MATHEMATICAL MODELING AND DYNAMIC SIMULATION

OF CATALYTIC FLUIDIZED BED REACTOR

BY

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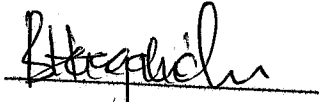
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DEPARTMENT OF CHEMICAL ENGINEERING

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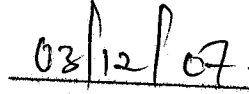
MINNA,

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DECLARATION

I, Bagudu Hadiza .Y. hereby declare that this project work was carried out by me under the supervision of Mr. E.A. Afolabi of the Department of Chemical Engineering, School of Engineering and Engineering Technology, Federal University of Technology, Minna, Niger state.

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BAGUDU HADIZA .Y.

2001/11499EH

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03/12/07

DATE

CERTIFICATION

This is to certify that I have thoroughly read and approved this work, which I found adequate both in scope and quality for the partial fulfillment of the requirement for the Award of Bachelor of Engineering (B.ENG) in Chemical Engineering.

_____   3 – 12 – 2007.

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EXTERNAL EXAMINER   **DATE**

DEDICATION

This research project is dedicated to the memory of my beloveth father, Late. Alhaji Bagudu Waziri, I pray that the Almighty Allah (SWT) grant him Eternal Rest and Al-Janat Firdaus.

ACKNOWLEDGEMENT

ABSTRACT

This research project "Mathematical modeling and dynamic simulation of catalytic fluidized bed reactor" was carried out in order to formulate mathematical equations that could be used in describing the dynamic behaviour of the fluidized bed reactor. The mathematical model equations were formulated, and simulated for the catalytic dehydrogenation of butane to butadiene using matlab. The results obtained from the programming were compared to those obtained from experiment.The dynamic time at which fluidization was achieved between the catalyst particle and reacting gas temperature and pressure was observed and discussed from the results and plots of catalyst particle and reacting gas temperature and pressure against time. The results of the comparison between the modeled equations and that of experiment showed that the R-square (coefficient of determination) value is 99.69%, adj. R-square (adjusted coefficient of determination) is 99.65% and the variance 0.0082952. this values show that there is closeness in the two results and that the model equation developed is accurate.

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CHAPTER ONE

GENERAL INTRODUCTION

Mathematical modeling and simulation has proven to be an insightful
productive process engineering tool. It can be used to design various processes
as a distillation process that will produce quality products in the most economic
ion possible, even under undesirable process disturbances. It can also be used
y in   project to aid in the process and control system design. Later in a project to
mplete detailed control system design and solve wide plant operability problems.
ter the project, the same simulation can be employed in operator training and plant
provement programs. (Grassi 1992).

A **fluidized bed reactor** (FBR) is a type of reactor device that can be
used to carry out a variety of multiphase chemical reactions. In this type of reactor, a
fluid (gas or liquid) is passed through a granular solid material (usually a catalyst
possibly shaped as tiny spheres) at high enough velocities to suspend the solid and
cause it to behave as though it were a fluid. This process, known as fluidization,
imparts many important advantages to the FBR. As a result, the fluidized bed reactor
is now used in many industrial applications.

The solid substrate (the catalytic material upon which chemical species react)
material in the fluidized bed reactor is typically supported by a porous plate, known as
a distributor. The fluid is then forced through the distributor up through the solid
material. At lower fluid velocities, the solids remain in place as the fluid passes
through the voids in the material. This is known as a packed bed reactor. As the fluid
velocity is increased, the reactor will reach a stage where the force of the fluid on the
solids is enough to balance the weight of the solid material. This stage is known as
incipient fluidization and occurs at this minimum fluidization velocity. Once this
minimum velocity is surpassed, the contents of the reactor bed begin to expand and

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around much like an agitated tank or boiling pot of water. The reactor is now a

ized bed. The characteristics and behaviour of fluidized beds are strongly

dent on both the solid and fluid properties.

Today fluidized bed reactors are still used to produce gasoline and other fuels,

with many other chemicals. Many industrially produced polymers are made

FBR technology, such as rubber, vinyl chloride, polyethylene, and styrenes.

ious utilities also use FBR's for coal gasification, nuclear power plants, and water

waste treatment settings. Used in these applications, fluidized bed reactors allow

a cleaner, more efficient process than previous standard reactor technologies.

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A model is a representation of an entity and or a process using physical terms

by the use of mathematical equations.

Simulation on the other hand is a model or composite of models for which

elected materials are uniformly varied. In the most familiar simulations, the

parameter that changes uniformly is time. At least one eqation in the model has time

as a variable and as it changes, the changes to all other variables authomatically occur

because all the equations are linked.

Therefore, mathematical modeling and simulation of catalytic fluidized bed

reactor is the mathematical representation or description of the behaviour of of

processes that take place in the fluidized bed reactor and the act of getting dynamic

response from the developed models from which selected parameters are uniformly

varied.

