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Kolmetz Handbook of Process Equipment Design

REACTOR SYSTEMS SELECTION, SIZING AND TROUBLESHOOTING

(ENGINEERING DESIGN GUIDELINES)

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TABLE OF CONTENTS

INTRODUCTION

Scope 5

General Design Consideration 6

I. Catalyst and Catalytic Reaction 6

A. Homogeneous catalysis 6

B. Heterogeneous catalysis 6

II. Reactor types 7

A. Ideal reactors 7

i. Batch Reactor 7

ii. Continuous Stirred-Tank Reactor (CSTR) 9

iii. Plug Flow Reactor (PFR) 9

B. Catalytic Reactors 10

i. Fixed-bed reactors 10

ii. Fluidized bed reactor 14

III. Advantages and Disadvantages of Reactor Types 16

IV. Mode Operation 18

A. Isothermal Operation 18

B. Adiabatic Operation 18

DEFINITIONS 19

NOMENCLATURE 21

Greek letters 23

THEORY 24

I. Reaction Rate 24

II. Reactor Sizing and Design 27

A. Design Equations For A Batch Reactor 27

B. Design Equations For A Continuous Stirrer-Tank Reactor 30

C. Design Equations For A Plug Flow Reactor 36

D. Design of Catalytic Reactors 38

i. Catalyst and Bed Characteristics 38

ii. Design Equations For A Fixed-Bed Reactor 46

iii. Design Equations For A Fluidized Bed Reactor 48

III. Reactor Performance Measures 54

APPLICATION

Example Case 1: Batch reactor sizing 56

Example Case 2: Continuous Stirred-Tank Reactor series sizing 61

Example Case 3: Fixed-bed sizing 68

Example Case 4: Fluidized bed sizing 77

REFERENCES 85

LIST OF TABLE

Table 1: Main fixed-tube reactor processes 11

Table 2: Advantages and disadvantages of reactor types 16

Table 3: Standard Stirred Tank Reactors 35

Table 4: Several catalysts in industrial processes 44

LIST OF FIGURE

Figure 1: Operation of batch reactor 8

Figure 2: Continuous Stirred Tank Reactor 9

Figure 3 : Plug flow reactor 10

Figure 4: Fixed bed reactor types 12

Figure 5 : Trickle-bed reactor 13

Figure 6 : Fluidized bed reactor 14

Figure 7 : Bubble column reactor 15

Figure 8 : Catalyst shapes 38

Figure 9 : Model used to describe the K-L bubbling gas fluidized bed 50

INTRODUCTION

Scope

Chemical kinetics and reactor design are very important to all industrial chemicals. Chemical kinetics is the study of chemical reaction rates and reaction mechanisms. The chemical reactor may be regarded as the very heart of a chemical process. It is the piece of equipment in which conversion of feedstock to desired products takes place and is thus the single irreplaceable component of the process. To find what a reactor is able to do, one needs to know the kinetics, the contacting pattern and the performance equations.

Generally, reactors are chosen that will meet the requirements imposed by the reaction mechanisms, rate expressions, and the required production capacity. An important factor in reactor operation is the outlet degree of conversion. Operating conditions such as temperature, pressure, and degree of agitation, are related for the most economic operation. The optimum reactor that will best meet the process requirements requires a review of whether the physical configuration is continuous, batch, tubular or catalytic reactors such as the fixed and fluidized beds.

This design guideline covers the basic elements in the field of reaction to allow the design of a reactor with the suitable process parameters; volume of reactor, conversion, time reaction and pressure drop. This design guideline includes; catalyst types, reactor types and calculation of reactor desing and sizing.

The design of reactor may be influenced by factors, including process requirements, advantages and disadvantages. All the important parameters use in the guideline are explained in the definition section which help the reader more understand the meaning of the parameters or the terms utilized.

In the application section of this guideline, four case studies are shown and discussed in detail, highlighting the way to apply the theory for the calculation. Example Calculation Spreadsheets are part of this guideline. This Example Calculation Spreadsheets are based on case studies in the application section to make them easier to understand.

