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SCHOOL OF BIO AND CHEMICAL ENGINEERING
DEPARTMENT OF CHEMICAL ENGINEERING

UNIT – I – PRINCIPLES OF CHEMICAL ENGINEERING – SCHA1101

UNIT-I

1.1 CHEMICAL ENGINEERING:

- What is Chemical Engineering?
- How and why Chemical Engineering develop?
- What do Chemical Engineers contribute to the society?
- How this profession got developed over last century?

Chemical engineers have been improving our well-being for more than a century. From the development of smaller, faster computer chips to innovations in recycling, treating disease, cleaning water, and generating energy, the processes and products that chemical engineers have helped create touch every aspect of our lives. Chemical engineers work in manufacturing, pharmaceuticals, healthcare, design and construction, pulp and paper, petrochemicals, food processing, specialty chemicals, microelectronics, electronic and advanced materials, polymers, business services, biotechnology, and environmental health and safety industries, among others. Within these industries, chemical engineers rely on their knowledge of mathematics and science—particularly chemistry— to overcome technical problems safely and economically. And, of course, they draw upon and apply their engineering knowledge to solve any technical challenges they encounter.

It is true that chemical engineers are comfortable with chemistry, but they do much more with this knowledge than just make chemicals. All engineers employ mathematics, physics, and the engineering art to overcome technical problems in a safe and economical fashion. Yet, it is the chemical engineer alone that draws upon the vast and powerful science of chemistry to solve a wide range of problems. The strong technical and social ties that bind chemistry and chemical engineering are unique in the fields of science and technology. The interconnection of chemists and chemical engineers has been beneficial to both sides and includes other engineering fields along with them.

Chemical engineering is based on applications of chemistry, physics, mathematics, economics, and increasingly, biology and biochemistry. Because of this broad-based foundation the chemical engineer is considered the universal engineer. Chemical engineering deals with unit operations. Industrial process requires a chemical engineer who has a complete and quantitative understanding of the engineering principles as well as the scientific principles on which the operations rest. ... Because many industries are based on some chemical or physical transformation of matter, the chemical engineer is much in demand."

1.2HISTORY OF CHEMICAL ENGINEERING:

- Chemical engineering profession began in **1888.**
- While, the term "chemical engineer" had been floating around technical circles throughout the 1880's, there was no formal education for such a person.
- The "chemical engineer" of those years was either a mechanical engineer who had gained some knowledge of chemical process equipment, a chemical plant foreman with a lifetime of experience but little education, or an applied chemist with knowledge of large scale industrial chemical reactions.
- An effort in 1880, by **George Davis**, to unite these varied professionals through a "**Society of Chemical Engineers**" proved unsuccessful.

- However, this muddled state of affairs was changed in 1888, when **Professor Lewis Norton** of the **Massachusetts Institute of Technology** introduced **"Course X"** (ten), thereby uniting chemical engineers through a formal degree.
- Other schools, such as the **University of Pennsylvania** and **Tulane University**, quickly followed suit adding their own four-year chemical engineering programs in **1892** and **1894** respectively.
- **William Page Bryant** was the first of seven students to graduate from "Course X" and thereby became the world's first formal chemical engineer in the year **1891.**
- The first formal class on chemical engineering, consisting of 12 lectures by George E. Davis in **1887.**
- **Massachusetts Institute of Technology** offered **"Course X"** in **1888**, the first four-year chemical engineering degree which was taught by Lewis M. Norton. The program offered a mixture of mechanical engineering and industrial chemistry.
- Chemical engineers gained a formal education in 1888, this was certainly no guarantee of success.
- Many prominent people saw no need for this new profession. Additionally, it was unclear what role chemical engineers would play in industry.
- To survive, chemical engineers had to claim industrial territory by defining themselves and demonstrating their uniqueness and worth. With this goal in mind, **the American Institute of Chemical Engineers (AIChE)** was formed in **June** of **1908.**
- However, AIChE also faced difficult challenges in defining its own territory. The old (since 1876) and powerful (5000 members) **American Chemical Society (ACS)** had already laid claim to all realms of American Chemistry, both pure and applied.
- After the formation of AIChE, the ACS launched its own "Division of Industrial Chemistry & Chemical Engineering" placing itself in direct competition with AIChE for the hearts and minds of the new engineers.

