Public Lecture Series

REACTOR DESIGN: THE DEVELOPMENT OF A SIMPLIFIED NOVEL OPTIMIZATION TECHNIQUE

J. A. OMOLEYE
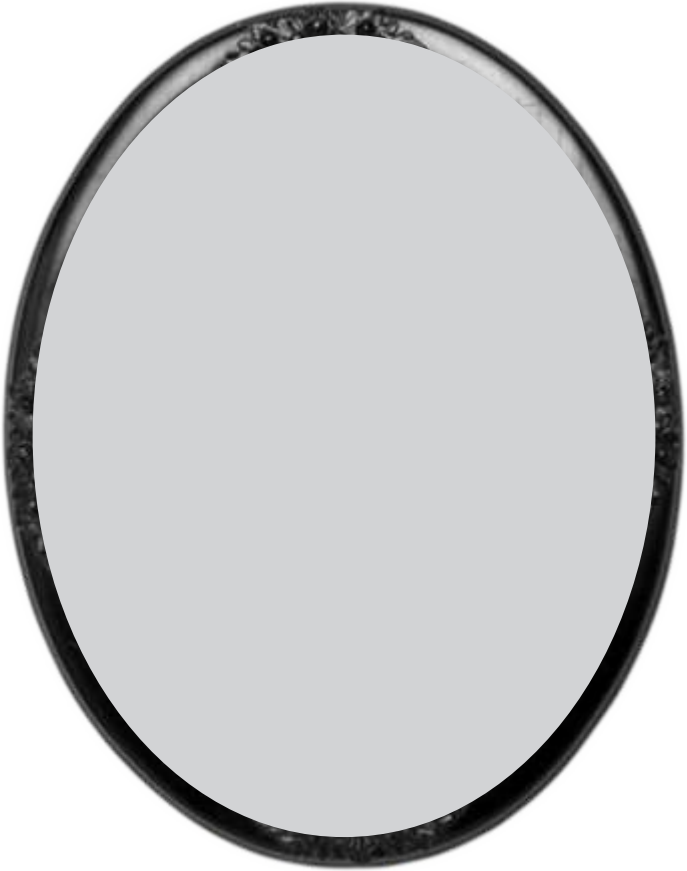
Professor J. A. Omoleye
Professor of Chemical Engineering,
Covenant University,
Canaanland, Ota.

Introduction

INTRODUCTION

REACTORS AND REACTIONS

Reactor as the name indicates has to do with Reaction - it is a vessel in which a reaction occurs. Reaction itself in Chemistry has to do with a chemical transformation taking place with atoms or molecules (compounds) or their combinations. Since there is usually a change in energy level , reaction is usually accompanied by heat absorption (Endothermic reactions) or heat evolution (Exothermic reactions) On a daily basis , apart from reactions initiated by man, there scores of natural reactions taking place on routine basis. The existence of man and other living things are dependent on some of these naturally occurring reactions. Failure of such reactions means termination life on earth. Some of these natural reactions include: isothermal enzymatic reaction in the intestine leading to food digestion and cell growth; Photosynthesis: a form of photochemical reaction upon which plants life depend; the absorption of the ultraviolet rays ozone in the stratosphere in its chemical decomposition to oxygen thus ensuring the continuous supply of oxygen on earth: the formation of petroleum oil from the transformation of cellulosic materials under high temperature and pressure underneath the earth over thousands of years.

Apart from the above natural reactions, there are other hundreds of industrial reactions today for the manufacture of one product or

another useful to man.

There are very few household and office equipments today that are not components of an industrial chemical reaction. All of these reactions take place in what we call Reactors. Rectors are in different sizes ranging from the tiny intestines of baby rat to those as large as the standard size of a room. In complexity, some are as simple as an open kettle with a stirrer and heater like soap making vessel while some are complex structures with inter-cooling and inter-heating coils. For some, energy supply is from electrical source, while some are from combustible fuel and for some others energy supply is from ultraviolet radiation from the sun. While some are designed for total mixing (Continuous Stirred Tank Reactor and Batch Reactor), others are designed in tube like manner for plug flow processes (Plug flow Reactors).there are both low and high pressure reactors depending on the kinetics of their reactions. Most industrial reactors are provided with Temperature and Pressure monitoring instruments. While some are operated batch-wise others are operated continuously from few minutes to as long as months with the feed coming in through the inlet pipe and the products going out through the exit pipe continuously. The materials of construction of a reactor must be resistant to the reactants, products and even by-products and also withstand the stress build-up from the pressure within.