1.1   AIMS AND OBJECTIVE OF STUDY

To formulate mathematical models and simulation program for the catalytic

fluidized bed reactor

1.2 SCOPE OF STUDY

(a)   Development of mathematical models for the catalytic fluidized bed reactor.

(b)   Development of matlab programs that can be used to predict the dynamic response of the catalytic fluidized bed reactor output variables (reactant fluid and catalyst temperature and pressure) to changes in the dynamic input variable (time).

(c)   Determination of the dynamic time where fluidization is achieved.

(d)   Comparison of the matlab programs with those obtained from experiment.

CHAPTER TWO

2.0   LITERATURE REVIEW

2.1   INTRODUCTION TO REACTORS

An industrial chemical reactor is a complex device in which heat transfer,

mass transfer, diffusion and friction may occur along with chemical reaction and it

must be safe and controllable. In large vessels, questions of mixing of reactants, flow

distribution, residence time distribution and efficient utilization of the surface of

porous catalyst also arise. (Perry 1998)

2.2   FLUIDIZED BED REACTORS

A fluidized bed reactor (FBR) is a type of reactor device that can be

used to carry out a variety of multiphase chemical reactions. In this type of reactor, a

fluid (gas or liquid) is passed through a granular solid material (usually a catalyst

possibly shaped as tiny spheres) at high enough velocities to suspend the solid and

cause it to behave as though it were a fluid. Fluidization occurs when small solid

paarticles are suspended in an upward flowing stream of fluid as shown in fig. 2.1
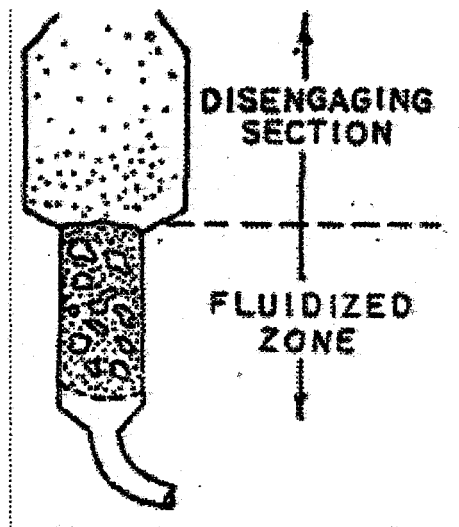
Figure 2.1 From Kunii and Levenspiel *Fluidization Engineering.*

The fluid velocity is sufficient to suspend the particles, but it is not large

enough to carry them out of the vessel. The solid particles swirl around the bed

rapidly The, creating excellent mixing among them. The material "fluidized" is almost always a solid and the "fluidizing medium" is either a liquid or gas. The characteristics and behavior of a fluidized bed are strongly dependent on both the solid and liquid or gas properties. Nearly all the significant commercial applications of fluidized-bed technology concern gas-solid systems.(H.S. Fogler 1981).

2.2.1 DESCRIPTION OF THE PHENOMENA

considering a vertical bed of solid particles supported by a porous or perforated distributor plate. The direction of gas flow is upward through this bed.
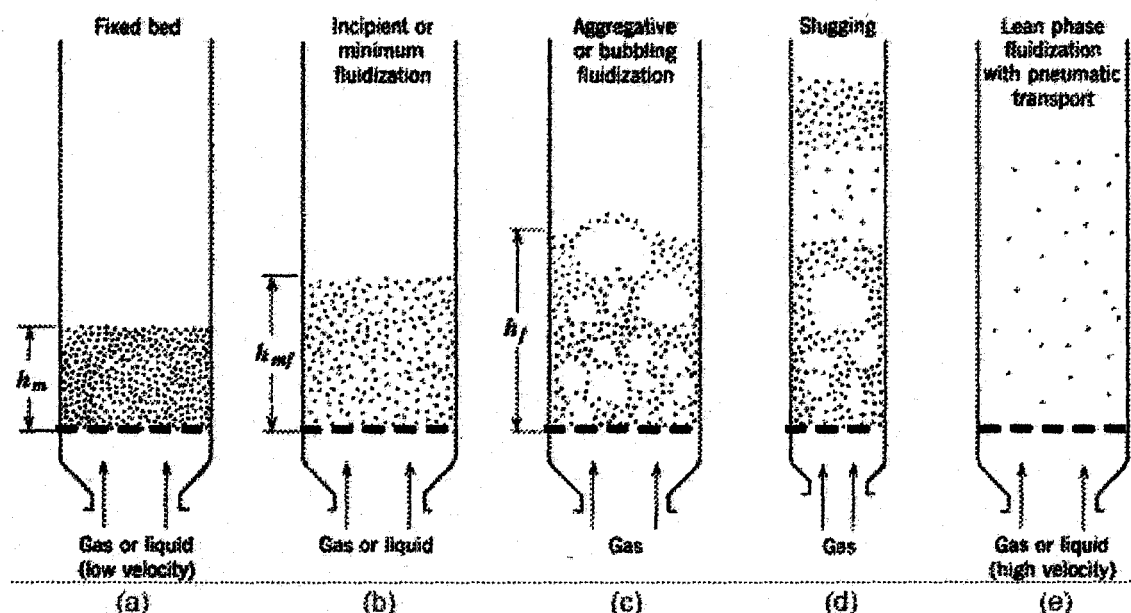
Figure 2.3.2 various kinds of contacting of a batch of solids by fluid. Adapted from Kuni&Levenspiel, Fluidized Engineering.