INTRODUCTION

General Design Consideration

I. Catalyst and Catalytic Reaction

Catalyst is a substance that affects the rate or the direction of a chemical reaction, but is not appreciably consumed in the process and cannot change the position of the thermodynamic equilibrium. There are many ways of chemical reactions type. In chemical reaction engineering probably the most useful scheme is the breakdown according to the number and types of phases involved, the big division being between the homogeneous and heterogeneous systems.

A. Homogeneous catalysis

Homogeneous catalysis is happened when the reactants and the catalyst are in the same phase. This catalysis is happened by movement of substance becomes complex substance and movement of molecular arrangement and catalyst ligan. Examples of this catalysis include the gas-phase decomposition of many substances, including diethyl ether and acetaldehyde, catalyzed by iodine, and liquid-phase esterification reactions, catalyzed by mineral acids[6].

B. Heterogeneous catalysis

When the catalyst and the reactants in different phases, then reaction is called heterogeneous catalysis. Because in this systems more than one phase is involved, the problems becomes more complex. Typical heterogeneous catalysts are inorganic solids such as metals, oxides, sulfides, and metal salts, but may also be organic materials such as organic hydroperoxides, ion exchangers, and enzymes. This catalysis system is easily applicated in industries, because pellet catalyst is easy to produce and simple to put it in reactor tube where reactant flows.

II. Reactor types

The different phases is a special concern for reactor designing. Basically configurations of reactor are described below. In terms of the physical configurations encountered, there are basically only two types of reactors: the tank and the tube. Both types can be used as continuous reactors or batch reactors. Most commonly, reactors are run at steady-state, but can also be operated in a transient state.

A. Ideal reactors

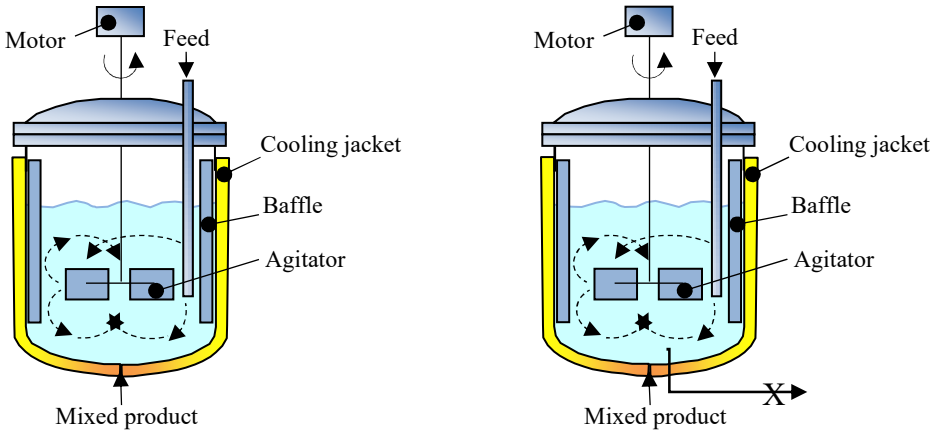
Ideal reactors have three ideal flow or contacting patterns. There are the main basic models used to estimate the most important process variables of different chemical reactors:

i. Batch Reactor

Batch reactor is one in which stirring is so efficient that the fluid elements will all have the same composition, but the composition will be time dependent. Nothing else is put in or taken out tank reactor until the reaction is completed. The tank is easily heated or cooled by an external jacket. Discontinuous step or pulse operation necessarily results in transient conditions. Batch reactors particularly are used in the manufacture of pharmaceuticals and fermentations.

Another operation mode that operate much like batch reactors in that reactors take place in a single stirred tank with similar equipment, is called semibatch. In this mode the tank is partially filled with reactants, and additional reactants are added progressively until the desired end composition is achieved. Alternatively, one may charge the reactants all at once and continuously remove products as products are formed.

These reactors can be illustrated in figure 1.



a. Batch reactor b. Semibatch reactor

Figure 1: Operation of batch reactor

ii. Continuous Stirred-Tank Reactor (CSTR)

A continuous stirred tank reactor (CSTR) differs from the batch reactor in that the feed mixture continuously enters and the outlet mixture is continuously withdrawn; at the same time an equal volume of reactor contents is discharged in order to maintain a constant level in the tank. Thus, the reaction rate at any point will be approximately the same. Also, the outlet concentration will be identical to the internal composition. The operation of this mode is normally one of steady-state.