1.3 AIChE AIChE (American Institute of Chemical Engineers):

- AIChE is the smallest of the societies representing one of the "big four" engineering fields (mechanical, electrical, civil, and chemical engineering).
- The Institute was formed in June of 1908 as the sole institutional home for chemical engineers.
- However, almost before the echoes of McKenna's founding keynote address had finished reverberating with the audience, the ACS had launched a new division; joining in a battle for the chemical engineer's heart, mind, and financial dues.
- Because of this, the AIChE spent the first third of its life as a very exclusive organization. While it contributed to industry through publications such as the "Transactions of AIChE" (which evolved into "Chemical Engineering Progress" in 1947 and still provides news and technical information today), or through scholastic accreditation.
- AIChE hardly represented the chemical engineering profession as a whole.

- It changed in the 1930's when membership requirements were relaxed, and chemical engineers joined in masses.
- Today there are five classes of membership (student, affiliate, associate, member, and fellow) through which nearly 60,000 chemical engineers have become members (see AIChE & THE FUTURE).
- The Institute has a yearly budget of around $21 million, which it spends providing technical education, safety training, career counseling, governmental advising, and social activities for its members.

1.4 ACS (American Chemical Society)

- ACS represents the best American chemistry has to offer.
- ACS grew rapidly after its founding in 1876 (even before chemical engineering existed).
- Because of its success, smaller factions within the society often felt they could go it alone, and splinter groups soon became a problem.
- At the turn of the century chemical engineers became one of these splinter groups, forming the AIChE in 1908.
- The ACS responded by creating the "Division of Industrial Chemistry & Chemical Engineering."
- Today the ACS remains at the center of American Chemical developments boasting 150,000 members.
- Through its "Chemical Abstracts" service and "Chemical & Engineering News" the ACS continues to provide valuable information to chemists & chemical engineers alike.
- Despite bitter feelings concerning the creation of the AIChE, today chemical engineers and chemists have a relationship unlike anything found in other engineering fields

1.5 GEORGE DAVIS (1880):

- George Davis was an Alkali Inspector from the "Midland" region of England.
- Throughout his long career Davis was going through many of the chemical plants in his region.
- Inside he was given intimate access to monitor pollution levels as necessitated by the Alkali Works Act of 1863.
- These rounds included the Lead-Chamber, Le Blanc, and Solvay processing plants which had undergone a revolution due to engineering efforts.
- This revolution in operation clarified the necessity for a new branch of engineering that was equally comfortable with both applied chemistry and traditional engineering.
- In 1880 George Davis acted upon these ideas and proposed the formation of a "Society of Chemical Engineers".
- In 1884 Davis became an independent consultant applying and synthesizing the chemical knowledge he had accumulated over the years.
- In 1887 he moulded his knowledge into a series of 12 lectures on chemical engineering, which he presented at the Manchester Technical School.

- This chemical engineering course was organized around individual chemical operations, later to be called "unit operations."
- Davis explored these operations empirically and presented operating practices employed by the British chemical industry.
- Because of this, some felt his lectures merely shared English know-how with the rest of the world.
- However, his lectures went far in convincing others that the time for chemical engineering had arrived. Some of these people lived across the Atlantic, where the need for chemical engineering was also real and immediate.

1.6 F. W. Atkinson

"Chemical engineering needs to be more sharply defined. Its scope is still in a somewhat indeterminate state and as yet its position as one of the professions is not clearly recognized."

1.7 Milton C. Whitaker

"The chemical engineer works in the organization, operation and management of existing or proposed processes with a view to building up a successful manufacturing industry... His fundamental training in chemistry, physics, mathematics, etc., must be thorough and must be combined with a natural engineering inclination and an acquired knowledge of engineering methods and appliances."

1.8 ARTHUR D. LITTLE

- He is the Consultant and co-founder with William Walker, of "Little and Walker" which later became "Arthur D. Little”
- He coined the term "**unit operations**" in **1915** and headed up AIChE's Committee on Chemical Engineering Education which emphasized the "unit operation" concept along with accreditation to standardize courses in chemical engineering programs.
- He said: "Any chemical process, on whatever scale conducted, may be resolved into a coordinate series of what may be termed 'unit operations', as pulverizing, dyeing, roasting, crystallizing, filtering, evaporation, electrolyzing, and so on.
- The number of these basic unit operations is not large and relatively few of them are involved in any particular process.
- The complexity of chemical engineering results from the variety of conditions as to temperature, pressure, etc., under which the unit operations must be carried out in different processes, and from the limitations as to material of construction and design of apparatus imposed by the physical and chemical character of the reacting substances."