There is a drag exerted on the solid particles by the flowing gas, and at low gas velocities the pressure drop resulting from this drag will follow the Ergun equation just as for any other type of packed bed. When the gas velocity is increased to a certain value however, the total drag on the particles will equal the weight of the bed, and the particles will begin to lift and barely fluidize. If ρ_c is density of the solid catalyst particles, A_c is the cross sectional area, h_s, is the height of the bed settled before the particles start to lift, h, is the height of the bed at any time, and ε_s and ε are

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the corresponding porosities, of the settled and expanded bed, respectively; then the mass of solids in the bed, W_s, is

$$W_s = \rho_c A_c h_s \left(1 - \varepsilon_s \right) = \rho_c A_c h \left(1 - \varepsilon \right) \quad \text{------------------(2.2.1)}$$

This relationship is a consequence of the fact that the mass of the bed occupied solely by the solid particles is the same no matter what the porosity of the bed. When the drag force exceeds the gravitational force, the particles begin to lift, and the bed expands (i.e., the height increases) thus increasing the bed porosity. This increase in bed porosity decreases the overall drag until it is again balanced by the total gravitational force exerted on the solid particles.

If the gas velocity is increased still further, expansion of the bed will continue to occur; the solid particles will become somewhat separated from each other and begin to jostle each other and move around in a restless manner. Increasing the velocity just a slight amount further causes instabilities, and some of the gas starts bypassing the rest of the bed in the form of bubbles. These bubbles grow in size as they rise up the column. Coincidentally with this, the solids in the bed begin moving upward, downward, and around in a highly agitated fashion appearing as a boiling frothing mixture. With part of the gas bubbling through the bed and the solids being moved around as though they were part of the fluid, the bed of particles is said to be "fluidized." It is in a state of aggregative, nonparticulate, or bubbling fluidization.

A further increase in gas velocity will result in slug flow and unstable chaotic operation of the bed. Finally at extremely high velocities, the particles are blown or transported out of the bed. The range of velocities over which the Ergun equation applies can be fairly large. On the other hand, the difference between the velocity at which the bed starts to expand and the velocity at which the bubbles start to appear can be extremely small and sometimes nonexistent. This observation means that if one steadily increases the gas flow rate, the first evidence of bed expansion may be the appearance of gas bubbles in the bed and the movement of solids. At low gas velocities in the range of fluidization, the rising bubbles contain very few solid

particles. The remainder of the bed has a much higher concentration of solids in it and is known as the *emulsion phase* of the fluidized bed. The bubbles are shown as the *bubble phase*. The cloud phase is an intermediate phase between the bubble and emulsion phases.

After the drag exerted on the particles equals the net gravitational force exerted on the particles, that is,

$$\Delta P = g\left(\rho_c - \rho_g\right)(1 - \varepsilon)h \text{ -----------------------(2.3.2)}$$

the pressure drop will not increase with an increase in velocity beyond this point. From the point at which the bubbles begin to appear in the bed, the gas velocity can be increased steadily over a quite appreciable range without changing the pressure drop across the bed or flowing the particles out of the bed. The bubbles become more frequent, and the bed, more highly agitated as the gas velocity is increased, but the particles remain in the bed. This region is bubbling fluidization. Depending on the physical characteristics of the gas, the solid particles, and the distributor plate; and the internals (e.g., heat exchanger tubes) within the bed, the region of bubbling fluidization can extend over more than an order of magnitude of gas velocities. In other situations, gas velocities in the region of bubbling fluidization may be limited; the point at which the solids begin to be carried out of the bed by the rising gas may be a factor of only three or four times the velocity at incipient fluidization. Eventually, if the gas velocity is continuously increased, it will become sufficiently rapid to carry the solid particles upward, out of the bed. When this begins to happen, the bubbling and agitation of the solids are still present, and this is known as the region of fast fluidization, and the bed is know as *fast-fluidized bed*. At velocities beyond this region, the particles are well apart, and the particles are merely carried along with the gas stream. Under these conditions, the reactor is usually referred to as a *straight through transport reactor* or STTR.