What is Optimum Reactor Design?

From the above description of a reactor, it is obvious that some can be simple in design while some others can be complex in design. This depends on the type of reaction going on inside the reactor. Reactors design generally has to do with the process of estimating the size (reactor volume,V or weight, W of catalyst) of reactor required for a given reaction, conversion level x, rate of production F, and the rate of reaction r. a simple reactor equation relating the above variables are.

Equation (1) above is mostly useful for the estimation of the size of a single reactor needed for a given reaction.

There are however, a number of useful industrial products today described by some exothermic reversible reactions. The rate of such reactions is highly influenced by the temperature of reaction in a peculiar way that a single reactor operating at a constant temperature might not be efficient for any meaningful production rate. For such reaction, multiple reactors each operating at different unique temperature is required for any reasonable production level.

The design of efficient and economic reactors for irreversible and endothermic reactions is a lot simpler than the design of reactor for exothermic reversible reactions. While the rate of reaction for the former is hastened by using a very high temperature, depending on the maximum allowable temperature based on the material of construction, the rate of reaction in the later is based on some complex

Design considerations. The process of determining the number, volume and the optimum temperature of each reactor required for the most economic operation of a reversible reaction system is described as the Optimum Reactor Design. This type of reactor design in most Universities is beyond the undergraduate syllabus.

Expectation from this Lecture

This lecture will briefly review the traditional approach to ordinary and optimum reactor designs (CSTR). We shall then discuss the works of this lecturer that has resulted in a more simplified approach to optimum reactor design. Finally we shall take a look at the application of this simplified new approach to separation processes, in particular the simplified design of a distillation column for a binary mixture.

REVIEW OF REACTOR AND TRADITIONAL DESIGN APPROACH

RATE $(-r_A)$ – TEMPERATURE (T) – CONVERSION (X_A) RELATIONSHIP

For a desired level of conversion (X_A) of reactants to the product, the data of T vs.-r_A are needed. These three essential variables in reactor design are related together through the rate equation. Traditionally the three variables for a given kinetics of reaction, are read on standard charts prepared for a simple transformation reaction (Levenspiel, 1972). Reactor design has to do with coming up with the specification of a reaction vessel that minimizes its volume and hence it's cost for a desired quantity and quality of products. In the reversible reaction system:

$$\left.\begin{array}{l} A = R \\ \\ A + B = R + S \end{array}\right\} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(1)$$
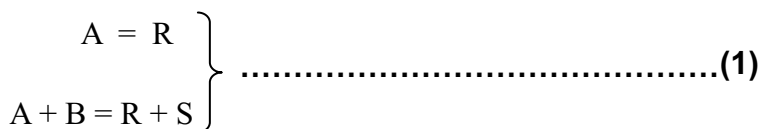
for a given rate of reaction, minimization of reactor volume hence its cost are dependent on the Conversion level desired and the Temperature of reaction. The minimization of the reactor volume for an endothermic reversible and non reversible reactions are easy to determine because the higher the temperature of reaction, the higher the rate of reaction and hence the smaller the volume of reactor required. However, if the above reaction is an exothermic reversible reaction, the story is quite different. There is a particular temperature, that guarantees the maximum rate of reaction and hence the minimum volume of reactor required for a given conversion of reactant or quality of the product. Even then, the route $(X_A$ vs. T) taken to the final conversion level also influences

the how small and economic the reactor will be.

THE ROUTE OF REACTION

The route of a reaction is the path of X vs. T taken by from the level of pure reactant (X=0) to the desired product at the final conversion (X=X_f). From figure 1, if the reaction is isothermal, the route is from point A to point B.