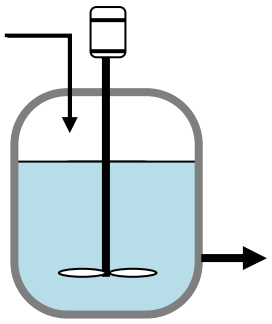


Figure 2 : Continuous Stirred Tank Reactor

iii. Plug Flow Reactor (PFR)

In a plug-flow reactor (PFR), the feed enters one end of a cylindrical tube and the product stream leaves at the other end or passes many short reactors in a tube bank. A PFR is usually operated continuously at steady-state, apart from startup and shutdown periods.

Characteristics of the PFR are when the inlet flow is fully turbulent and the entrance region (where the velocity profile is developing) is a small fraction of the total length; no radial variation in reaction rate (concentration), concentration changes with length down

the reactor; and a PFR typically has a higher efficiency than a CSTR of the same volume.

A Plug flow reactor can be seen in figure 3.

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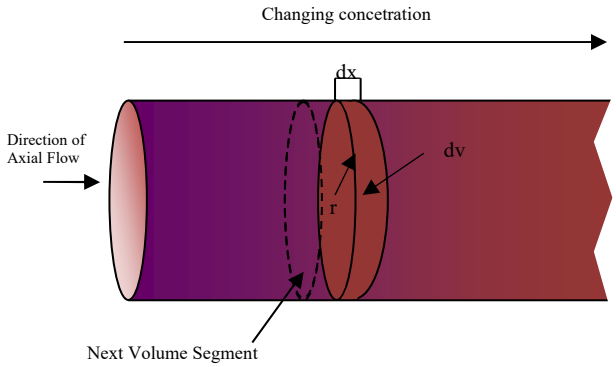


Figure 3: Plug flow reactor

B. Catalytic Reactors

Heterogeneous catalytic reactors are the most important single class of reactors utilized by the chemical industry. These may be divided into two broad types, the fixed bed reactors and the fluidized-bed reactors.

i. Fixed-bed reactors

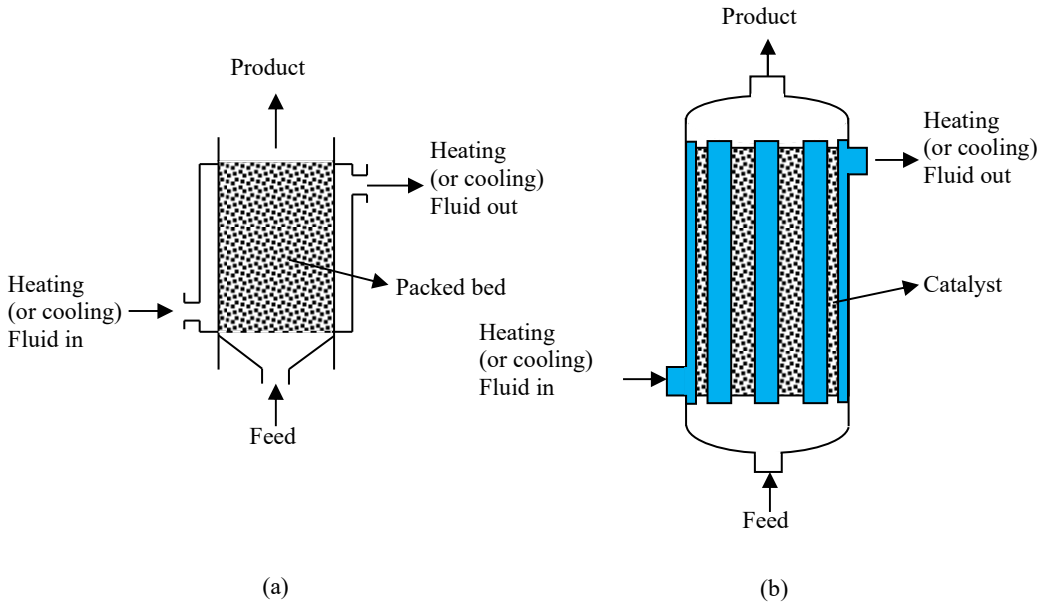
In the chemical industry fixed-bed reactors are the standard type of reactors for heterogeneously catalyzed gas phase reactions (two phase reactors). Multiple layers of these screens constitute the catalyst bed that are used in commercial processes for the oxidation or synthesis. Applications of fixed bed reactor can be described in table 1.

