REACTOR DESIGN CONSIDERATIONS

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INTRODUCTION

In size and appearance Reactors may often seem to be one of the least impressive items of equipment, but its demands and performance are usually the most important factors in the design of the whole plant.

When a new metallurgical process is being developed, at least some indication of the performance of the reactor is needed before any economic assessment of the project as a whole can be made.

As a general statement of the basic objectives in designing a reactor, we can say that the aim is to produce a ***specified product*** at a ***given rate*** from ***known reactnts.***
In proceeding further however a number of important decisions must be made and there may be scope for considerable ingenuity in order to achieve the best result.

Subsequently, the aim is to reach logical conclusions concerning the following
(a) The overall size of the reactor, its general configuration and the more important dimensions of any internal structures.
(b) The exact composition and physical condition of the products emerging from the reactor. The composition of the products must of course lie within any limits set in the original specification of the process.
(c) The temperatures prevailing within the reactor and any provision which must be made for heat transfer.
(d) The operating pressure within the reactor and any pressure drop associated with the flow of the reaction mixture.

Reactor design involves all the basic principles of chemical engineering with the addition of chemical kinetics. Mass transfer, heat transfer and fluid flow are all concerned and complications arise when, as **so** often is the case, interaction occurs between these transfer processes and the reaction itself. In designing a reactor it is essential to weigh up all the various factors involved and, by an exercise of judgement, to place them in their proper order of importance. Often the basic design of the reactor is determined by what is seen to be the most troublesome step. It may be the chemical kinetics; it may be mass transfer between phases; it may be heat transfer; or it may even be the need to ensure safe operation.

Byproducts and their Economic Importance

Before taking up the design of reactors in detail, let us first consider the very important question of whether any byproducts are formed in the reaction. Obviously, consumption of reactants to give unwanted, and perhaps unsaleable, byproducts is wasteful and will directly affect the operating costs of the process. Apart from this, however, the nature of any byproducts formed and their amounts must be known **so** that plant for separating and purifying the products from the reaction may be correctly designed. The appearance of unforeseen byproducts on start-up of a full-scale plant can be utterly disastrous. Economically, although the cost of the reactor may sometimes not appear to be great compared with that of the associated separation equipment such as distillation columns, etc., it is the composition of the mixture of products issuing from the reactor which determines the capital and operating costs of the separation processes.

Pyrometallurgy

Pyrometallurgy is a branch of extractive metallurgy. it consists of the thermal treatment of minerals and metallurgical ores and concentrates to bring about physical and chemical transformations in the materials to enable recovery of valuable metals. Pyrometallurgical treatment may produce products able to be sold such as pure metals, or intermediate compounds or alloy, suitable as feed for further processing. Examples of elements extracted by pyrometallurgical processes include the oxides of less reactive elements like iron, copper, zinc, chromium, tin and manganese.
Pyrometallurgical processes are generally grouped into one or more of the following categories.

- calcining
- roasting
- smelting
- refining

Most pyrometallurgical processes require energy input to sustain the temperature at which the process takes place. The energy is usually provided in the form of combustion or from electrical heat. When sufficient material is present in the feed to sustain the process temperature solely by exothermic reaction (i.e. without the addition of fuel or electrical heat), the process is said to be "autogenous". Processing of some sulfide ores exploit the exothermicity of their combustion

Calcining

Calcination is thermal decomposition of a material. Examples include decomposition of hydrates such as ferric hydroxide to ferric oxide and water vapor. The decomposition of calcium carbonate to calcium oxide and carbon dioxide as well as iron carbonate to iron oxide:

$$CaCO_3 \rightarrow CaO + CO_2$$

Calcination processes are carried out in a variety of furnaces, including shaft furnance, rotary kilns, and fluidized bed reactor.

