Basic Principles of Process Calculations in Chemical Engineering (ChEg2106)

Prerequisites: No prerequisite for this course

Lecture 1: Introduction to Basic Principles of Chemical Engineering

Week 1

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Lecture learning outcomes

At the end of the lecture, you will be able to:

- identify the basic principles of chemical engineering,
- explain the basic concepts of unit processes and unit operations, and
- describe the insights of sustainability and engineering ethics.

Presentation outlines

- Basic principles of chemical engineering
- Unit operations
- Unit processes
- Sustainability and engineering ethics
- Summary

1.1. Basic principles of chemical engineering

Chemical engineering is the branch of engineering that deals with the **process of converting raw materials into more useful products** using basic sciences, mathematics and economics.

It involves processes that include reactions followed by purification of the products.

These processes may consist of chemical reactions followed by concentration of the products, biological reactions followed by systems that recover and purify the products, or various reactions and recovery of methods. i.e. chemical engineering deals with processes that produce a wide range of products.

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It is a discipline influencing numerous areas of technology.

Chemical engineers are responsible for the **conception, design, operation and control of processes** for purpose of **production, transformation and transportation** of materials.

The activities are started with experimentation in the laboratory and pilot design, which is followed by implementation of technology to full scale production.

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Chemical engineering has several **basic principles**.

Some of the basic principles of chemical engineering are the followings:

- **Material and energy balances:** Both material and energy balances account for the mass and energy entering and leaving a process system.
- **Thermodynamics:** It helps to determine how energy is transferred and transformed in chemical processes.
- **Fluid Mechanics:** This principle helps to study the behavior of fluids (liquids and gases) flow and pressure drop across flow pipes, which is essential for designing process equipment.

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- **Heat transfer:** It helps to understand how heat moves through materials for designing processes that involve heating or cooling.
- **Mass transfer**: It involves the movement of mass from one location to another via various mechanisms, which is vital in separation processes.
- **Chemical reaction**: It helps to design chemical reactors, which accounts reaction kinetics and mechanisms to maximize yield and efficiency.
- **Safety and environmental considerations:** This principle considers the safety of processes and their environmental impact by performing hazard analysis, risk assessment, and waste management.

Chemical engineering processes are categorized into **unit operations** and **unit processes.**

1.2. Unit operations

Unit operations refer to physical steps in processes that involve the transfer of mass, energy, or momentum without changing the chemical identity of the substances involved.

Unit operations deal with physical changes and transport phenomena.

Unit operations are the basis of chemical engineering.

Unit operations can be classified into **mechanical**, **thermal** and **mass transfer** unit operations.

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- **Mechanical unit operations**: These are physical operations which are used for size reduction, size enlargement and separation.

There are numerous mechanical unit operations.

Some of the mechanical unit operations are crushing, grinding, milling, screening, flotation, magnetic separation, gravity separation, sedimentation, filtration and centrifugal separation.

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- **Thermal unit operations:** These are physical operations which are used for thermal applications with heat energy transfer.

Thermal unit operations can be applied with heat exchange between hot and cold materials for heating or cooling .

Thermal unit operations are used for energy utilization in the processes using various heat exchangers such as double pipe heat exchanger, shell and tube heat exchanger, plate and frame heat exchanger or cooler.

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Thermal unit operations are applied for heating (for boilers to generate steam, for distillation to separate volatile liquids, and for evaporator to concentrate solutes by removing solvents).

The rate of heat transfer is described by equation (1.1).

$$Q = UA\Delta T \tag{1.1}$$

Where: Q is rate of heat transfer (W) , U is overall heat transfer coefficient ($W/m^2.K$), A is surface area of hear transfer (m^2), and ΔT is the log mean temperature difference (K) of hot and cold streams.

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- **Mass transfer unit operations**: These are material transfer unit operations by diffusion and convective transport.

Some of the mass transfer unit operations are **distillation**, **leaching**, **evaporation**, **drying**, **adsorption** and **absorption**.

The rate of mass transfer is determined using equation (1.2).

$$J_i = AK_L(C_{ib} - C_{is}) \qquad (1.2)$$

Where: J_i is rate of mass transfer of species i, A is mass transfer area, K_L is mass transfer coefficient, C_{ib} is concentration of at the bulk fluid, and , C_{is} is concentration of at the surface.

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Distillation: It is used to separate liquid mixtures based on their boiling point and volatility differences.