Table 1 : main fixed-tube reactor processes

Basic Chemical Industry	Petrochemical Industry	Petroleum Refining
Steam reforming : primary secondary Water-gas-shift CO-methanation Ammonia synthesis Sulfuric synthesis Acid synthesis Methanol synthesis Oxo synthesis	Ethylene oxide Ethylene dichloride Vinylacetate Butadiene Maleic anhydride Phthalic anhydride Cyclohexane Styrene Hydrodealkylation	Catalytic reforming Isomerization Polymerization (Hydro)desulfurization Hydrocracking

Fixed-bed reactors can be operated under adiabatic or nonadiabatic conditions that depend of temperature change. Because of the necessity of removing or adding heat, it may not be possible to use a single large-diameter tube packed with catalyst. In this event the reactor may be built up of a number of tubes encased in a single body to prevent excessive temperatures.

There are types of fixed-bed reactors as shown in figure 4.



Packed bed Multitube

Figure 4 : Fixed bed reactor types

a. Trickle-Bed Reactors

A trickle-bed reactor is a three-phase (gas-liquid-solid) reactor in which the solid (catalyst) is a fixed bed of particles catalyzing a gas-liquid reaction. Liquid reactants or reactants dissolved in a solvent are flowing downward through the catalyst bed and the gaseous reactants are conducted in the cocurrent direction.

Trickle-bed reactors are widely used for hydrogenations in the petroleum industry, including hydrodesulfurization (HDS) of heavy oils and gasoline, hydrodenitrogenation (HDN), hydrocracking, and hydrofinishing of lubricating oil[3].

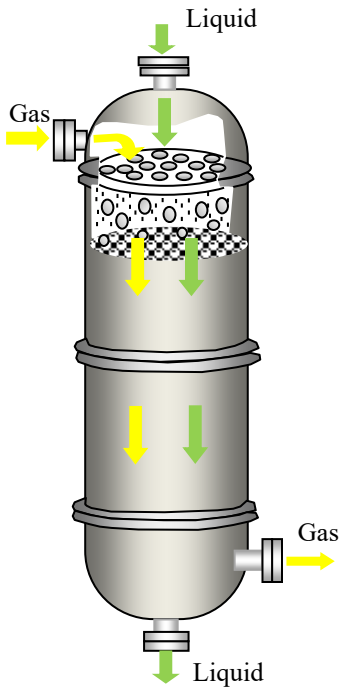


Figure 5: Trickle-bed reactor

ii. Fluidized bed reactor

A fluidized bed is a bed of solid particles that are supported by the drag of upward flowing gas or liquid when the volume flow rate of the fluid exceeds a certain limiting value, the minimum fluidization volume flow rate. The catalyst particles are held suspended in the fluid stream at this or higher flow rates. Depending on the volume flow rate of the fluid different types of fluidized beds form as shown in figure 6.