If the reaction is adiabatic, the route is from point C to point B; however, it can be decided to combine isothermal and adiabatic routes through point C to D and then E to B. The route taken, determines the size of the reactor required. Moreover, while it is possible to use only one reactor following either route AB or CB, two reactors with inter-cooling system are required for route CDEB: one reactor operating adiabatically from the starting point C to E followed by some heating, and the second reactor operating isothermally from point E (conversion X_2) to the final conversion X_3 at point B.

The total volume of reactor needed through route AB will be different from the total volume of reactor needed through route CB and also different from the volume through route CDEB. Along each route, the table of -r_A vs X_A can be obtained from X_A=0 to X_A= X_f using the relevant chart shown in fig.1. This table is needed in a reactor design to obtain the needed volume of reactor foe a given quantity and quality of product per unit time.
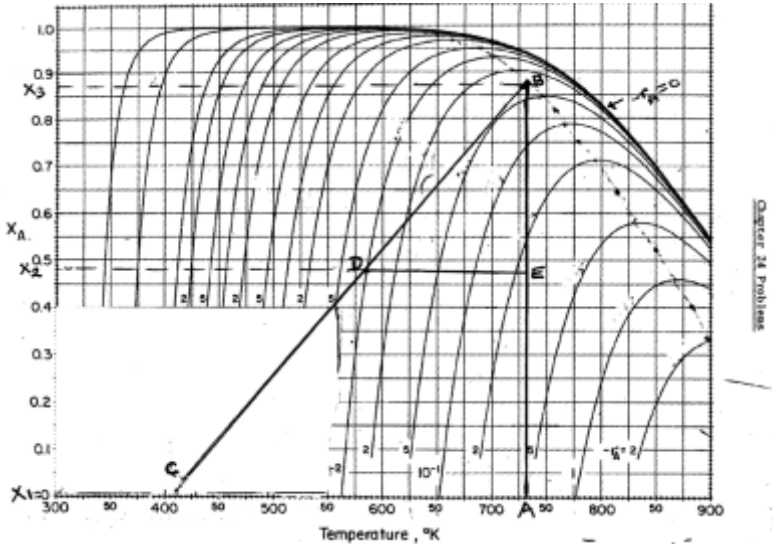
Figure1; Chart of Rate – Temperature – Conversion (Levenspiel, 1979)

OPTIMUM TEMPERATURE PROGRESSION (OTP) ROUTE

There is a reaction path that is different from the ones described thus far. It guarantees the smallest possible volume and as such the most economic route for a given reversible reaction. This path is called the optimum Temperature Progression (OTP) path. In fig1, it can be observed that for each rate curve, there is a particular temperature, at which the maximum possible conversion is achieved. Joining all such maximum conversion peaks at various temperatures (see dotted curve on fig 1) gives us what is called the Optimum Temperature progression path or route. A reactor design trailing this path offers the least possible ideal and the most economic reactor volume required for any given conversion and molar flow rate of the reactants. The challenge with the optimum temperature progression path design is that a single Continuous Stirred Tank Reactor can not be used since every conversion level achieved in the cause of the reaction is at different temperature as predicted on the reaction path in fig.1

BATTERY OF REACTORS IN SERIES

For certain obvious reason, it is sometimes necessary to use a battery of reactors for some reaction systems. The use of a battery of reactors might be required to suppress the concentration of a reactant for better selectivity: or to reduce the overall size of the required reactor for a given conversion or in order to follow closely the optimum temperature progression path, of an exothermic reversible reaction system. For either of the above cases, it is necessary, in practice, to obtain a reactor arrangement pattern that guarantees the minimum overall reactor volume.

The question is how many reactors will be required in series along the path that will minimize the overall practical volume and at what intermediate outlet conversions? There is an optimum number of reactors in series at certain specific conversions that will model a single ideal reactor operating along the OTP. Optimum reactor design had traditionally being an up-hill task, as such; trial and error graphical approach had always been adopted.