Figure 2.2.3 below presents the pressure drop across a bed of solid particles as a function of gas velocity. The region covered by the Ergun equation is the rising

portion of the plot (Section I: $1 < U_0 < 4$ cm/s). The section of the figure where the

pressure drop remains essentially constant over a wide range of velocities is the

region of bubbling fluidization (Section II: $4 < U_0 < 50$ cm/s). Beyond this are the

regions of fast fluidization and of purely entrained flow.
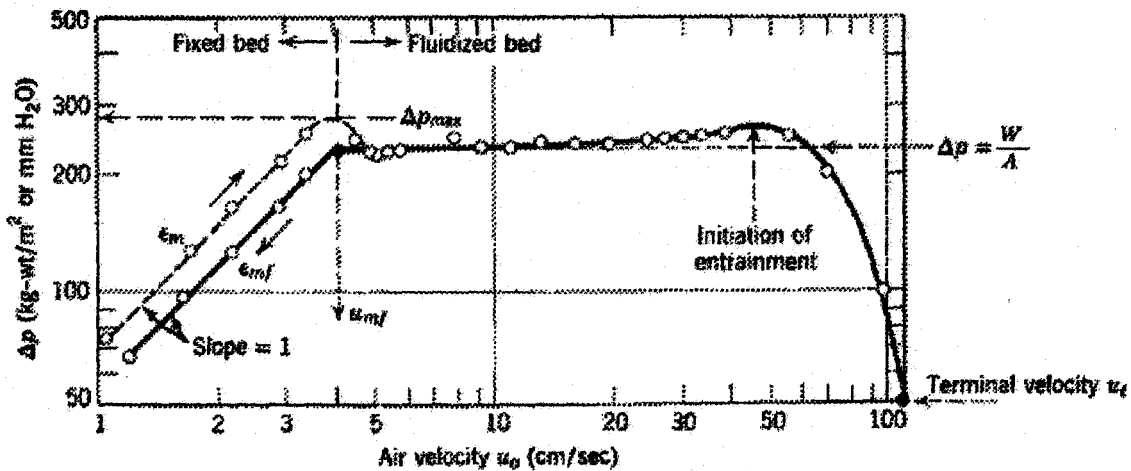
Figure 2.2.3 From Kunii and Levenspiel, FluidizationEngineering.

2.2.2 DESCRIPTIVE BEHAVIOUR OF A FLUIDIZED BED REACTOR (THE MODEL OF KUNII AND LEVENSPIEL).

At gas flow rates above the point of minimum fluidization, a fluidized bed

appears much like a vigorously boiling liquid; bubbles of gas rise rapidly and burst on

the surface, and the emulsion phase is thoroughly agitated. The bubbles form very

near the bottom of the bed, very close to the distributor plate and as a result the design

of the distributor plate has a significant effect on fluidized-bed characteristics.

Literally hundreds of investigators have contributed to what is now regarded as

a fairly practical description of the behavior of a fluidized bed; chief among these is

the work of Davidson and Harrison. Early investigators saw that the fluidized bed had

to be treated as a two-phase system – an emulsion phase and a bubble phase (often

called the dense and lean phases). The bubbles contain very small amounts of solids.

They are not spherical; rather they have an approximately hemispherical top and a

pushed-in bottom. Each bubble of gas has a wake that contains a significant amount

of solids. These characteristics are illustrated in Figure 2.3.4, which were obtained

from x-rays of the wake and emulsion, the darkened portion being the bubble phase.

As the bubble rises, it pulls up the wake with its solids behind it. The net flow of the solids in the emulsion phase must therefore be downward.
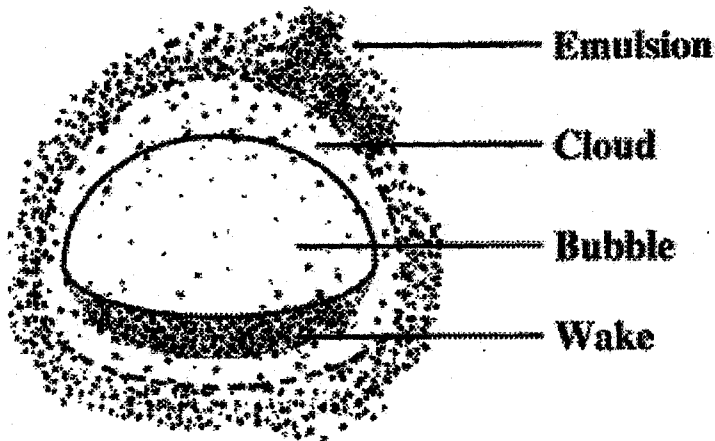
Figure 2.2.4 Schematic of bubble, cloud, and wake.

The gas within a particular bubble remains largely within that bubble, only penetrating a short distance into the surrounding emulsion phase. The region penetrated by gas from a rising bubble is called the cloud. Davidson found that he could relate the velocity of bubble rise and the cloud thickness to the size of bubble. Kunii and Levenspiel combined these observations with some simplifying assumptions to provide a practical, useable model of fluidized-bed behavior. Their assumptions are as follws:

(a) The bubbles are all of one size.

(b) The solids in the emulsion phase flow smoothly downward, essentially in plug flow.