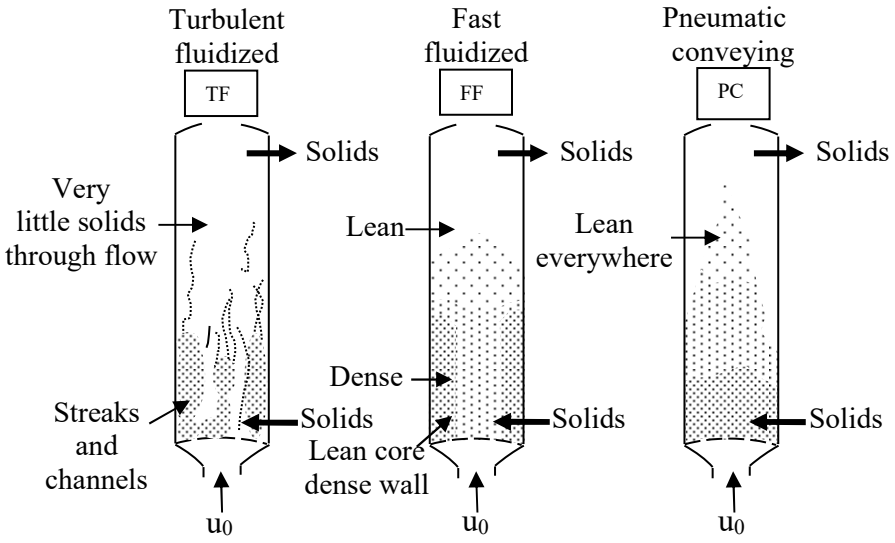


Figure 6: Fluidized bed reactor

Another common fluidized bed reactor type is the fluid catalytic cracking (FCC) that typically used in the refinery industries. FCC converts straight-run atmospheric gas oil, vacuum gas oils, and heavy stocks recovered from other operations into high-octane gasoline, light fuel oils, slurry oil, and olefin-rich light gases.

The invention of the fluidized bed with its suspended and rapidly mixing solids completely overcame dangerously rapid catalyst deactivation occurs or operation in the explosive regime is required that may be happened in fixed-bed reactor.

a. Bubble Column Reactor

Bubble columns are mainly continuously operating three-phase reactors. The reactant liquid contains suspension catalyst particles in a bubble column reactor is stirred by the reactant gas introduced continuously through a gas distributor installed at the bottom of the reactor such nozzles, perforated plates (sparger) or tubes. The reactant gas is bubbled through the liquid, dissolves, and then diffuses to the catalyst surface. This reactor is typically used for coal liquefaction, oxo processes and oil fats hydrogenation.

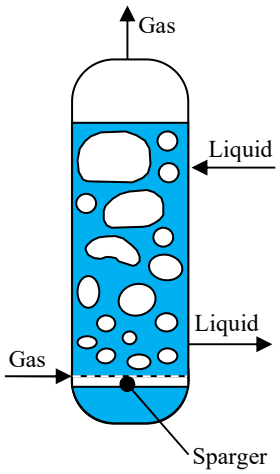


Figure 7: Bubble column reactor

III. Advantages and Disadvantages of Reactor Types

The following table is advantantages and disadvantages of reactor types as shown in Table 2.

Table 2: advantages and disadvantages of reactor types

Reactor Types	Advantages	Disadvantages
Batch	High conversion per unit volume for one pass	Operating cost may be relatively high
	More flexible for multiproduct (multiprocess) operation	Product quality more variable
	Easy to shut down and clean for fouling service	Difficulty of large scale production
Continuous Stirrer-Tank	Better for indefinitely long production runs of one product or set of products	Lowest conversion per unit volume
	Good process control and obtaining uniformity of product less difficult	Loss of production in lengthy stoppages can be costly
	Low operating (labor) cost	The rate of heat transfer per unit volume of reaction mixture is generally lower than in tubular reactors
Plug Flow Reactor	Large scale production	Shutdown and cleaning may be expensive
	Good heat transfer	Difficult temperature control
	Low operating (labor) cost	Undesired thermal gradients may exist

Continue Table 2

Reactor Types	Advantages	Disadvantages
Fixed-Bed Reactor	The highest conversion per weight of catalyst of any catalytic reactor	The catalysts often require regeneration after a relatively short period of operation
	do not need to be separated from the liquid by filtration	It is difficult to control the heat-transfer in the catalyst bed
Fluidized Bed Reactor	Uniform temperature distribution (due to intensive solid mixing)	Expensive catalyst separation and purification of reaction products
	Catalyst can be continuously regenerated with the use of an auxiliary loop	Erosion of internals resulting from high solids velocities
	High heat-transfer coefficient between bed and immersed heating or cooling surfaces	catalyst regeneration or replacement is relatively difficult to accomplish
Trickle-Bed Reactor	Fast diffusion of gases through the liquid film to the catalyst surface	Poor heat transfer
	Lower back-mixing	Partial utilization of the catalyst in case of the incomplete wetting
	No problems with catalyst separation	Possibility of “brooks” formation
Bubble Column Reactor	Good heat transfer, temperature control, catalyst utilization, and simple design	The difficult catalyst separation

The real reactors from these ideals often have deviations consider such as recycle reactors, staged reactors, and other flow pattern combinations. All deviations from ideal performance fall into two classifications. The first is a flow arrangement in which elements of fluid do not mix, but follow separate paths through the reactor (segregated flow). The second is a flow arrangement whereby adjacent elements of fluid partially mix (micromixing). The effects of these deviations on the conversion can be evaluated, provided know the distribution of residence times in the fluid leaving the reactor and the extent of micromixing [1].