1.9 Ralph McKee

Said that "The Committee have written a prescription, and it is our duty to see that the prescription is filled and given to the patients"

1.10 Unit operation :

In transforming matter from inexpensive raw materials to highly desired products, chemical engineers became very familiar with the physical and chemical operations necessary in this metamorphosis. Examples of this include: filtration, drying, distillation, crystallization, grinding, sedimentation, combustion, catalysis, heat exchange, extrusion, coating, and so on. These "unit operations" repeatedly find their way into industrial chemical practice, and became a convenient manner of organizing chemical engineering knowledge. Additionally, the knowledge gained concerning a "unit operation" governing one set of materials can easily be applied to others.

Whether one is distilling alcohol for hard liquor or petroleum for gasoline, the underlying principles are the same! The "unit operations" concept had been latent in the chemical engineering profession ever since George Davis had organized his original 12 lectures around the topic. However, it was Arthur Little who first recognized the potential of using "unit operations" to separate chemical engineering from other professions. While mechanical engineers focused on machinery, and industrial chemists concerned themselves with products, and applied chemists studied individual reactions, no one, before chemical engineers, had concentrated upon the underlying processes common to all chemical products, reactions, and machinery. The chemical engineer, utilizing the conceptual tool that was unit operations, could now claim to industrial territory by showing his or her uniqueness and worth to the American chemical manufacturer.

1.11 Some important process of chemical engineering

Le Blanc Process

A method for converting common salt into soda ash using sulfuric acid, limestone and coal as feedstock’s (raw materials) and thereby creating hydrochloric acid as a by-product. It was invented in 1789 by Nicholas Le Blanc (1742-1806), a French industrial chemist. In 1794, just prior to the French Revolution, the French government seized Le Blanc's process and factory without payment. Although vast fortunes where accumulated through his process, Le Blanc died in poverty. In many ways, his process began the modern chemical industry. While the precise chemistry involved in the process remained obscure for nearly 100 years, it was later found to consist of several steps:

a) 2 NaCl (salt) + H_2SO_4 (sulfuric acid) => Na_2SO_4 (saltcake, intermediate) + 2 HCl (hydrochloric acid gas, a horrible waste product)

b) Na_2SO_4 (saltcake) + Ca_2CO_3 (calcium carbonate, limestone) + 4 C(s) (coal) => Na_2CO_3 (soda ash extracted from black ash) + CaS (dirty calcium sulfide waste) + 4 CO (carbon monoxide)

Solvay process

It was perfected in 1863 by a Belgian chemist named Ernest Solvay. The chemistry was based upon a half century old discovery by A. J. Fresnel who in 1811 had shown that Sodium Bicarbonate could be precipitated from a salt solution containing ammonium bicarbonate. This chemistry was far simpler than that devised by Le Blanc, however to be used on an industrial scale many engineering obstacles had to be overcome. Sixty years of attempted scale-up had failed until Solvay finally succeeded. Solvay's contribution was there for one of chemical engineering. The heart of his design embodied an 80 foot tall high-efficiency carbonating tower in which ammoniated brine trickled down from above and carbon dioxide rose from the bottom. Plates and bubble caps helped create a large surface area over which the two chemicals could react forming sodium bicarbonate. Solvay's process had several advantages over the Le Blanc process which it rapidly replaced:

1) Continuous operation

2) A product which was easier to purify

3) No dirty, hazardous, and hard to dispose of bi-products.

Sulfuric Acid (Oil of Vitriol) & "Fuming" Sulfuric Acid (Oleum) (H_2SO_4)

During the 19th Century sulfuric acid was necessary in the production of alkali salts and dyestuffs, two giants of the day. Today the largest single use is in the manufacture of fertilizers. It is also necessary in petroleum purification, steel production, electroplating, and automobile batteries. The production of TNT (trinitrotoluene), nitroglycerin, picric acid, and all other mineral and inorganic acids require sulfuric acid. "Fuming" sulfuric acid contains excess amounts of sulfur trioxide and fumes when exposed to air; hence its name.