Roasting

Roasting consists of thermal gas–solid reactions, which can include oxidation, reduction, chlorination, sulfation, and pyrohydrolysis.
The most common example of roasting is the oxidation of metal sulfide ores. The metal sulfide is heated in the presence of air to a temperature that allows the oxygen in the air to react with the sulfide to form sulfur dioxide gas and solid metal oxide. The solid product from roasting is often called "**calcine**". In oxidizing roasting, if the temperature and gas conditions are such that the sulfide feed is completely oxidized, the process is known as "**dead roasting**". Sometimes, as in the case of pre-treating reverberatory or electric smelting furnace feed, the roasting process is performed with less than the required amount of oxygen to fully oxidize the feed. In this case, the process is called "**partial roasting**" because the sulfur is only partially removed. Finally, if the temperature and gas conditions are controlled such that the sulfides in the feed

react to form metal sulfates instead of metal oxides, the process is known as "**sulfation roasting**". Sometimes, temperature and gas conditions can be maintained such that a mixed sulfide feed (for instance a feed containing both copper sulfide and iron sulfide) reacts such that one metal forms a sulfate and the other forms an oxide, the process is known as "**selective roasting**" or "**selective sulfation**".

Smelting

Smelting involves thermal reactions in which at least one product is a molten phase.
Metal oxides can then be smelted by heating with coke or chorcoal, a reducing agent that liberates the oxygen as carbon dioxide leaving a refined mineral. Concern about the production of carbon dioxide is only a recent worry, following the identification of the enhanced green house effect.
Carbonate ores are also smelted with charcoal, but sometimes need to be calcined first.
Other materials may need to be added as flux aiding the melting of the oxide ores and assisting in the formation of a slag, as the flux reacts with impurities, such as silicon compounds.
Smelting usually takes place at a temperature above the melting point of the metal, but processes vary considerably according to the ore involved and other matters.

Refining

Refining is the removal of impurities from materials by a thermal process. This covers a wide range of processes, involving different kinds of furnace or other plant.
The term "**refining**" can also refer to certain electrolytic processes. Accordingly, some kinds of pyrometallurgical refining are referred to as "**fire refining**".

Metallurgical reactors

CLASSIFICATION OF REACTORS AND CHOICE OF REACTOR TYPE

Homogeneous and Heterogeneous Reactors

Chemical reactors may be divided into two main categories, homogeneous and heterogeneous. In homogeneous reactors only one phase, usually a gas or a liquid, is present. If more than one reactant is involved, provision must of course be made for mixing them together to form a homogenous whole. Often, mixing the reactants is the way of starting **of** the reaction, although sometimes the reactants are mixed and then brought to the required temperature.
In heterogeneous reactors two, or possibly three, phases are present, common examples being gas-liquid, gas-solid, liquid-solid and liquid-liquid systems. In cases where one of the phases is a solid, it is quite often present as a catalyst; gas-solid catalytic reactors particularly form an important class of heterogeneous chemical reaction systems. It is worth noting that, in a heterogeneous reactor, the chemical reaction itself may be truly heterogeneous, but this is not necessarily **so.**
In a gas-solid catalytic reactor, the reaction takes place on the surface of the solid and is thus heterogeneous. However, bubbling a gas through a liquid may serve just to dissolve the gas in the liquid where it then reacts homogeneously; the reaction is thus homogeneous but the reactor is heterogeneous in that it is required **to** effect