CONTINUOUS STIRRED TANK REACTOR DESIGN

Fundamental Design Equations

To estimate the volume of a reactor or the weight of catalyst required for a given reaction system, the basic equation used is:

$$V/F_{Ao} = \int dX_A/-r_A \qquad (2a)$$

For isothermal CSTR, equation (1) transforms to:

$$V/F_{AO} = \Delta X_A/(-r_A) \qquad \text{(since } -r_A \text{ is constant)}$$

Where   V = volume of reactor
        W = weight of catalyst

F_{Ao} = molar flow rate of reactor
X_A = change in conversion
$-r_A$ = rate of reaction

Equation (2) is the design equation for a single reactor either operating isothermally or adiabatically.

For N mixed flow reactors in series, the residence time and hence the reactor volume can be obtained from:

(a) 1st order Reaction (equal residence time)

$$C_{AN}/C_{Ao} = 1/(1+k\tau)^N \qquad (3)$$

Where N = number of reactors in series
C_{AN} = concentration of reactant A out of Nth or the last reactor
C_{Ao} = initial concentration into the first reactor
= residence time

(b) For any Kinetics, (if the intermediate conversions are given, i.e.
i.e. X_{A1}, X_{A2}, X_{A3},.......X_{AN} known and τ_1, τ_2, τ_3, etc are required
Substitute the various conversions into the rate equation to determine the various the rates and then plug both the various rates and their equivalent conversions into equation (2) to determine the various volumes of the reactors.

(c) Optimized Design Technique following a chosen path

The design approach in (a) and (b) above whereby the number of reactors in series are predetermined do not guarantee an economic design since the number of reactors chosen in series may not be the optimized one that ensures the minimum number
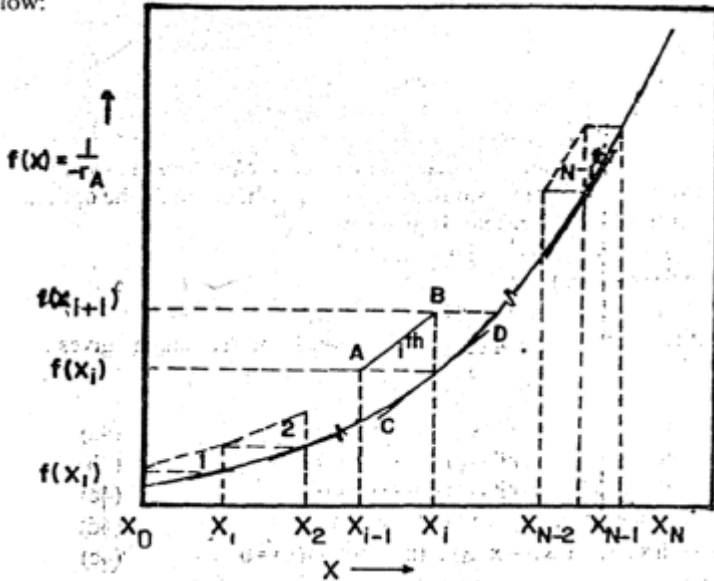
of reactors.

Figure 2: Graphical Trial and Error Method of Optimized Reactor Design

Consider the reaction with the rate – conversion path shown in fig.2. The number of reactors required in series is minimized as the triangles so constructed are maximized. The triangles are maximized when the slope of the tangent CD at ith reactor is equal to the slope of the diagonal AB.   .

This condition can be fulfilled by guessing an outlet conversion X_1, from the first reactor that ensures that the two slopes are equal. When the condition is fulfilled for the first reactor, we proceed to make a guess of the outlet coversion X_2 from the second reactor and ensure the two slopes are also equal through a right guess.

This process continues till the maximum conversion X_N

desired is reached. Whatever number of triangles is obtained, gives the minimum number of reactors required in series for the process along the chosen path of reaction. The various conversions obtained from this operation can be used as in (b) above to determine the various optimized reactor volumes needed.

(a) Optimized Design Technique trailing Optimum Temperature Progression path

The battery of reactors in (a) to (c) could be designed to operate along any
$-r_A$-T-X_A path, but only one path guarantees the least possible residence time or volume of each reactor in the battery and that is the Optimum Temperature Progression path (dotted curve on fig1). This path gives us the maximum rate of reaction at each conversion level. The data of $-r_A$ vs. X_A along the OTP path, is processed the same way as it's done in (c) above except that the temperatures used for calculating optimum rate (if not read on the chart) are the optimum ones (Omoleye, et al 1987). The volume of each reactor obtained is the least possible for the reaction because the technique of design is optimized and the reaction path followed is the OTP or the locus of maximum rate with conversion.