A continuous distillation is shown in **Figure 1.1** **(Coulson & Richardson’s, 1999, pg. 493).**

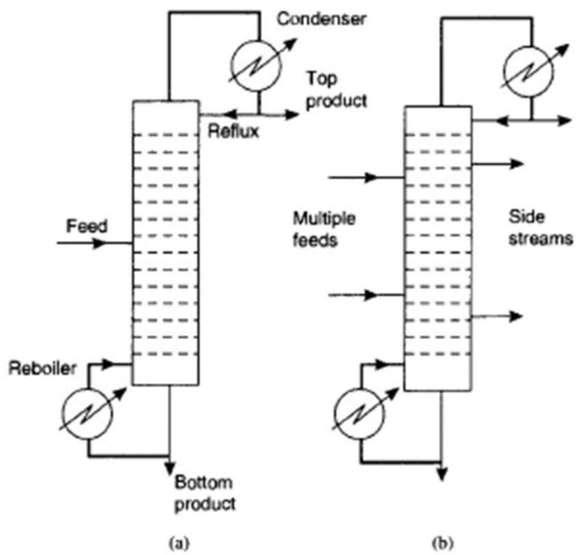

Figure 1.1. Distillation column (a) basic column (b) multiple feeds and side streams

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Distillation is applied in various industries such as petroleum refining, alcohol production and water purification.

In petroleum refining, it is used to separate crude oil into fractions like gasoline, diesel, and kerosene.

In alcohol production, it is used to separate and purify ethanol from fermentation mixtures.

In water purification, it is used to remove impurities from water through distillation for drinking or industrial use.

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Leaching: It is a separation process that involves the extraction of soluble constituents from a solid by means of a solvent **(Coulson & Richardson's, 1999, pg. 445).**

The leaching process effectiveness depends on solvent to solid ration, temperature, concentration of solvent, contact time, and agitation.

Leaching process can be also a unit process, if there is chemical reaction.

Leaching is used in various industries such as food, agriculture and minerals processing industries.

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- In **food industry**, it is used to extract essential oils, colors, and flavors from plant materials.

- In **agriculture**, it is used to leach nutrient from fertilizers into soil.

- In **minerals processing industry**, it is used to extract metals from ores using acid solutions.

For example, cyanide leaching for gold from gold mining, acid leaching for aluminum from kaolinite or clay materials.

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Evaporation: It is the removal of a solvent by vaporization from solids that are not volatile **(Coulson & Richardson’s, 1999, pg. 432).**

It is the process by which liquid molecules transition into the gas phase.

It is a natural process where liquid turns into vapor at temperatures below boiling point.

It is driven by molecular kinetic energy and influenced by environmental factors.

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- Evaporation is widely applied in processing industries such as sugar processing and salt production industries.

- In **sugar processing industry**, it is used to concentrate the sugar by removing water from a solution.

For example, sugar solution from sugarcane juice is concentrated using multiple effect evaporators.

- In **salt processing industry**, it is used to concentrate salt by removing water from a brine solution.

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Drying: It is a process that involves heat transfer and mass transfer to remove moisture from solid materials for preservation, quality enhancement, and preparation for further processing **(Coulson & Richardson's, 1999, pg. 424)**.

It helps to extend shelf life of materials by preventing microbial growth and spoilage.

The quality, texture, and taste of food products can be improved by achieving the desired moisture content.

It is used to removing moisture which decreases the weight of materials for easier handling and transportation.

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Drying process is **applied** in numerous industries such as **food**, **pharmaceuticals**, **textiles** and s**ugar** industries.

- In food industry, it is used to dry fruits, vegetables, crop grains, meats, and herbs for preservation, convenience and further processing.
- In **pharmaceuticals industry**, it is used to dry active ingredients and formulations to ensure stability and efficacy.
- In **textiles industry**, it is used to remove moisture from fabrics after washing or dyeing processes.
- In **sugar industry**, it is used to dry sugar crystals before sieving and packaging.

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Adsorption: It is used to separate impurities from a product, and pollutants from waste water using solid adsorbent materials based on surface charge affinity.

It is a physical phenomenon that occurs when gas or liquid molecules are brought into contact with a solid surface, the adsorbent.

Some of the molecules may condense (the adsorbate) on the exterior surface and in the cracks and pores of the solid.

If interaction between the solid and condensed molecules is relatively weak; the process is called **physical adsorption.**

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If the interaction is strong (similar to a chemical reaction), it is called **chemisorption**.