1.13 Petrochemicals

At the birth of our Nation (1776) energy was used primarily to heat houses and cook food; requiring only timber and coal. Water power was sufficient for the textile factories and grain mills that existed, while animal power helped till the fields and provide transportation. However, as the Industrial Revolution (18th Century to today) rolled along, larger quantities of mechanical energy were soon required. Several inventions helped meet these needs, but in the process they also consumed vast quantities of fossil fuels.

Petroleum is so important to our society that it has rightfully earned the title "black gold." When used to supply energy, petroleum is converted into; gasoline, fuel oils, lubricants, kerosene, and jet fuels. However, it is also necessary for; plastics, waxes, asphalt, and all nature of fine organic chemicals. Because of its value as a raw material, some claim that petroleum is too valuable to burn! About half of all American chemical engineers are employed by the petroleum industry; and a huge industry it is. The petroleum industry is one of the main reasons chemical engineers have enjoyed such success.

- Small amounts of petroleum have been used throughout history.
- The Egyptians coated mummies and sealed their mighty Pyramids with pitch.
- American Indians used petroleum for paint, fuel, and medicine.
- Ancient Persians and Sumatrans also believed petroleum had medicinal value.
- Yet despite its usefulness, for thousands of years petroleum was very scarce.
- For those digging wells to get drinking water the petroleum was seen as a nuisance. However, some thought the oil might have large scale economic value.
- **George Bissell**, a lawyer, thought that petroleum might be converted into kerosene for use in lamps.

Early Refining

- By 1860 there were 15 refineries in operation. Known as "tea kettle" stills, they consisted of a large iron drum and a long tube which acted as a condenser.
- Capacity of these stills ranged from 1 to 100 barrels a day. A coal fire heated the drum, and three fractions were obtained during the distillation process.
- The first component to boil off was the highly volatile naphtha. Next came the kerosene, or "lamp oil", and lastly came the heavy oils and tar which were simply left in the bottom of the drum.
- These early refineries produced about 75% kerosene, which could be sold for high profits. (Giddens, p.14) Kerosene was so valuable because of a whale shortage that had began in 1845 due to heavy hunting.
- This shortage of natural sources meant that kerosene was in great demand. Almost all the families across the country started using kerosene to light their homes.
- However, the naphtha and tar fractions were seen as valueless and were simply dumped into Oil Creek.
- Later these waste streams were converted into valuable products.
- In **1869 Robert Chesebrough** discovered how to make petroleum jelly and called his new product Vaseline.
- The heavy components began being used as lubricants, or as waxes in candles and chewing gum.
- Tar was used as a roofing material. But the more volatile components were still without much value.
- Limited success came in using gasoline as a local anesthetic and liquid petroleum gas (LPG) in a compression cycle to make ice.
- The success in refined petroleum products greatly spread the technique.
- By 1865 there were 194 refineries in operation.

1.15 Various compounds in petroleum industries:

- Hydrocarbons
- Bitumen
- Organic compounds
- Inorganic compounds
- Aromatic compounds
- Aliphatic
- Petrol
- Natural gas
- Liquefied petroleum gas
- Gasoline
- Naptha
- Kerosene
- Diesel
- Gas oil
- Heavy fuel oil
- Asphalt
- Tar

1.16Modern Petroleum Refining

Petroleum refineries are marvels of modern engineering. Within them a maze of pipes, distillation columns, and chemical reactors turn crude oil into valuable products. Large refineries cost billions of dollars, employ several thousand workers, operate around the clock, and occupy the same area as several hundred football stadiums. The U.S. has about 300 refineries that can process anywhere between 40 and 400,000 barrels of oil a day. These refineries turn out the gasoline and chemical feedstock's that keeps the country running.

Locating an oil field is the first obstacle to be overcome. The first explorers used Y-shaped divining rods and other supernatural, but ineffective, means of locating petroleum. Today geologists and petroleum engineers employ more tried and true methods. Instruments to aid the search include; geophones (uses sound), gravimeters (uses gravity), and magnetometers (uses the Earth's magnet field). While these methods narrow the search tremendously, a person still has to drill a exploratory well, or wildcat well, to see if the oil actually exists. Success brings visions of gushers soaring skyward, however today wells are capped before this happens.