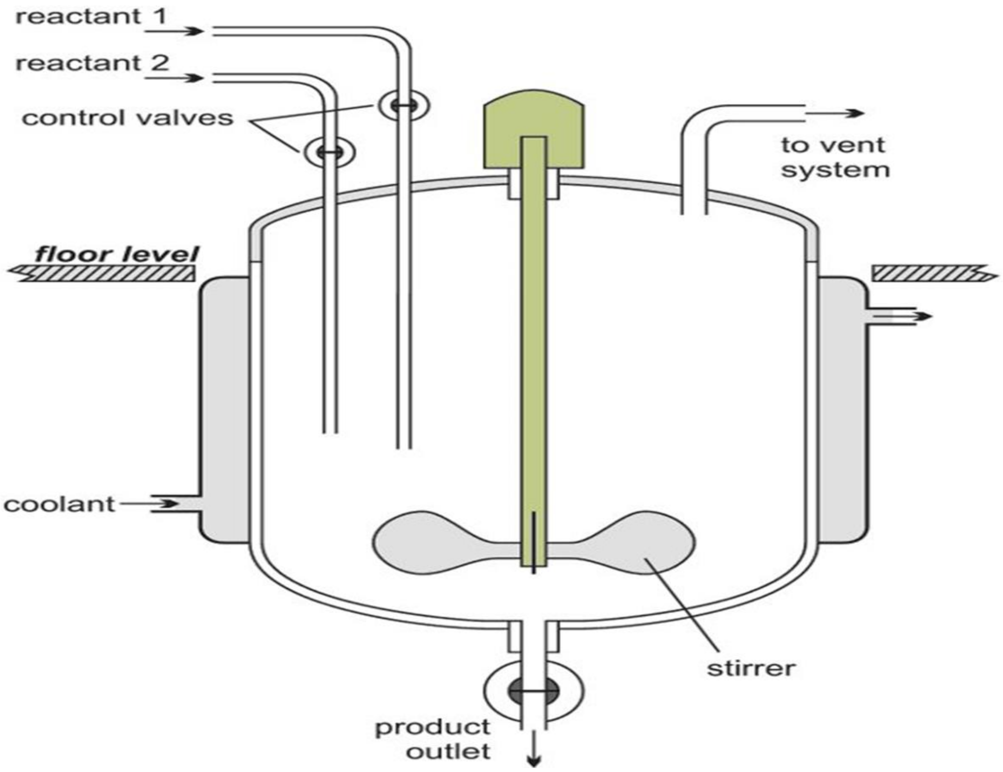
contact between two phases-gas and liquid. Generally, heterogeneous reactors exhibit a greater variety of configuration and contacting pattern than homogeneous reactors. Initially, therefore, we shall be concerned mainly with the simpler homogeneous reactors, although parts of the treatment that follows can be extended to heterogeneous reactors with little modification.

Batch Reactors and Continuous Reactors

Another kind of classification which cuts across the homogeneous-heterogeneous division is the mode of operation-batchwise or continuous. Batchwise operation, is familiar to anybody who has carried out small-scale preparative reactions in the laboratory.

BATCH REACTORS

A batch reactor is like a giant washing machine. There is a big vat where all of the reagents are put and a big agitator that keeps them stirring. A batch reactor is great if a company wants to make small amounts of specialty chemicals one "batch" at a time, but not if they want to make the same thing over and over. This is because the reactor must be emptied and cleaned after every batch is made. This takes a lot of time and money, and every batch can be just a little bit different due to small changes in reaction conditions, equipment aging, or because the operator drops a little bit of something foreign into the reactor.



Batch reactor

Benefits of batch reactors

Batch reactors are very versatile and are used for a variety for different unit operations (batch distillation, storage, crystallisation, liquid-liquid extraction etc.) in addition to chemical reactions. There is a large installed base of batch reactors within industry and their method of use is well established.

Batch reactors are excellent at handling difficult materials like slurries or products with a tendency to foul.

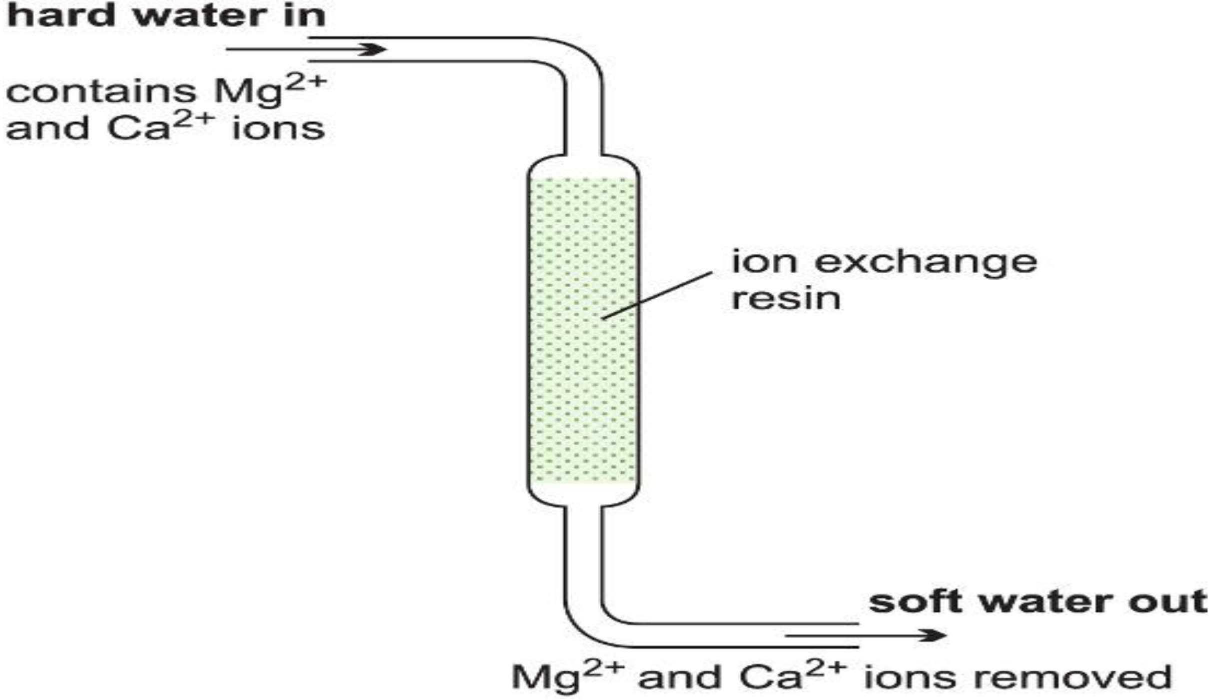
Batch reactors represent an effective and economic solution for many types of slow reactions.

