple calculations that use publicly available relationships. HAZOP studies elucidate the mechanisms by which a specific accident occurs. This is a method for identifying and classifying incidents. The usual HAZOP study does not use probabilities or numbers. Instead, the review committee relies on their knowledge to determine the most suitable course of action.

Equipment failures or faults in a process can arise from the intricate interplay of various components. The graphical representation of risk is commonly presented, as shown in Figure 11.4. Each company establishes its thresholds for acceptable and unacceptable risks.

QRA or LOPA are commonly used to assess the actual risk associated with a process or plant. Alternative methods are occasionally used, but QRA and LOPA are the prevailing approaches. A suitable adaption of fault trees, event trees or both is used to estimate the release frequency.

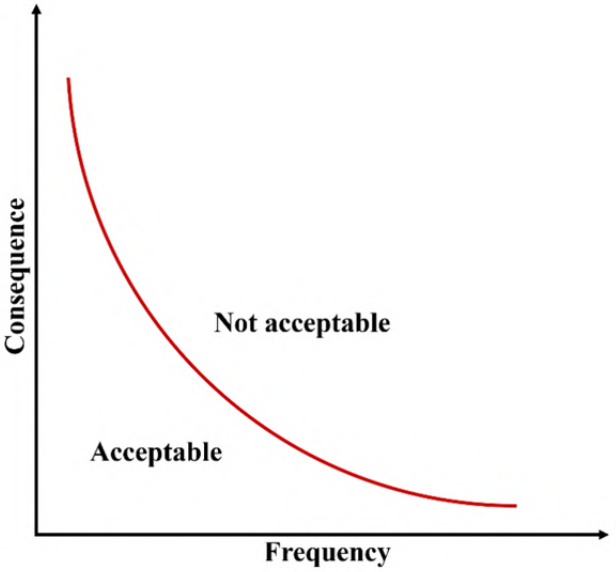


Figure 11.4. *Overview of risk (prepared for this work). For a color version of this figure, see www.iste.co.uk/kumararya/chemicalengineering2.zip*

11.9. Quantitative risk analysis

The QRA method is used to identify areas where modifications can be made to reduce risk in operations, engineering or management systems. The level of complexity in a QRA is determined by the study's objectives and the accessible information. QRAs are most effective when implemented from the beginning of a project, during the conceptual review and design phases, and consistently maintained throughout the entire life cycle of the facility (Freeman 1990). The QRA method is developed to help managers evaluate the overall risk of a process. QRAs are used to assess potential risks in situations where qualitative methods are insufficient for comprehending the risks. QRA is highly effective in evaluating risk reduction strategies (Hendershot 1996).

There are several essential steps to follow in a QRA study. Steps in this process include outlining all potential event sequences and incidents, assessing their consequences (usually through fire and explosion modeling or dispersion modeling), estimating the frequency of incidents (using fault trees or event trees) and finally combining the impacts and frequencies to obtain an overall risk estimate. Visual representations of this danger can subsequently be made, as shown in Figure 11.4. In most cases, QRA is a labor-intensive procedure that requires specialized knowledge

and a significant commitment to time and money. When unnecessary complexity is present, LOPA approaches may be a better choice.

11.9.1. *Layer of protection*

LOPA is a tool used to analyze and assess risk semi-quantitatively. This approach uses streamlined techniques to analyze the outcomes and determine the probabilities (Al-Dhafeeri 2018). A method is designed to decrease the occurrence of bad events by implementing many layers of protection. Shields, blast barriers, essential process control, safety instrumented operations, relief valves, active devices and human involvement are all potential components of the protective layers (Clarin 2013). Figure 11.5 provides a visual representation of the layers of protection. The protective layers and their consequences are subsequently evaluated based on predetermined risk tolerance criteria.

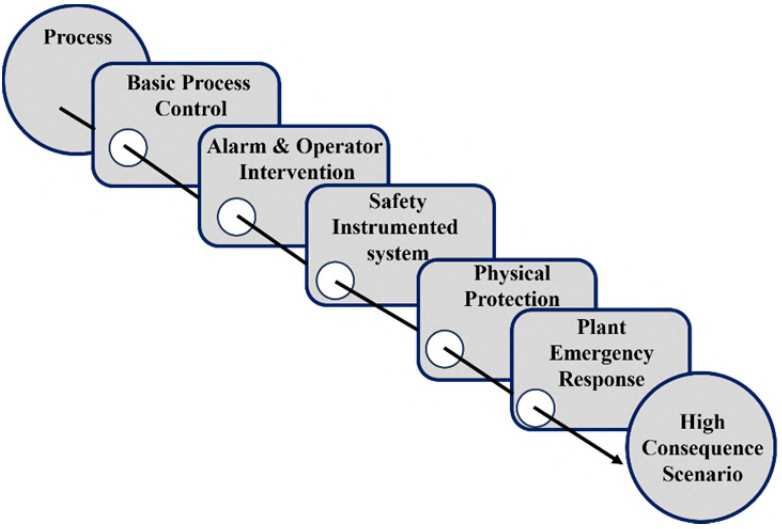


Figure 11.5. *A layer of protection to reduce the likelihood of a particular accident scenario (prepared for this work)*