Drilling

There are three main types of drilling operations; cable-tool, rotary, and off-shore. Cable-tool drilling involves a jack-hammer approach were a chisel dislodges earth and hauls up the loose sediment. Rotary drilling works at much greater depths, and involve sinking a drill pipe with a rotating steel bit in the middle. Off-shore drilling involves huge semisubmersible platforms which lower a shaft to the ocean floor, containing any oil which is located. All crude oil contains some amount of methane or other gases dissolved in it. Once the drilling shaft makes contact with the oil it releases the pressure in the underground reservoir. Just like opening a can of soda pop, the dissolved gases fizz out of solution pushing crude oil to the surface. The dissolved gases will allow about 20% recovery of oil. To get better recovery water is often pumped into the well, this forces the lighter oil to the surface. Water flooding allows recoveries of about 50%. The addition of surfactant allows even more oil to be recovered by preventing much of it from getting trapped in nooks and crannies. Yet, it is impossible to get all of the oil out of a well.

Transportation

Because crude oil is a liquid it is much easier to move than natural gas or coal. Coal is nice and dense, so it does not require large holding containers, but it cannot be pumped. Conveyor belts and cranes cannot compete with pipelines for economic efficiency. Natural gas can be pumped using expensive compressors, but it requires enormous holding tanks. A recent trick has been to inject huge amounts of water into salt strata. The water dissolves the salt, leaving truly enormous caverns. The natural gas is then pumped in and stored until needed. The ease in transporting oil is one of the reasons we have become so dependent upon it. Pound for pound natural gas and coal just cannot compete.

Distillation

Oil contains a complex mixture of hydrocarbons. The first step in obtaining something of value from this muck is to de-salt and de-water it. Then the oil is heated and sent into a huge distillation column operating at atmospheric pressure. Heat is added at the reboiler, and removed at the condenser, thereby separating the oil into fractions based upon boiling point. A typical atmospheric column can separate about 4,000 cubic meters (25,000 barrels) of oil per day. The bottom fraction is sent to another column operating at a pressure of about 75 mm Hg (one tenth of an atmosphere). This column can separate the heaviest fraction without thermally degrading (cracking) it. Whereas atmospheric columns are thin at tall, vacuum columns are thick and short, to minimize pressure fluctuations along the column. Vacuum columns can be over 40 feet in diameter.

Catalytic Reforming

Catalytic Reforming produces high octane gasoline for today’s automobiles. Gasoline and naphtha feedstocks are heated to 500 degrees Celsius and flow through a series of fixed-bed catalytic reactors. Because the reactions which produce higher octane compounds (aliphatic in this case) are endothermic (absorb heat) additional heaters are installed between reactors to keep the reactants at the proper temperature. The catalyst is a platinum (Pt) metal on an alumina (Al2O3) base. While catalysts are never consumed in chemical reactions, they can be fouled, making them less effective over time. The series of reactors used in Catalytic Reforming are therefore designed to be disconnected, and swivelled out of place, so the catalyst can be regenerated.

Fluidized Catalytic Cracking

Catalytic Cracking takes long molecules and breaks them into much smaller molecules. The cracking reaction is very endothermic, and requires a large amount of heat. Another problem is that reaction quickly fouls the Silica (SiO2) and alumina (Al2O3) catalyst by forming coke on its surface. However, by using a fluidized bed to slowly carry the catalyst upwards, and then sending it to a regenerator where the coke can be burned off, the catalyst is continuously regenerated. This system has the additional benefit of using the large amounts of heat liberated in the exothermic regeneration reaction to heat the cracking reactor. The FCC system is a brilliant reaction scheme, which turns two negatives (heating and fouling) into a positive, thereby making the process extremely economical.

Hydro processing

Hydro processing includes both hydrocracking and hydro treating techniques. Hydro treating involves the addition of hydrogen atoms to molecules without actually breaking the molecule into smaller pieces. Hydro treating involves temperatures of about 325 degrees Celsius and pressures of about 50 atmospheres. Many catalysts will work, including; nickel, palladium, platinum, cobalt, and iron. Hydrocracking breaks longer molecules into smaller ones. Hydrocracking involves temperatures over 350 degrees Celsius and pressures up to 200 atmospheres. In both cases, very long residence times (about an hour) are required because of the slow nature of the reactions.