CONTINUOUS REACTORS

In a continuous process, the reactor is basically a long tube. The raw materials go in one end, react on their way through the tube, not stopping along the way, and the finished product comes out the other end. A continuous process works well, because it can easily make large amounts of a product with little attention from a careless factory worker, and the product usually tends to be of similar quality throughout the process. The down side is, like in the initial production of Butyl rubber, if the tube gets clogged, the whole system has to be shut down for cleaning, which can cost a lot of time and money.

OR

Continuous reactors (alternatively referred to as flow reactors) carry material as a flowing stream. Reactants are continuously fed into the reactor and emerge as continuous stream of product. Continuous reactors are used for a wide variety of chemical and biological processes within the food, chemical and pharmaceutical industries. A survey of the continuous reactor market will throw up a daunting variety of shapes and types of machine. Beneath this variation however lies a relatively small number of key design features which determine the capabilities of the reactor. When classifying continuous reactors, it can be more helpful to look at these design features rather than the whole system.



Benefits of continuous reactors

The rate of many chemical reactions is dependent on reactant concentration. Continuous reactors are generally able to cope with much higher reactant concentrations due to their superior heat transfer capacities. Plug flow reactors have the additional advantage of greater separation between reactants and products giving a better concentration profile.

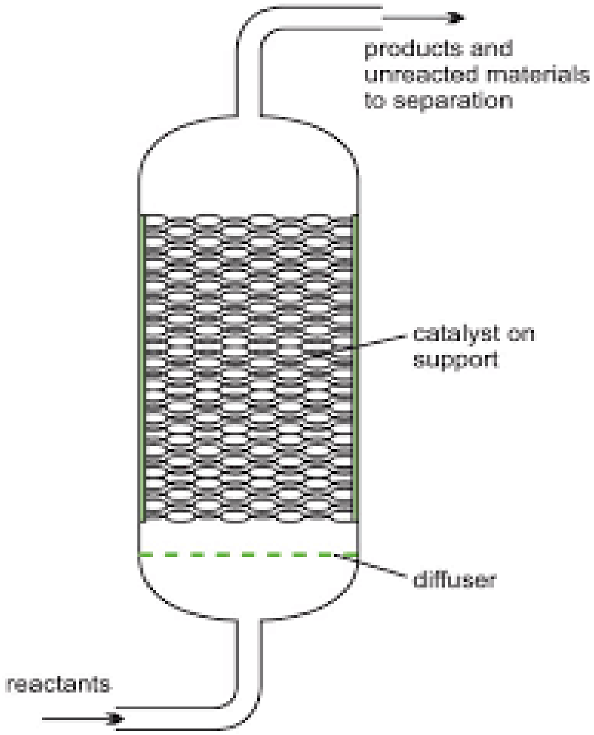
The small size of continuous reactors makes higher mixing rates possible.

The output from a continuous reactor can be altered by varying the run time. This increases operating flexibility for manufacturers.