Some examples of adsorption processes are:

- decolorizing of petroleum fractions,
- decolorizing of vegetable and animal oils, and of crude sugar syrups,
- clarification of beverages and pharmaceutical preparations,
- purification of process effluents and gases for pollution control, and
- impurity removal from air prior to low-temperature fractionation.

(Himmelblau, 2023, pg. 707)

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Absorption: It is a separation technique used to remove a specific component from mixture of gases or liquid mixtures by transferring it into a liquid phase.

It is used to separate gases mixtures using solvents based on selective solubility of gases in the solvent.

It is widely utilized in chemical process industries for recovering of materials

The absorption rate is determined by concentration gradients of the gases in the gas stream and solvent stream.

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Absorption is often employed to capture harmful gases such as CO_2 and SO_2 from industrial emissions before they are released into the atmosphere.

It helps in purifying gases by removing impurities or unwanted components, improving product quality.

The difference in concentration between the gas and the liquid drives the absorption.

In some cases, absorption is part of a chemical reaction where the absorbed species reacts with the solvent or other components.

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Absorption process is used many industries such as **chemical**, **environmental**, **natural gas processing**, and **food and beverage industries**.

- In chemical industry, it is used to capture and recycle solvents or reactants.
- In environmental protection, it is used to treat exhaust gases and reduce air pollutants.
- In natural gas processing, it is used to remove CO_2 and H_2S from natural gas streams.
- In food and beverage industry, it is used to remove unwanted flavors or odors.

Activity 1.1

a) Describe the basic principles of chemical engineering.

b) Explain unit operations.

Cont’d

Activity 1.1, Answers:

a) Describe the basic principles of chemical engineering.

Chemical engineering has several basic principles. Some of the basic principles of chemical engineering are material and energy balances, thermodynamics, fluid mechanics, heat transfer, mass transfer, chemical reaction, and safety and environmental considerations.

b) Explain unit operations.

Unit operations refer to physical steps in processes that involve the transfer of mass, energy, or momentum without changing the chemical identity of the substances involved.

Unit operations can be **mechanical**, **thermal** and **mass transfer** unit operations.

1.3. Unit processes

Unit processes are specific chemical transformations that occur in chemical manufacturing processes.

Unit processes are concerned with chemical changes (reactions).

Unit processes focus on the chemistry of the reaction and transformation of reactants into products.

For examples, synthesis of ammonia (Haber process), esterification, oxidation, reduction, polymerization, and synthesis of inorganic materials are some of the unit processes.

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There are three types of unit processes **(Richard M. Felder, 2005, pg. 84).**

These are: **batch process**, **semi-batch** or semi-continuous process, and **continuous process**.

- **Batch process:** in which production rate changes with time.

There is no feed in flow to the system or product withdrawals from the system until production is completed.

Batch process is used for the **production of specialty chemicals** and small-scale production.

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Batch process is used **to scale-up laboratory experiments** to pilot-plant operation or to full-scale production.

The material balances equation of a batch process for species, i, is given by equation (1.3):

Rate of accumulation of species, i = rate of generation of species, i

$$\frac{-dNi}{dt} = (-r_i)\text{V} \qquad (1.3)$$

Where: N is mole of species i (mol), t is process/ reaction time (min), r_i is rate of reaction of species i (mol/L. min), and V is volume of mixture (L).

Cont'd

Moreover, the energy balance equation of a batch process is given by equation (1.4):

$$\{\boldsymbol{Rate\ of\ accumulation\ of\ energy\ within\ the\ system}\}$$
$$= \{\boldsymbol{Rate\ of\ heat\ energy\ addition\ to\ from\ the\ surroundings}\}$$
$$- \{\boldsymbol{Rate\ of\ work\ done\ by\ the\ system\ on\ the\ surroundings}\}$$

$$\frac{dE}{dt} = \dot{Q} - \dot{W} \qquad (1.4)$$

Where: E is the total of energy (J) , t is time (s), Q is rate of addition of heat (J/s), and W is work done by the system (J/s).

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- **Semi-batch (semi-continuous) process:** Production rate changes with time.

There are either feed flows in to a system or product withdrawals from a system.

It combines features of both batch and continuous processes.

It is useful for processes that require the addition of materials during the reaction.

For batch component, some reactants are added at the beginning, and the process can be operated until the required conversion is achieved.

For continuous component, other reactants can be fed continuously during chemical reactions.