1.17 10 Greatest Achievements of Chemical Engineering

- ✓ The Atom, as Large as Life
- ✓ The Plastic Age
- ✓ The human reactor
- ✓ Wonder drugs for the masses
- ✓ Synthetic fibers
- ✓ Liquefied air
- ✓ Environment
- ✓ Food
- ✓ Petrochemicals
- ✓ Running on synthetic rubber

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COMPONENTS OF CHEMICAL ENGINEERING

UNIT-II

2.1 Role and Importance of Basic Sciences in Engineering

- In this chapter, examples of the interaction between these disciplines will be discussed as they arise in different applications.
- A common misconception which prevails is that chemical engineering is based primarily on chemistry. It is not true. In fact, chemical engineering involves a combination of principles of mathematics, physics, chemistry, biology, and even economics.
- Biology comes in since some processes such as fermentation involve microorganisms and are biochemical in nature.
- Economics is necessary so that the cost of production can be addressed. This ensures that a technological concept is also economically viable.
- All systems must satisfy the principles of conservation of mass, momentum, and energy.
- These principles are used to solve problems concerning the design of equipment (such as a reactor or a distillation column) for a desired performance level or predicting performance for a specific design.
- First, we will see different examples wherein we use physics and mathematics to analyze a situation.
- Physics is used to formulate equations and mathematics is used to solve equations. Equations arise from the applications of the fundamental laws which any system must conform to.
- The three fundamental laws all systems must obey are the *laws of conservation of mass, momentum,* and *energy*.
- One of the main responsibilities of the chemical engineer is to understand how to apply these laws to specific systems and problems and obtain useful information from them.
- This equation will arise in different forms in different situations or applications. It is used to analyse the behaviour of different systems in various contexts.
- Applications of this equation in different situations give rise to different kinds of mathematical equations: algebraic equations, ordinary differential equations, and partial differential equations.

2.2 Safety Issues in the Scale-up

One of the important responsibilities and challenges of a chemical engineer is the scale-up of a process. The manufacturing steps are first demonstrated at the laboratory scale and it is the primary responsibility of the chemical engineer to come up with a process which will enable high volumes of production.

Consider a reaction which has been successfully demonstrated in the laboratory as capable of producing 5 moles of a compound in a reactor of size 2 litres (say a beaker or a conical flask). These numbers are hypothetical and are used to illustrate the idea. It is now desired that at the commercial scale 5,000 moles of this compound be produced. You are asked to determine the size of the reactor.

let us assume that the reactor is being designed for a batch operation. One might be tempted to think that a 2,000 litre reactor would serve the purpose. Under this assumption, an increase in amount produced by a factor of 10^3 can be achieved by increasing the reactor volume by the same factor.

Here we have assumed that the moles produced depend linearly on the volume. Under this assumption an increase in the amount produced by a factor of 1,000 can be achieved by increasing the reactor volume by the same factor. However, this assumption is frequently invalid since different processes occurring in the system scale with size in different ways. For instance, if we have a homogeneous chemical reaction which is exothermic the heat is generated throughout the volume. The reaction is accompanied by heat generation and heat loss to the ambience. Hence increasing the size of the vessel would result in the heat generation being proportional to the volume, i.e. it increases as a cube of the length scale (radius if the vessel is spherical). However, the surface area across which heat loss to the ambient occurs increases only as the square of the length scale (radius) since it is proportional to the surface area.

Hence increasing the volume of the vessel implies that the rate of heat generation increases much more than the rate of heat loss. Consequently, this would result in a higher temperature prevailing in the reactor at the commercial (larger) scale as opposed to the lab (smaller) scale. This has implications on the reaction rate which is dependent nonlinearly (exponentially) on temperature through the Arrhenius temperature dependency.

The point being made here is in the larger reactor as the reaction progresses the temperature prevailing would be different from that in a smaller reactor. The bigger reactor may have to be designed to ensure that the temperature is the same as that in the lab scale or there could be undesirable side reactions giving unwanted products reducing the reaction efficiency. If the objective is to keep the temperature same it is necessary to provide additional provisions in the larger reactor to remove the extra heat being generated. A second problem that can arise is maintaining spatially uniform conditions in the larger reactor. In a smaller vessel it may be easier to have spatial uniformity. The spatial variations in a larger reactor may result in the performance of the larger reactor being different from what is expected. Hence, during the scale-up these issues have to be kept in mind and addressed.

The scale-up issues pose challenges for several systems, in particular exothermic reactions which exhibit runaway behavior.