Fixed bed reactors

A fixed bed reactor is a cylindrical tube filled with catalyst pellets with reactants flowing through the bed and being converted into products. The catalyst may have multiple configuration including: one large bed, several horizontal beds, several parallel packed tubes, multiple beds in their own shells. The various configurations may be adapted depending on the need to maintain temperature control within the system. Serial connection of two reactors with option to dose oxidant between the stages enable under optimal conditions to increase the product yield in oxidation catalysis. By dosing intermediates or products between the stages, valuable information could be found concerning the reaction pathways.

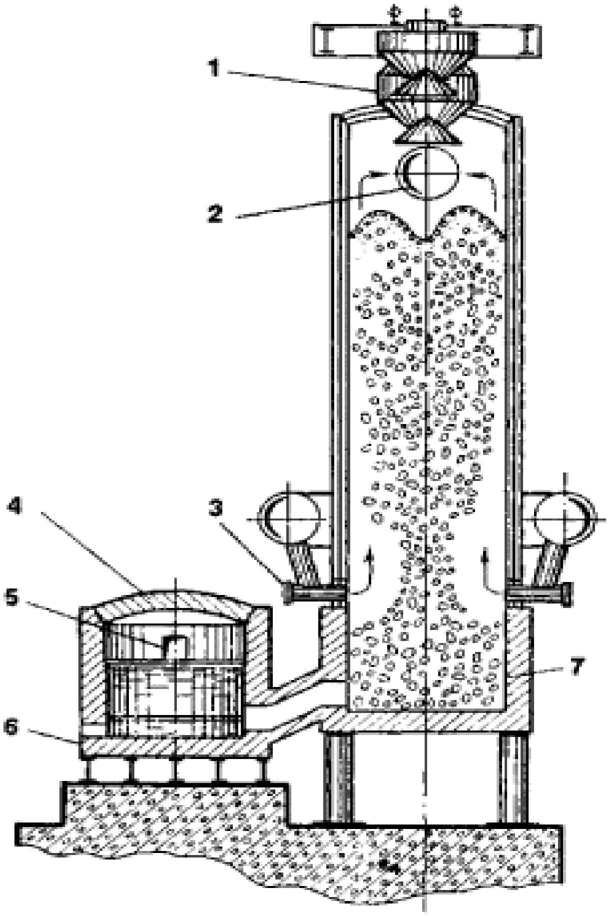
The catalyst pellets may be spherical, cylindrical, or randomly shaped pellets. They range from 0.25 cm to 1.0 cm in diameter. The flow of a fixed bed reactor is typically downward. Packed bed reactor.



Fixed bed reactors

furnace that has an upright working chamber of circular, elliptical, or rectangular cross section and is used to smelt or roast lumped materials. The heat required for the smelting or roasting process is produced by the combustion of a fuel either directly in the furnace or in an external firebox from which hot combustion products are supplied to the furnace.

Moderate velocities of the gaseous combustion products are characteristic of shaft furnaces. At such velocities, the bulk of the lumped materials is not entrained by the ascending gas stream and, in contrast to the case of a fluidized-bed furnace, maintains aerodynamic stability. The countercurrent motion of the charge (from the top to the bottom) and of the gases forced through the charge (from the bottom to the top) and the direct contact between the charge and the hot gases result in good heat exchange and the generation of low-temperature exhaust gases. Consequently, shaft furnaces are characterized by a high thermal efficiency and a relatively high output. Such furnaces are widely used to smelt iron ores, pig iron, and the raw materials employed in non-ferrous metallurgy, as well as to roast, for example, iron ore and limestone.