.

CHAPTER 2

THE RATE–TEMPERATURE – CONVERSION: DERIVATION OF EQUATIONS FOR A GENERAL CLASS OF REVERSIBLE REACTIONS

Very frequently, practising chemical engineers have to contend with the design of vessels for chemical reactions having significant heat changes. The accompanying temperature change influences the reactor size (or space time). As pointed out by Levenspiel (1972, 1979), for both endothermic and irreversible reactions, the ideal optimum reactor size is obtained by operating isothermally at the maximum allowable temperature. However, for a reversible exothermic reaction, the ideal optimum reactor size is obtained by following the locus of the maximum rates (often termed the optimum temperature progression, OTP) on the rate-temperature conversion (r-T-X_A) chart. Such a chart is provided in Levenspiel (1972, 1979).

This r-T-X_A chart, while permitting a visual appreciation of the nature of the rate-temperature-conversion profiles, and hence the OTP, is specific to the reaction type.

$$A \rightleftharpoons R \qquad (1)$$

with first-order kinetics.

Probably for proprietary reasons, the r-T-X_A charts for other types of reactions besides that given by Eq. (1) and for different kinetics were provided neither by Levenspiel (1972, 1979) nor in the open literature. Consequently, it becomes almost impossible for a designer confronted with other types of reactions and kinetic rate expressions to utilize Levenspiel's traditionally-easy-to-use graphical design procedure. In fact, it is desirable to have a general mathematical basis for the construction of such charts so that the practising engineer may have at his disposal tools for generating the r-T-X_A profiles for any reaction of interest.

In our research pursuits, we have therefore endeavoured to provide:

(a) an analytical treatment for the generation of r-T-X_A charts for a class of reversible reactions.
(b) the mathematical relations which describe the locus of the maximum rates for the class of exothermic reactions considered in (a).

In what follows, we demonstrate that under certain conditions, our generalized relation is reducible to those on which the Levenspiel chart was probably based. Additionally, with the palpable infiltration of computers into chemical engineering, our formularies may be easily incorporated into packages for computer-aided reactor design.

In addition to the rigor and the time consuming nature of

the graphical method, the need for a faster result makes this systematic analytical method more advantageous. In this work, we present a systematic analytical method of optimal design of a battery of CSTR that is easy to use and gives result

very fast. Additionally, analytical expression for the optimum temperature progression for all the types of reactions considered was also derived for exothermic reactions. The work also illustrates how this formula can be used to generate the charts and to procure the ideal optimum reactor size.

The traditional design approach reviewed in chapter 1 had been in use for many years and needs review for adaptation to computerization.

The General Class of Reversible Reactions

Most chemical reactions of industrial significance fall within the general class of reversible reactions given by

Type I: $aA \rightleftharpoons rR$

Examples: polymerization, isomerization reactions

Type II: $aA + bB \rightleftharpoons rR$

Examples: oxidation, hydrogenation, halogenation reactions

Type III: $aA + bB \rightleftharpoons rR + sS$

Examples: esterification, saponification, neutralization reactions

Type IV: $aA \rightleftharpoons rR + sS$

Examples: decomposition, dehydrogenation, sublimation reactions

Let k_1 and k_2 denote the forward and backward rate constants respectively. The general rate expression, $-r_A$, for any type of reaction may be easily written

$$-r_A = K_1 \prod_{i=1}^{M} C_i^{\alpha_i} - K_2 \prod_{j=1}^{N} C_j^{\beta_j} \qquad (2)$$

where

$$k_1 = A_1 \exp(-E_1/RT)$$
$$k_2 = A_2 \exp(-E_2/RT)$$

Also, for a constant density system (which is the premise throughout this paper), the concentration of any species, k, C_k, during the course of reaction is given by

$$C_k = C_{A_0}(\theta_k + v_k \chi_A)$$

where the variables are as defined in the Nomenclature.