The consequences and effects of LOPA are categorized, frequencies are estimated and the effectiveness of the protective layers is also approximated (Ouazraoui et al. 2013; bt Razali 2009). We chose the approximate values and categories to ensure our results are conservative. Therefore, it is crucial to ensure that the outcomes of an LOPA are consistently more cautious than those obtained from a QRA (Myers 2013; Chastain et al. 2017). If the LOPA results are deemed

unsatisfactory or there is a level of uncertainty in the results, it may be necessary to conduct a comprehensive QRA (Xu 2023). Caution should be exercised when using the findings from both approaches. Nevertheless, the outcomes of QRA and LOPA studies are particularly encouraging when evaluating different options (Arendt and Lorenzo 2000).

Various companies use different criteria to determine the demarcation between acceptable and unacceptable risks (Fischhoff 1981). The number of casualties, fires, the maximum frequency of a specific consequence category and the required number of separate protective levels for this category are all potential components of the criteria (Necci et al. 2015).

The primary goal of LOPA is to determine whether the various levels of protection are sufficient for a particular accident scenario. One or more levels of protection may be required in a given situation, depending on the complexity of the process and the possible severity of an accident (Girgin et al. 2019). It is crucial to remember that, in a particular case, the outcome can be avoided by the successful operation of only one layer. Given that no layer is 100% secure, it is crucial to have enough levels to reduce risk to an acceptable level.

In an LOPA study, the main procedures are as follows:

1) Identifying a single consequence (a simple way to determine consequence categories is discussed later).

2) The second step is to consider an accident scenario with a single cause–consequence pair and determine what the cause was.

3) The third step is to determine how often the initial event of the scenario occurs (a straightforward approach is detailed below).

4) Finding all of the possible safeguards for this specific outcome and calculating the on-demand failure probability for each safeguard.

5) Estimating the frequency of mitigated consequences for this initiating event by combining the frequency of the initiating event with the on-demand failure probabilities for independent protective layers.

6) Estimating the risk by plotting the consequence against the frequency of the consequence (see Figure 11.4). Assessing the level of risk and determining whether it is acceptable; otherwise, safeguards must be implemented.

This procedure can be repeated for a variety of other results and scenarios. This method is routinely used in several different variants.

11.9.2. *Outcome*

The main concern about the chemical process sector is that containment is lost and hazardous materials are released. This can be caused by various events such as a vessel leak, pipeline rupture, gasket failure or relief valve release. Dispersion modeling and in-depth analysis are used to quantify the consequences of these releases, specifically in terms of downwind effects caused by fires, explosions or toxicity. In an LOPA study, the consequences can be estimated using different methods. These methods include a semi-quantitative approach that does not directly consider human harm, qualitative estimates that consider human harm and quantitative estimates that also consider human harm. This method is much more straightforward to use than QRA. While the technique is user-friendly, it effectively highlights issues that require further attention, such as a QRA. It also identifies issues that may be downplayed due to their minimal impact.

11.10. Conclusion

To guarantee a secure and conducive work environment, it is necessary to identify potential dangers, evaluate the associated risks and establish ways to control them. Identifying potential hazards requires conducting routine inspections, documenting incidents, gathering input from employees and following manufacturer guidelines. Evaluating the likelihood and severity of identified hazards, implementing control measures, and reviewing and updating assessments are part of the risk assessment process. It is crucial for effective risk management in various fields, with specific methods and tools varying depending on the context and industry. Eradicating dangers, replacing them with safer options, putting engineering controls in place, creating administrative controls and supplying PPE are part of the effective risk control procedures. Employees must be adequately educated about possible dangers and the control actions that must be taken through clear and thorough documentation and communication. It is essential to have employee participation in training, reporting systems and decision-making. Continuous improvement is achieved by consistently evaluating, gaining insights from incidents and implementing feedback mechanisms. By implementing these processes, organizations can establish work environments that prioritize safety, minimize the chances of accidents, and safeguard the health and well-being of employees.

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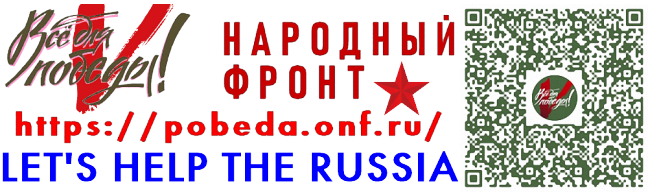
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LOBRY Claude
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