(c) The emulsion phase exists at minimum fluidizing conditions. The gas occupies the same void fraction in this phase as it had in the entire bed at the minimum fluidization point. In addition, because the solids are flowing downward, the minimum fluidizing velocity refers to the gas velocity relative to the moving solids, that is,

$$u_e = u_{mf}/\varepsilon_{mf} - u_s \underline{\hspace{2cm}}(2.2.3)$$

(The ε_{mf} is present in this equation because u_{mf} is the superficial velocity, i.e., based on an empty tube cross section.) The velocity of the moving solids, u_s, is positive in the downward direction here, as in most of the fluidization literature. The velocity of

the gas in the emulsion, u_e, is taken as a positive in the upward direction, but note that it can be negative under some conditions.

(d) In the wakes, the concentration of solids is equal to the concentration of solids in the emulsion phase, and therefore the gaseous void fraction in the wake is also the same as in the emulsion phase. Because the emulsion phase is at the minimum fluidizing condition, the void fraction in the wake is equal to ε_{mf}. The wake, however, is quite turbulent, and the average velocities of both solid and gas in the wake are assumed to be the same and equal to the upward velocity of the bubbles.

Several of these assumptions had been used by earlier investigators, particularly Davidson and Harrison. With the possible exception of (c), all these assumptions are of questionable validity, and rather obvious deviations from them are observed routinely. Nevertheless, the deviations apparently do not affect the mechanical or reaction behavior of fluidized beds sufficiently to diminish their usefulness.

2.2.3 Mass Transfer In Fluidized Beds

There are two types of mass transport important in fluidized-bed operations. The first is the transport between gas and solid. In some situations this can affect the analysis of fluidized-bed behavior significantly, and in others it might not enter the calculations at all. In the treatment of this type of transfer, it will be seen that this type of transport is quite similar to gas-solid mass transfer in other types of operations.

The second type of mass transfer is unique to fluidized-bed operations. It concerns the transfer of material between the bubbles and the clouds, and between the clouds and the emulsion. In almost every type of fluidized-bed operation, there are significant gas phase concentration differences between the various elements of the fluidized bed. Consequently, calculations involving this type of mass transfer occur in almost every fluidized-bed analysis.

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A → B
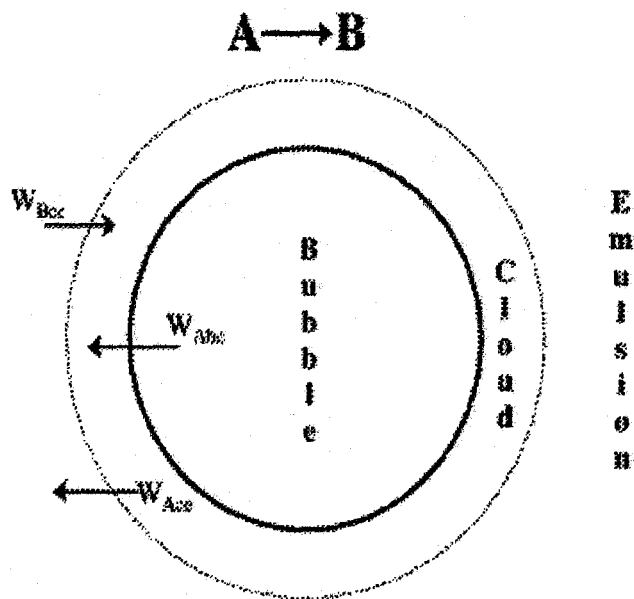
Figure 2.2.5 Transfer between bubble, cloud, and emulsion.

2.2.3(a) Gas-Solid Mass Transfer

In the bubble phase of a fluidized bed, the solid particles are sufficiently separated so that in effect there is mass transfer between a gas and single particles. The most widely used correlation for this purpose is the 1938 equation of Fröessling for mass transfer to single spheres.

$$Sh = 2.0 + 0.6 \left(Re\right)^{1/2} \left(Sc\right)^{1/3} \text{-----------------(2.2.4)}$$

The relative velocity between the solid particle and the gas used in calculating the Reynolds number will be taken as $u0$. In the emulsion phase, the equation would be one that applied to fixed-bed operation with a porosity in the bed equal to ε_{mf} and a velocity of umf. The equation recommended by Kunii and Levenspiel is

$$Sh = 2.0 + 1.5 \left(Sc\right)^{1/3} \left[\left(1-\varepsilon\right)\left(Re\right)^{1/2}\right] \text{-----------------(2.2.5)}$$

for $5 < Re < 120$, and $\varepsilon < 0.8$

Mass transfer coefficients obtained from these relationships may then be combined with mass transfer among the various phases in the fluidized bed to yield the overall behavior with regard to the transport of mass. Owing to the small particle sizes and high surface area per volume of solids used in fluidized beds, the mass

transfer from the gas to the solid surface is usually quite rapid and consequently it