(1) charging device,

(2) gas outlet,

(3) tuyere,

(4) outside crucible,

(5) slag notch,

(6) matte hole,

(7) inside crucible

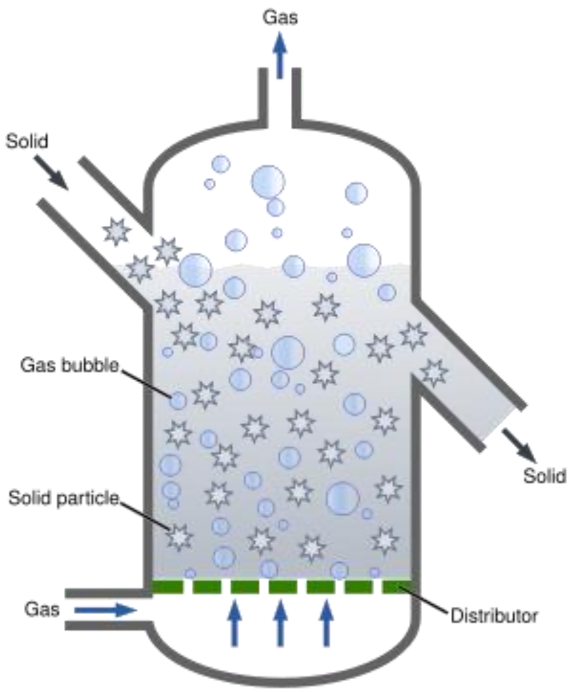
A shaft furnace

The shaft furnaces used in nonferrous metallurgy Figure are designed for continuous operation. They are low because of the need to carry out smelting without the reduction of substantial amounts of iron oxides and are narrow; the length of the furnaces is 8–15 m. The main components of such a furnace are as follows: a top, through which the charge is loaded and the gaseous combustion products are discharged; a shaft equipped with tuyeres, through which either a blast for fuel combustion or hot gases are supplied; and an inside crucible with a refractory lining, where the molten products collect. The smelts are tapped through an outside crucible or directly from the inside crucible to a forehearth for the stripping of the slags. The forehearth is often equipped for electric heating.

Formerly, shaft furnaces were constructed from metal jackets, through which water for cooling circulated. Later, evaporative cooling came to be used instead of water cooling. The shaft is constructed of thick-walled tubing welded into units. Shaft furnaces are usually not lined since iron slags in nonferrous metallurgy readily dissolve refractory materials.

Fluidized bed reactors

A fluidized bed reactor suspends small particles of catalyst by the upward motion of the fluid to be reacted. The fluid is typically a gas with a flow rate high enough to mix the particles without carrying them out of the reactor. The particles are much smaller than those for the above reactors. Typically on the scale of 10-300 microns. One key advantage of using a fluidized bed reactor is the ability to achieve a highly uniform temperature in the reactor.



Fluidized bed reactors

Rotatory Kilns

Rotary kilns have the capability to handle feed materials in a wide array of forms ranging from slurries (Wet Process) through to dry granular materials (Dry Process).

Rotary kiln is just another name for rotary kiln equipment. Rotary kiln equipment consists of: cylinder, belt, supporting wheel, blocking wheel, transmission device, sealing device, brick block ring, block ring, chain, metal heat exchange. Device, manhole door, fire hood and connection accessories.

Working principle of rotary kiln

(1) There are chemical and physical reactions inside the rotary kiln, and the calcination phase is divided into three phases, the preheating phase, the calcination phase, and the cooling phase. When the limestone is calcined, the heat between the material and the calcination zone is exchanged back and forth in the area of the rotary kiln, so that the moisture of the raw material is evaporated, and under the condition of uneven heating, the volume expands and the ultimate compressive strength decreases. When the internal temperature reached 700 degrees Celsius, it entered the calcination zone.

(2) The calcination zone is in the middle of the rotary kiln.

When the material enters the area, the fuel starts to burn under the condition of the blower's combustion. Can release a lot of heat, so the temperature in the kiln will rise slowly, when the temperature reaches a certain range. At this point, temperature control is required. For example, the decomposition rate of limestone and the gas generated in this case will be relatively large, which is conducive to the calcination of raw meal into clinker. The generated gas is discharged by the air flow, at this time the clinker begins to enter the cooling zone.

(3) The cooling zone is in the lower half of the kiln body of the rotary kiln equipment. At this time, the residual clinker will not be decomposed in this area. At this time, the material after being calcined can be cooled. The relative position of each area is also relatively stable. Can not be separated indiscriminately, it is necessary to operate according to changes in raw material and fuel conditions. The materials can be better utilized after cooling inside the kiln body.

Uses of rotatory kiln:

- In the building materials industry, in addition to calcining cement clinker, rotary kiln is also used for calcining clay, limestone, and slag drying; etc

- In the production of refractory materials, rotary kiln is used as the raw material to stabilize the size and increase the strength. , And then processed.
- In the chemical industry, rotary kiln is used to produce soda, calcined phosphate fertilizer, barium sulfide, etc. In the 1960s, a new process for producing phosphoric acid using a rotary kiln was invented
- In terms of environmental protection, developed countries in the world have used cement kilns to incinerate hazardous waste and garbage for more than 20 years. This not only reduces waste and harmless it, but also uses waste as fuel to save pulverized coal. Recycling of waste.