IV. Mode Operation

It is also important to determine whether the mode of operation involves either an isothermal or an adiabatic in design consideration of reactor.

A. Isothermal Operation

For a liquid-phase reaction, or gas-phase reaction at constant temperature and pressure with no change in the total number of moles, the density of the system may be considered to remain constant, is called isothermal operation. Isothermal operation is attained due to this well mixed condition to achieve uniform condition. Uniform isothermal temperatures is main problem the fixed bed design therefore, it is included in adiabatic operation.

B. Adiabatic Operation

Adiabatic operation happened when no heat is added or removed from the reactor (i.e., Q = 0), and the heat given up by the reaction is entirely used within the system to change its enthalpy. As result, the temperature increases for an exothermic reaction and decreases for an endothermic reaction.

DEFINITION

Adiabatic operation - Operation happened when no heat is added or removed from the reactor (i.e., Q = 0), and the heat given up by the reaction is entirely used within the system to change its enthalpy.

Batch reactor - one in which stirring is so efficient that the fluid elements will all have the same composition, but the composition will be time dependent.

Catalyst - a substance that affects the rate or the direction of a chemical reaction, but is not appreciably consumed in the process and cannot change the position of the thermodynamic equilibrium.

Continuous stirred tank reactor - happened when the feed mixture continuously enters and the outlet mixture is continuously withdrawn; at the same time an equal volume of reactor contents is discharged in order to maintain a constant level in the tank.

Conversion - the ratio of the amount of A reacted at some point (time or position) to the amount introduced into the system, and is a measure of consumption of the reactant.

Deactivation - decrease the activity of a catalyst as a function of time.

Fluidized bed - a bed of solid particles that are supported by the drag of upward-flowing gas or liquid.

Heat of reaction - the energy absorbed by the system when the products after reaction are restored to the same temperature as the reactants.

Heterogeneous catalysis – happened when the catalyst and the reactants in different phases

Homogeneous catalysis - happened when the reactants and the catalyst are in the same phase.

Isothermal operation – Operation reaction at constant temperature and pressure with no change in the total number of moles, the density of the system may be considered to remain constant.

Liquid slugging - a condition which occurs when liquid is allowed to enter one or more cylinders. Where extreme cases of flooded start or liquid flood back occur.

Minimum fluidization velocity - velocity at which pressure drop becomes constant and bed height starts to increase.

Order – Concentration power number in reaction rate

Plug flow reactor – happened when the conditions at any point in the reactor are independent of time, and the linear velocity of the reacting mixture is the same at every point in a cross-section perpendicular to the flow direction.

Pressure drop - decrease in pressure from one point in a pipe or tube to another point downstream. Pressure drop occurs with frictional forces on a fluid as it flows through the tube.

Reaction rate - the amount of product formed or the amount of reactant consumed per unit volume of the gas or liquid phase per unit time.

Residence time - the time it takes a molecule 'to pass through a reactor

Selectivity (S) - the ratio of the desired product to the amount of limiting reactant that has undergone chemical change

Space time - time required to process one reactor volume of feed measured at specified conditions

Yield - the amount of the desired product formed divided by the amount of the reactant feed