seldom limits the reaction.
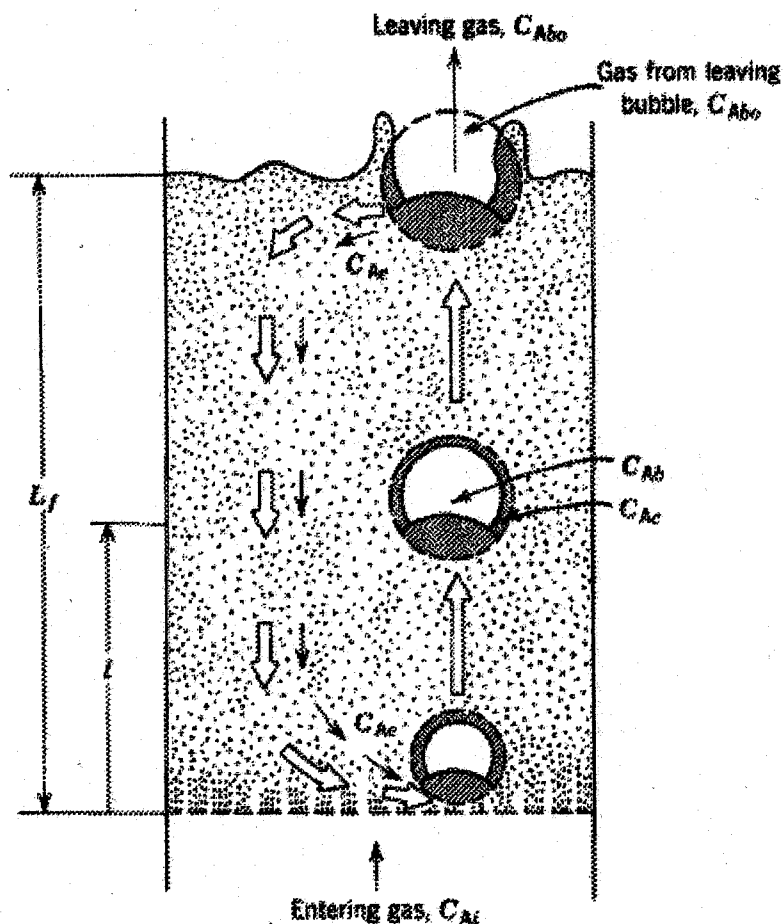
Figure 2.2.6 Sketch of flow pattern in a fluidized bed for downflow of emulsion gas,
$ue/u0 < 0$ or $u0/umf > 6$ to 11. Adapted from Kunii & Levenspiel,
Fluidized
Engineering,

2.2.3(b)   Mass Transfer Between The Fluidized-Bed Phases

For the gas interchange between the bubble and the cloud, Kunii and

Levenspiel defined the mass transfer coefficient Kbc (s^{-1}) in the following manner:

$$W_{Abc} = K_{bc} \left(C_{Ab} - C_{Ac} \right) \text{----------------}(2.2.6)$$

Where C_{Ab} and C_{Ac} are the concentration of A in the bubble and cloud

respectively, (mole/dm3) and W_{Abc} represents the number of moles of A transferred

from the bubble to the cloud per unit time per unit volume of bubble (mole/dm3/s).

The concept of basing all mass transfer (and later, all reaction) on the bubble volume

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proves to simplify the calculations markedly. For the products, (e.g., B in $A \rightarrow B$) the rate of transfer into the bubble from the cloud is given by a similar equation

$$W_{Bcb} = K_{cb} \left(C_{Bc} - C_{Bb} \right) \text{-----------------------}(2.2.7)$$

The mass transfer coefficient K_{bc} can also be thought of as an exchange volume q between the bubble and the cloud.

$$W_{Bcb} = q_b C_{Ab} - q_c C_{Ac} = q_o \left(C_{Ab} - C_{Ac} \right) \text{--------------------}(2.2.8)$$

where q_b = Volume of gas flowing from the bubble to the cloud per unit time per unit volume of bubble

q_c = Volume of gas flowing from the cloud to the bubble per unit time per unit volume of bubble

q_o = Exchange volume between the bubble and cloud per unit time per unit volume of bubble (i.e., K_{bc}; $q_o = q_c = q_b$)

Using Davidson's expression for gas transfer between the bubble and the cloud, and then basing it on the volume of the bubble, Kunii and Levenspiel obtained this equation for evaluating K_{bc}:

$$K_{bc} = 4.5 \left(\frac{u_{mf}}{d_b} \right) + 5.85 \left(\frac{D_{AB}^{1/2} \; g^{1/4}}{d_b^{5/4}} \right) \text{-----}(2.2.9)$$

where u_{mf} is in cm/s, d_b is in cm, D_{AB} is the diffusivity (cm^2/s) and g is the gravitational constant (980 cm/s^2). We note that $K_{bc} = K_{cb}$ -----(2.2.10) and a typical value of K_{bc} is 2 s^{-1}.

Similarly, these authors defined a mass transfer coefficient for gasinterchange between the cloud and the emulsion:

$$W_{Ace} = K_{ce} \left(C_{Ac} - C_{Ae} \right) \text{-------------}(2.2.11)$$

$$W_{Bce} = K_{ce} \left(C_{Be} - C_{Bc} \right) \text{--------------}(2.2.12)$$

where W_{Ace} is the moles of A transferred from the cloud to the emulsion per unit time per unit volume of bubble. Note that even though this mass transfer does not involve the bubble directly, it is still based on the bubble volume.