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The general material balance equation of species, i, for a semi-batch process is given by equation (1.5):

{Rate of accumulation} = {rate of inputs} – {rate of outputs} + {rate of generation}

$$\frac{dN_i}{dt} = F_{i0} - F_i + (-r_i V) \qquad (1.5)$$

If species, i, is batch in the feed and continuous in the output stream, the material balance equation (1.5) will be reduced to equation (1.6):

$$\frac{dN_i}{dt} = -F_i + (-r_i V) \qquad (1.6)$$

Cont'd

If species, i, is continuous in the feed and batch in the outputs stream, the material balance equation (1.5) will be reduced to equation (1.7):

$$\frac{dN_i}{dt} = F_{i0} + (-r_i V) \qquad (1.7)$$

Where: N is mole of species i (mol), t is process time, F_{io} is molar flow rate of species i in the feed stream (mol/s), F_i is molar flow rate of species i in the output stream (mol/s), r_i is rate of reaction (mol/L.s) and V is volume of mixture (L).

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The general energy balance equation of a semi-batch process is given by equation (1.8):

$$\frac{dE}{dt} = Q - \dot{W}_S + \sum_{i=1}^{m} F_{io}H_{io} - \sum_{i=1}^{m} F_iH_i \qquad (1.8)$$

If species, i, is continuous in the feed and batch in the outputs stream, the energy balance equation (1.8) will be reduced to equation (1.9):

$$\frac{dE}{dt} = Q - \dot{W}_S + \sum_{i=1}^{m} F_{io}H_{io} \qquad (1.9)$$

Where: E is total energy, Q is addition of heat, t is reaction time, W_s is work done by the system, F_{io} is molar flow rate of species, i in the input, and H_{io} is specific enthalpy of species, i in the input.

Cont'd

If species, i, is batch in the feed and continuous in the outputs stream, the energy balance equation (1.8) will be reduced to equation (1.10):

$$\frac{dE}{dt} = \dot{Q} - \dot{W}_S - \sum_{i=1}^{m} F_i H_i \qquad (1.10)$$

Where: E is total energy, Q is addition of heat, t is reaction time, W_s is work done by the system,, F_i is molar flow rate of species, i in the output stream, and H_i is specific enthalpy of species, i in the output stream.

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- **Continuous process**: Process variables/ parameters do not change with time.

There is feed in flow to the system and product withdrawals from the system until production is completed.

A simple continuous process of materials flow is illustrated in **Figure 1.2**

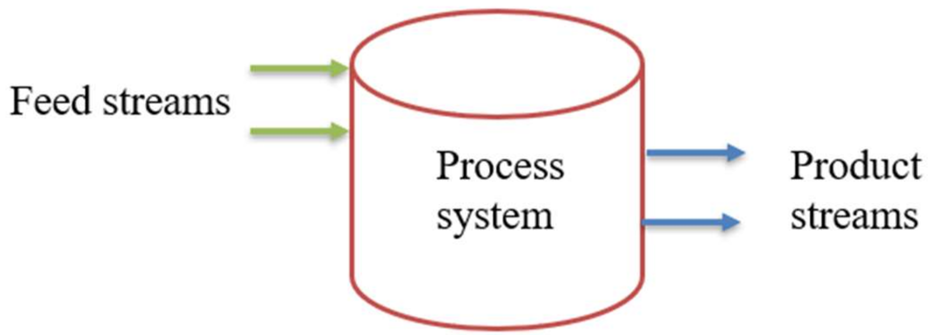

Figure 1.2 A Continuous process materials flow

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The material balances equation of species, i, for a continuous process is given by equation (1.11):

{Rate of inputs} – {rate of outputs} + {rate of generation} = 0

$$F_{i0} - F_i + (-r_i V) = 0 \qquad (1.11)$$

Where: F_{io} is molar flow rate of species i in the feed stream (mol/s), F_i is molar flow rate of species i in the output stream (mol/s), r_i is rate of reaction (mol/L.s) and V is volume of mixture (L).

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The energy balances equation of species, i, for a continuous process is given by equation (1.12):

{Rate of inputs} - {rate of outputs}= 0

$$\dot{Q} - \dot{W}_S + \sum_{i=1}^{m} F_{io}H_{io} - \sum_{i=1}^{m} F_iH_i = 0 \qquad (1.12)$$

Where: Q is addition of heat, W_s is work done by the system, F_{io} is molar flow rate of species, i in the input stream, H_{io} is specific enthalpy of species, i in the input stream, F_i is molar flow rate of species, i in the output stream, and H_i is specific enthalpy of species, i in the output stream.