NOMENCLATURE

A	Deactivation rate, ◦F/bpp
A_c	Area per unit volume of individual particle, in^2 (mm^2)
A_J	Cross-sectional area of jacket, ft^2 (m^2)
c	Product stoichiometric coefficient, dimensionless
C_A	Final reactant consentration, mol/liter (mol/m^3)
C_{An}	*n*th reactant consentration, mol/liter (mol/m^3)
C_{A0}	Initial reactant consentration, mol/liter (mol/m^3)
c_P	Specific heat capacity of the system, Btu/lb.°F (J/g.°C)
C_p	Molar heat capacity of the system, Btu/lbmol°F (J/mol.°C)
D	Diameter of tube, ft (m)
d_b	Diameter of bubble, ft (m)
D_{bed}	Diameter of bed, ft (m)
D_m	Transport diffusivity across the bubble cloud, ft^2/s (m^2/s)
D_p	Effective particle diameter, ft (m)
d_p	Catalyst particle diameter, in (mm)
D_s	Desulfurization activity, dimensionless
D^0_S	Initial desulfurization activity
F_{A0}	Molar flow rate of species A, mol/h
F_t	Total molar flow rate, mol/h
G	Gravitational constant, (32.2 ft/sec^2 or 9.82 m/s^2)
G	Mass velocity, $lb/s.ft^2$ ($kg/s.m^2$)
K	Reaction rate constant, depends order
K”’	Effective rate constant for the fluidized bed, depends order
K_{bc}	Exchange coefficient between bubble-cloud, s^{-1}
K_{ce}	Exchange coefficient between cloud-emulsion, s^{-1}
L	Depth of the packed bed, ft (m)
L_f	Height of bed at bubbling fluidized conditions, ft (m)
L_{mf}	Height of bed at minimum fluidization conditions, ft (m)
n_{A0}	Initial number of moles of A, mol
n_t	Total mol in system, mol
Pr(C)	Rate of production, mol C/h
q_0	Initial volumetric flow rate, ft^3/hr (m^3/hr)

q	Final volumetric flow rate, ft^3/hr (m^3/hr)
r_A	Reaction rate of A, depends order
$(-r_A)_n$	Reaction rate in *n*th reactor, depends order
Re*	Modified reynold number, dimensionless
t	Reaction time, h
T	Temperature of operation, °F (°C or K)
T_c	Catalyst life, bpp
td	Down-time, h
T_J	Jacket temperature, °F (°C or K)
T_o	Inlet temperature, °F (°C or K)
T_s	Temperature of the surroundings outside the tube, °F (°C)
U	Overall heat transfer coefficient, Btu/h.ft².°F(W/m².°C)
u_b	Velocity of bubbles, ft/s (m/s)
u_{br}	Velocity of a single bubble, ft/s (m/s)
u_{mf}	Superficial gas velocity at minimum fluidization, ft/s (m/s)
u_0	Superficial gas velocity in the bed, ft/s (m/s)
v	Superficial linear velocity, ft/s (m/s)
V	Volume of Reactor, L or gal (m^3)
V_{bed}	Volume of bed, ft^3 (m^3)
V_n	*n*th reactor volume, gal (m^3)
W_c	Mass of catalyst, lb (kg)
x_{An}	Fractional conversion of A in *n*th reactor, dimensionless
x_{An-1}	Fractional conversion of A in *n-1*th reactor, dimensionless
X_{A1}	Initial fractional conversion of A, dimensionless
X_{A2}	Final fractional conversion of A, dimensionless
$(-\Delta H_{RA})$	Reaction enthalpy, Btu/mol (J/mol)
ΔP	Pressure drop, psi (kPa)

Greek Letters

α	Ratio of wake volume to bubble volume, dimensionless
$\bar{C}_A$	Concentration of A seen by the solids, mol/L (mol/m^3)
$\dot{Q}$	Rate of heat transfer, J/s (W)
$\dot{m}$	Mass flow rate, lb (kg)
$\bar{t}$	Residence time, h
τ	Space time, h
ε_B	Void fraction of bed, dimensionless
ε_f	Void fraction of bed in bubbling fluidized condition, dimensionless
ε_{mf}	Void fraction of bed in minimum fluidization condition, dimensionless
δ	Bed fraction in bubbles, m^3 bubbles/m^3 bed
ρ	Fluid density, lb/ft^3 (kg/m^3)
ρ_B	Bed density, lb/ft^3 (kg/m^3)
ρ_p	Particle density, lb/ft^3 (kg/m^3)
μ	Fluid viscosity, cP (Pa.s)
ϕ_s	Irregular shape particles factor, dimensionless
π	pi (3.142)