Using Higbie's penetration theory and his analogy for mass transfer from a bubble to a liquid, Kunii and Levenspiel16 developed an equation for evaluating Kce:

$$K_{ce} = 6.77\left(\frac{\varepsilon_{mf} D_{AB} u_b}{d_b^3}\right)^{1/2} \quad \text{------------(2.2.13)}$$

where u_b is velocity of bubble rise in cm/s and the other symbols are as defined. A typical value of Kce is $1s^{-1}$. Kce can also be thought of as the exchange volume between the cloud and the emulsion. With knowledge of the mass transfer coefficients, the amount of gas interchange between the phases of a fluidized bed can be calculated and combined to predict the overall mass transfer behavior or reaction behavior of a fluidized-bed process.

2.2.4 Reaction Behavior in a Fluidized Bed

To use the Kunii-Levenspiel model to predict reaction rates in a fluidized bed reactor, the reaction rate law for the heterogeneous reaction per gram (or other fixed unit) of solid must be known. Then the reaction rate in the bubble phase, the cloud, and the emulsion phase, all per unit of bubble volume, can be calculated. Assuming that these reaction rates are known, the overall reaction rate can be evaluated using the mass transfer relationships presented in the preceding section. All this is accomplished in the following fashion. We consider an nth order, constant-volume catalytic reaction. In the bubble phase.

$$r_{Ab} = -k_b C_{Ab}^n \quad \text{----------------(2.2.14)}$$

in which the reaction rate is defined per unit volume of bubble. In the cloud,

$$r_{Ac} = -k_c C_{Ac}^n \quad \text{----------------------(2.2.15)}$$

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and similarly in the emulsion,

$$r_{Ae} = -k_e C_{Ae}^n \qquad \text{------------------------}(2.2.16)$$

where k_e, k_c and k_b are the specific reaction rates in the emulsion cloud, and bubble respectively. In the latter two equations, the reaction rate is also defined per unit volume of bubble.

2.2.5 HISTORY AND CURRENT USES

Fluidized bed reactors are a relatively new tool in the industrial engineering field. The first fluidized bed gas generator was developed by Fritz Winkler in Germany in the 1920s, One of the first United States fluidized bed reactors used in the petroleum industry was the Catalytic Cracking Unit, created in Baton Rouge, LA in 1942 by the Standard Oil Company of New Jersey (now ExxonMobil). This FBR and the many to follow were developed for the oil and petrochemical industries. Here catalysts were used to reduce petroleum to simpler compounds through a process known as cracking. The invention of this technology made it possible to significantly increase the production of various fuels in the United States.

Today fluidized bed reactors are still used to produce gasoline and other fuels, along with many other chemicals. Many industrially produced polymers are made using FBR technology, such as rubber, vinyl chloride, polyethylene, and styrenes. Various utilities also use FBR's for coal gasification, nuclear power plants, and water and waste treatment settings. Used in these applications, fluidized bed reactors allow for a cleaner, more efficient process than previous standard reactor technologies.

2.2.6 ADVANTAGES

The increase in fluidized bed reactor use in today's industrial world is largely due to the inherent advantages of the technology.

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- **Uniform Particle Mixing:** Due to the intrinsic fluid-like behavior of the solid material, fluidized beds do not experience poor mixing as in packed beds. This complete mixing allows for a uniform product that can often be hard to achieve in other reactor designs. The elimination of radial and axial concentration gradients also allows for better fluid-solid contact, which is essential for reaction efficiency and quality.

- **Uniform Temperature Gradients:** Many chemical reactions produce or require the addition of heat. Local hot or cold spots within the reaction bed, often a problem in packed beds, are avoided in a fluidized situation such as a FBR. In other reactor types, these local temperature differences, especially hotspots, can result in product degradation. Thus FBRs are well suited to exothermic reactions. Researchers have also learned that the bed-to-surface heat transfer coefficients for FBRs are high.

- **Ability to Operate Reactor in Continuous State:** The fluidized bed nature of these reactors allows for the ability to continuously withdraw product and
- introduce new reactants into the reaction vessel. Operating at a continuous process state allows manufacturers to produce their various products more efficiently due to the removal of startup conditions in batch processes.

2.2.7 DISADVANTAGES

As in any design, the fluidized bed reactor does have it draw-backs, which any reactor designer must take into consideration.

- **Increased Reactor Vessel Size:** Because of the expansion of the bed materials in the reactor, a larger vessel is often required than that for a packed bed reactor. This larger vessel means that more must be spent on initial startup costs.

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- **Pumping Requirements and Pressure Drop:** The requirement for the fluid to suspend the solid material necessitates that a higher fluid velocity is attained in the reactor. In order to achieve this, more pumping power and thus higher energy costs are needed. In addition, the pressure drop associated with deep beds also requires additional pumping power.

- **Particle Entrainment:** The high gas velocities present in this style of reactor often result in fine particles becoming entrained in the fluid. These captured particles are then carried out of the reactor with the fluid, where they must be separated. This can be a very difficult and expensive problem to address depending on the design and function of the reactor. This may often continue to be a problem even with other entrainment reducing technologies.