2.3 Runaway

In an exothermic reaction as the reaction proceeds, heat is liberated. This causes a further increase in the temperature which in turn makes the reaction proceed faster. This results in a greater heat release accompanied by a further increase in temperature. Consequently, the temperature rise in the system is very rapid. However, this does not proceed indefinitely as the reactants get consumed. Finally, when no reactants are left, the reaction stops. A sudden rapid increase in the temperature of the reactor sustaining an exothermic reaction is called a ***runaway behavior***.

2.4 Lab Scale and Commercial Scale

The demand for a product can be a few hundred tons per year. Under these circumstances, this large volume can be produced by carrying out the reaction in tens of thousands of the small reactors in the Laboratory. This would mean that the production is carried out in parallel. This would be a very inefficient way of doing things as it would require a large equipment inventory, it would be highly labor intensive, etc.

It is for this reason that most plants that we see in the industry are large in size. Here the plant operation becomes economical when it has a large capacity. This is the so-called ***economies of scale*** where the utilization of energy, raw materials, etc. on a per unit product formed basis is very efficient

There are several challenges (mixing, rate of heat generation, and heat loss) when the size of units is increased. New physical phenomena arise when the scale is increased and these have to be accounted for. Hence increasing the size is usually not done in one step. The scale of the plant operation or the size of the plant is not increased by three orders of magnitude, for instance.

The system behavior in an intermediate scale called the ***pilot plant*** is first analyzed. This has a production capacity which is in between the lab scale and the commercial scale. For instance, it could be a plant with a capacity of tens of tons. The process is first extended from the lab scale to the pilot-plant scale. There is a significant amount of learning or knowledge which is gained at this stage. This is achieved at a moderate cost, since the costs for building the pilot plant and running it are much lower than that of building and running a commercial plant. This knowledge is then used to scale up further to the commercial scale. Sometimes pilot-plant level tests may be done at two intermediate scales before going for commercial production

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2.5 Challenges involved in the scaling-up

- The operating conditions (initial concentrations of the reactants, initial temperature, etc.) which were safe for the pilot plant may be unsafe for the commercial scale reactor.
- These challenges make it important for us to obtain a good understanding of all the processes (reaction, mixing, and heat transfer, etc.) which are taking place in the system so that the scale-up can be done in a reliable way with minimum scope for any error.

2.6 Batch reactor

A batch reactor is a dynamic system. Here as the reaction progresses, heat is liberated if the reaction is exothermic and the temperature increases as a function of time. Hence, the accumulation term cannot be set to zero since we do not have a steady state. The energy balance equation is

Accumulation = In – Out + Generation

For a batch system there is no inflow or outflow of reactants or products across the reactor. The generation term represents the heat lost by the reactor to the ambient if the reactor is not insulated and the heat generated by the exothermic reaction. This term is high when the reaction rate and the heat of reaction are high. When this is higher than the outflow term, we have a net accumulation of heat resulting in an. Increase in the temperature with time. If the outflow term is more than the generation term the accumulation term is negative and this results in a decrease in temperature as a function of time.

2.7 DIMENSIONAL ANALYSIS:

Many practical flow problems of different nature can be solved by using equations and analytical procedures, as discussed in the previous modules. However, solutions of some real flow problems depend heavily on experimental data and the refinements in the analysis are made, based on the measurements. Sometimes, the experimental work in the laboratory is not only time-consuming, but also expensive. So, the dimensional analysis is an important tool that helps in correlating analytical results with experimental data for such unknown flow problems. Also, some dimensionless parameters and scaling laws can be framed in order to predict the prototype behavior from the measurements on the model. The important terms used in this module may be defined as below

Dimensional Analysis:

The systematic procedure of identifying the variables in a physical phenomenon and correlating them to form a set of dimensionless groups is known as dimensional analysis.

Dimensional Homogeneity:

If an equation truly expresses a proper relationship among variables in a physical process, then it will be dimensionally homogeneous. The equations are correct for any system of units and consequently each group of terms in the equation must have the same dimensional representation. This is also known as the law of dimensional homogeneity.

Dimensional variables:

These are the quantities, which actually vary during a given case and can be plotted against each other. Dimensional constants: These are normally held constant during a given run. But they may vary from case to case. Pure constants: They have no dimensions, but, while performing the mathematical manipulation, they can arise.