Reverberatory furnances:

A reverberatory furnace is a metallurgical or process furnace that isolates the material being processed from contact with the fuel, but not from contact with combustion gases. The term reverberation is used here in a generic sense of rebounding or reflecting, not in the acoustic sense of echoing.

Construction and working

Today, the reverberatory furnace mostly consists of rectangular steel box which is lined with castables processing non-wetting properties or refractory bricks. There is a vertically lifting door at one end and burners are placed usually on the other side of the furnace. Opposite to the burners there is a pouring spout and the exhaust gas duct. Roofs are also made of the same refractory brick which are durable and it further helps generate higher temperatures which leads to faster refining. However, as new technical innovations continue to be forged, they are changing and improving not only the basic construction materials but also the production capacity of this furnace.

As for the operation, in a reverberatory furnace, heat is generally passed over the hearth which consists the ore mixture. The main method of heat transfer is through the radiation from the refractory bricks present in the walls and the roof. Additional heating is supplied from the burner to the ore. The roof of the furnace is also slightly arched and remains slanted towards the bridge of flues that deflects the flame for reverberation. The mixture is heated constantly until it melts. Meanwhile, the molten impure metal is collected in the hearth which is thick and made of a strong material that can also resist any disintegration by the slag. The process is repeated in the furnace until the ore concentrate is tapped at regular intervals. The collected material is then sent to a converter for further refinement.

Electric furnaces

Electric furnace, heating chamber with electricity as the heat source for achieving very high temperatures to melt and alloy metals and refractories. The electricity has no electrochemical effect on the metal but simply heats it.

There are three tyoes of electric furnaces described below:

Type 1. Electric-Arc Furnace

It is most commonly used type of electric arc furnace, and is shown in Fig. 4.4. The heat is produced by an electric arc and is transferred by direct radiation or by reflected radiation off the internal lining of the furnace.

Electric-Arc Furnace

An electric arc is generated about midway between two graphite electrodes. One of which is stationary and another is movable to control the length of the arc and so as to heat produced. Electric-arc furnaces are generally used for melting ferrous metals like steels, gray cast iron etc., and to a lesser extents, some non-ferrous metals.

Type 2. Induction Furnace

Induction furnace consists of an electric-induction coil that is built into the walls of the furnace. An alternating current in the coil induces current in any metallic object that obstructs the electromagnetic flux. Induction furnaces use both high and low frequency current.

Electric Induction Furnace

They are successfully used in industry to induce alternating current in solid metal to melt it. Induction furnaces are used to melt ferrous and nonferrous alloys like steel, aluminum alloys etc. Fig. 4.5 shows a typical induction furnace.

Some advantages of these furnaces are:

(a) Uniformly distribution of temperatures within the molten metals.
(b) Possibility of controlling the furnace atmosphere.
(c) Provides better flexibility.

Type 3. Resistance Furnace

A typical resistance furnace is shown in Fig. 4.6. The solid metal is placed on each of the two inclined hearths and is subjected to heat radiation from the electric-resistance coils located above. When the metal melts, it flows down into a reservoir.

The molten metal can be lifted out through the spout (hole) by tilting the whole furnace. Resistance furnace is used mainly for melting aluminum and its alloys and for low melting temperature Resistance

Retention time in reactor:

Retention is defined as the time duration for which the material has stayed within the reactor.

It is necessary to know the retention time to calculate the degree of reaction along with kinetic data.It is easy to find out retention time in batch reactor, such as fixed-bed or as steel converter as all materials has stayed within the reactor for the same time but in continuous reactors like a shaft furnaces or fluidized-bed furnace, it becomes more difficult.

In perfect displacement or plug flow, the retention time is same for each piece of material and is given by (M/m) hour where

m =feeding rate

M =mass inside the reactor

The material along the walls will, due to friction, tend to descend more slowly than in the middle.

In continuous reactor as soon as the raw ore enters the reactors it is mixed completely with the bed content .At the same time the bed overflows continoulsy, and the composition of the overflow is the same as that of the bed.Calculation of actual retention time for each ore particle in continuous reactor relative to the mean retention time.