Activity 1.2

a) **What is the difference between unit processes and unit operations?**

b) **Describe unit processes (batch process, semi-batch process and continuous process).**

Cont'd

Answers:

a) What is the difference between unit processes and unit operations?

Unit operations are physical steps in processes that involve the transfer of mass, energy, or momentum without changing the chemical identity of the substances involved **while** **unit processes** are chemical transformations that occur with changing the chemical identity of the substances involve.

Cont'd

b) Describe unit processes (batch process, semi-batch process and continuous process).

Unit processes involve chemical changes of materials with changing their chemical identity.

Unit processes are categorized into batch, semi-batch and continuous.

- **Batch process:** in which there is no feed in flow to the system or product withdrawals from the system until production is completed.
- **Semi-batch process:** in which there is either feed flows in to the process system or product withdrawals from the process system.
- **Continuous process**: in which there is feed flows in to the process system and product withdrawals from the process system with continuous manner.

1.4. Sustainability and engineering ethics

1.4.1. Sustainability

Sustainability is one of the ways that chemical engineering can contribute to society today and into the future **(Himmelblau, 2023, pg. 26-31).**

A **sustainable product** is a product that meets the current needs without compromising the ability of future generations to meet their needs while protecting human health and the needs of society.

In chemical engineering, sustainability should be an integral part of future designs.

Therefore, the challenge for you as a future engineer is to develop new approaches that make sustainability as economically viable as possible.

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The sustainability of process designs and products can be evaluated using a life-cycle analysis.

A life-cycle analysis is a comprehensive method for developing a sustainable process design.

It considers the effect of a product on the environment, and all the steps used to produce a product and what happens to the product after its useful life has ended.

It is an excellent method to assess the sustainability of materials used in a project.

It shows that the initial impact on sustainability is the extraction of the material and its refining.

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- If the extracted materials concentration is low, it will require more energy to refine it.
- When the useful life of the product ends, the product must be disposed of and/or recycled.
- The recycling process recovers all or part of the product material, which can be used for production of other products in the future.
- Each step from raw material extraction to recycling materials requires the use of resources and has an environmental impact.

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1.4.2. Engineering ethics

Engineering ethics is a collection of moral principles applied in engineering practices **(Himmelblau, 2023, pg. 35-36)**

It is also the rules of fair play that engineers operate under while serving the public, their employer, the client, and the profession.

Engineering offers great potential for contributing to the public good, but at the same time, it can cause great harm if it is not applied correctly and ethically.

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Numerous engineering societies adopted formal codes of ethics.

The codes make it clear that engineers are responsible for protecting the safety of the public.

The public health, welfare, and safety make it the interest of the employer and the client.

In addition, engineers should work only on projects for which they have the necessary education or experience.

- Remember that whenever you sign your name to a document, you are confirming the accuracy and validity of it with your reputation.

Activity 1.3

a) What is sustainability in chemical engineering perspectives?

b) How do we develop a sustainable process design?

c) What is engineering ethics?

Cont'd

Answers:

a) What is sustainability in chemical engineering perspectives?

Sustainability is one of the ways that chemical engineering can contribute to society today by satisfying the current needs without compromising the ability of future generations to meet their needs while protecting human health and the needs of society.

Cont’d

b) How do we develop a sustainable process design?

A sustainable process design is developed by making a life-cycle analysis.

A life-cycle analysis is a comprehensive method for developing a sustainable process design, which considers the effect of a product on the environment.

c) What is engineering ethics?

Engineering ethics is a collection of moral principles applied in engineering practices.

It is also the rules of fair play that engineers operate under while serving the public, their employer, the client, and the profession.

1.5. Summary

- Unit operations are physical steps in processes that involve the transfer of mass, energy, or momentum without changing the chemical identity of the substances involved.
- Unit processes are chemical transformations that occur in chemical manufacturing processes.
- Sustainability is one of the ways that chemical engineering can contribute to society today and into the future
- Engineering ethics is a collection of moral principles applied in engineering practices.

References

- Basic Principles and Calculations in Chemical Engineering, Himmelblau, Pearson Education Inc, 9th edition, 2023.
- Chemical Engineering Design, Volume 6, Coulson & Richardson's, R. K. Sinnott, 3rd edition, 1999.
- Elementary Principles of Chemical Processes, Richard M. Felder, John Wiley & Sons, 3rd edition, 2005.

Thank you!