Primary dimensions and their associated primary SI and English units

Dimension	Symbol*	SI Unit	English Unit
Mass	m	kg (kilogram)	lbm (pound-mass)
Length	L	m (meter)	ft (foot)
Time†	t	s (second)	s (second)
Temperature	T	K (kelvin)	R (rankine)
Electric current	I	A (ampere)	A (ampere)
Amount of light	C	cd (candela)	cd (candela)
Amount of matter	N	mol (mole)	mol (mole)

2.8 Buckingham pi Theorem

The dimensional analysis for the experimental data of unknown flow problems leads to some non-dimensional parameters. These dimensionless products are frequently referred as *pi terms*. Based on the concept of *dimensional homogeneity*, these dimensionless parameters may be grouped and expressed in functional forms. This idea was explored by the famous scientist Edgar Buckingham (1867-1940) and the theorem is named accordingly.

Buckingham pi theorem, states that if an equation involving *k* variables is dimensionally homogeneous, then it can be reduced to a relationship among $\square k \, \square \, r \, \square$ independent dimensionless products, where *r* is the minimum number of reference dimensions required to describe the variable. For a physical system, involving *k* variables, the functional relation of variables can be written mathematically as,

$$y \,\square\, f \,\square\, x_1 , x_2 \; , x_k \,\square$$

From equation, it should be ensured that the dimensions of the variables on the left side of the equation are equal to the dimensions of any term on the right side of equation. Now, it is possible to rearrange the above equation into a set of dimensionless products (*pi terms*), so that

$$\pi_1=\varphi(\pi_2,\pi_3.....,\pi_{k-r})$$

here, $\varphi(\pi_2,\pi_3.....,\pi_{k-r})$ is a function of π_2 through π_{k-r}. The required number of *pi* terms is less than the number of original reference variable by r. these reference dimensions are usually the basic dimensions M, L and T (Mass, Length and Time).

2.9 Non-Dimensional numbers in Fluid Dynamics

Forces encountered in flowing fluids include those due to inertia, viscosity, pressure, gravity, surface tension and compressibility. These forces can be written as follows;

Inertia force: $m a = \rho V \frac{dV}{dt} \propto \rho V^2 L^2$

Viscous force: $\tau A = \mu A \frac{du}{dy} \propto \mu V L$

Pressure force: $(\Delta p) A \propto (\Delta p) L^2$

Gravity force: $mg \propto g \rho L^3$

Surface tension force: σL

Compressibility force: $E_v A \propto E_v L^2$

Parameter	Mathematical expression	Qualitative definition	Importance
Prandtl number	$P_r = \frac{\mu c_p}{k}$	$\frac{\text{Dissipation}}{\text{Conduction}}$	Heat convection
Eckert number	$E_c = \frac{V^2}{c\ T_{p0}}$	$\frac{\text{Kinetic energy}}{\text{Enthalpy}}$	Dissipation
Specific heat ratio	$\gamma = \frac{c_p}{c_v}$	$\frac{\text{Enthalpy}}{\text{Internal energy}}$	Compressible flow
Roughness ratio	$\frac{\varepsilon}{L}$	$\frac{\text{Wall roughness}}{\text{Body length}}$	Turbulent rough walls
Grashof number	$G_r = \frac{\beta(\Delta T) g L^3 \rho^2}{\mu^2}$	$\frac{\text{Buoyancy}}{\text{Viscosity}}$	Natural onvection
Temperature ratio	$\frac{T_w}{T_0}$	$\frac{\text{Wall temperature}}{\text{Stream temperature}}$	Heat transfer
Pressure coefficient	$C_p = \frac{p - p_\infty}{(1/2)\rho V^2}$	$\frac{\text{Static pressure}}{\text{Dynamic pressure}}$	Hydrodynamics, Aerodynamics
Lift coefficient	$C_L = \frac{L}{(1/2) A \rho V^2}$	$\frac{\text{Lift force}}{\text{Dynamic force}}$	Hydrodynamics,Aero dynamics
Drag coefficient	$C_D = \frac{D}{(1/2) A \rho V^2}$	$\frac{\text{Drag force}}{\text{Dynamic force}}$	Hydrodynamics, Aero dynamics

Surface tension force: □ L

Compressibility force: $E_v A$ □ $E_v L^2$