We assume that at a given time $t=0$ a small quantity n_0 ,of trace ore is introduced and we will follow this material for calculation of retention time after a, certain time t, the quantity remaining in the reactor is n and its concentration is n/M . The rate at which it overflows is $-\frac{dn}{dt}=(\frac{n}{M})m$, where m , the total rate of overflow, is expressed in term of and equal to the feeding rate. If the expression is integrated we get

$$-\int\frac{dn}{n}=\frac{m}{M}\int dt=\frac{1}{t_m}\int dt$$

Inserting the limits $n=n_0$ at $t=0$, and $n=n$ at $t=t$ we get

$$\frac{n}{n_0}=e^{-\frac{t}{t_m}}=e^{-\theta}=r$$

In this expression r gives the fraction of the original material which remain in the reactor at the time t and thus has a retention time equal to or larger than t, and $\frac{t}{t_m}$ is the relative retention time, which will be denoted θ.

Granulated materials

A granular material is a conglomeration of discrete solid, macroscopic particles characterized by a loss of energy whenever the particles interact. The constituents that compose granular material are large enough such that they are not subject to thermal motion fluctuations

Corresponding to the fluid- and solid-like modes, they show different flow regimes: quasi-static regime, rapid flow regime, and a transitional regime that lies in between. These features give rise to another state of matter that is poorly understood. The development of a general theory to describe the packing (statics) and flow (dynamics) of granular materials has been a problem challenging the scientific community for years.

Heat transfer in reactor

Heat transfer is a result of the 2nd law of thermodynamics which states that heat will flow from high to low temperature until equal temperatures are obtained.

The rate of heat transfer is determined partly by the temperature difference between the source and sink.

The main heat transfer mechanisms are

1.Conduction

2.Convection

3.Radiation

In metallurgical reactors heat transfer is of importance in the calculation of the heat losses through the reactors wall to the surrounding atmosphere from gases to reaction mixture.One or more than one heat transfer mechanisms can be possibly acting on a reactor.

Heat exchanger recator

Heat exchanger reactors remain an active research area with much development

required before they are fully implemented outside a number of existing niche areas.

Many, if not most, of process reactions for high added-value products are conducted in stirred tank reactors, consisting of a large tank with rotating paddle. The mixing process has a high energy demand and yet, because of its highly nonuniform nature, is not efficient. When reactions with a high intrinsic speed are undertaken in such reactors, the rate of mixing is insufficient to match the reaction rate. Hence, the reaction is slowed down and by-product formation is increased

Chemical reactions in flow system:

In flow chemistry, a chemical reaction is run in a continuously flowing stream rather than in batch production. In other words, pumps move fluid into a tube, and where tubes join one another, the fluids contact one another. If these fluids are reactive, a reaction takes place. Flow chemistry is a well-established technique for use at a large scale when manufacturing large quantities of a given material.

Choosing to run a chemical reaction using flow chemistry, either in a microreactor or other mixing device offers a variety of pros and cons.

Advantages

- Reaction temperature can be raised above the solvent’s boiling point as the volume of the laboratory devices is typically small
- Safety is increased
- Flow reactions can be automated with far less effort than batch reactions. This allows for unattended operation and experimental planning. By coupling the output of the reactor to a detector system, it is possible to go further and create an automated system which can sequentially investigate a range of possible reaction parameters (varying stoichiometry, residence time and temperature) and therefore explore reaction parameters with little or no intervention.

Continuous flow reactors:

Continuous reactors are typically tube like and manufactured from non-reactive materials such as stainless steel, glass and polymers. Mixing methods include diffusion alone (if the diameter of the reactor is small e.g. <1 mm, such as in microreactors) and static mixers. Continuous flow reactors allow good control over reaction conditions including heat transfer, time and mixing.

The residence time of the reagents in the reactor (i.e. the amount of time that the reaction is heated or cooled) is calculated from the volume of the reactor and the flow rate through it:

$$Residence\ time = \frac{Reactor\ \ Volume}{Flow\ Rate}$$

Therefore, to achieve a longer residence time, reagents can be pumped more slowly and/or a larger volume reactor used. Production rates can vary from nano liters to liters per minute.