- **Lack of Current Understanding:** Current understanding of the actual behavior of the materials in a fluidized bed is rather limited. It is very difficult to predict and calculate the complex mass and heat.

- **Erosion of Internal Components:** The fluid-like behavior of the fine solid particles within the bed eventually results in the wear of the reactor vessel. This can require expensive maintenance and upkeep for the reaction vessel and pipes.

2.3 MATHEMATICAL MODELING

Mathematical model is the mathematical representation of an entity and/or process using mathematical equations to describe the behaviour of the process.

Mathematical models can be useful in all phase of chemical engineering from research and development to plant operation and even in bussiness and economic studies. Mathematical modeling is very much an art, it takes experience, practice, and brain power to be a good mathematical modeler.(luyben 1998)

2.3.1 principle of modeling

The formulationn of mathematical model is analogue to the formulation of scientific hypothesis. The principle involved in the formulation of mathematical model are stated below,

2.3.2 Basis

The law of conservation of mass, energy, and momentum forms the basis for mathematical models. They are usually stated in their varying forms.

2.3.3 Assumption

The formulation of mathematical models involve making simplifying assumptions that are reasonable. The process is called optimum sloppiness, a term that refers to a compromise between making a vigorous description of a system and getting an answer that is good enough. Assumptions made in the formulation stage imposes limitations on the model and should always be considered when evaluating its predicted results.

2.3.4 mathematical consistency of model

In order to obtain solution for a model, its degree of freedom must be zero. That is, the number of variables must be equal to the number of equations describing the system. It is important that the unit of all terms in the equation be consistent.

2.3.5 solution of the model equation

Available solution techniques should be considered in the development of the models, for it would amount to a waste of time and energy developing an equation without any way of solving it.

2.3.6 verification

proving that the formulated models describe the real world situation is an important part of mathematical modeling. One way of achieving this objective is by computer simulation.

2.3.7 IMPORTANCE OF MATHEMATICAL MODELING

It is quite often the case that we have to design the control system for a chemical process before the real process is being constructed. In such case, we cannot rely on the experimental procedures and we need a different representation of the chemical process we examine.

Mathematical model and simulation can result in considerable saving of both time and money. When it is impractical to experiment with the real system. Mathematical modeling and simulation can be used to explore the effect of changes on a system. It can also result in increase in the fundamental knowledge about a system since it usually involves a considerable analysis of the system. Mathematical models and simulation can be useful in all phase of chemical engineering ;

(a) research and development: Determining chemical kinetics mechanism and parameters from laboratory or pilot plant reaction data, exploring the effect of different operating condition for optimization and control studies, aiding in scale up calculations.

(b) Design; exploring the sizing and arrangement of sizing equipment for dynamic performance, studying the interaction of various parts of the process, particularly when material recycle or heat integration is used , evaluating alternative process and control structures and strategies, simulating start up, shut down and emergency situations and procedures.

(c) Plant operation; trouble shooting control and processing problems, aiding in start up and operator training, studying the effects of and the requirements for expansion (bottle neck removal) projects, optimizing plant operation. It is usually much cheaper, safer, and faster to conduct the kinds of studies listed above on mathematical model than experimentally on an operating unit. This is not to say that plant tests are not necessary.

2.4   computer simulation

computer simulation means the running of a special program on a suitable type of computer which generates time response of the model that imitates the behaviour of the process being studied. There are two types of simulation methods namely, analogue and digital simulations.

The powerful range of values that digital computer can handle, eliminates the problems of scaling and other problems associated with analogue. The two principal difficulties with digital simulation are numerical integration of ordinary differential equations and how to obtain solution of simultaneous linear equation. Simulation can be carried out with the aid of the computer using softwares like Msexcel, polymath, mathcad, hysys, Aspen, chem.Office and so on.

CHAPTER THREE

3.0 MATHEMATICAL MODELS AND SIMULATION OF THE CATALYTIC FLUIDIZED BED REACTOR

figure 3.2 section of a bubbling fluidized bed

figure 3.0 Basic diagram of a fluidized bed reactor

using facts from literature to describe rection in the fluidized bed, the reactant gas enters from the bottom of the bed and flows up the reactor in the form of bubbles. The gas velocity is sufficient to suspend the particle, but it is not large enough to carry them out of the vessel.

3.1 Model Assumptions

(1) The catalyst particles are assumed to be small enough so that heat and mass transfer resistances can be lumped at the particle surface.

(2) The reaction takes place in the porous volumecatalyst.

(3) All particles have the same temperature and partial pressure.

(4) The reaction is irreversible.

From the above assumptions and the laws of conservation of mass energy and momentum, mass and energy balances can be written for the gas and particles.

3.2 Mathematical models of catalytic fluidized bed reactor (Catalytic dehydrogenation of butane to butadiene).

Equation of reaction for the dehydrogenation of butane to butadiene is
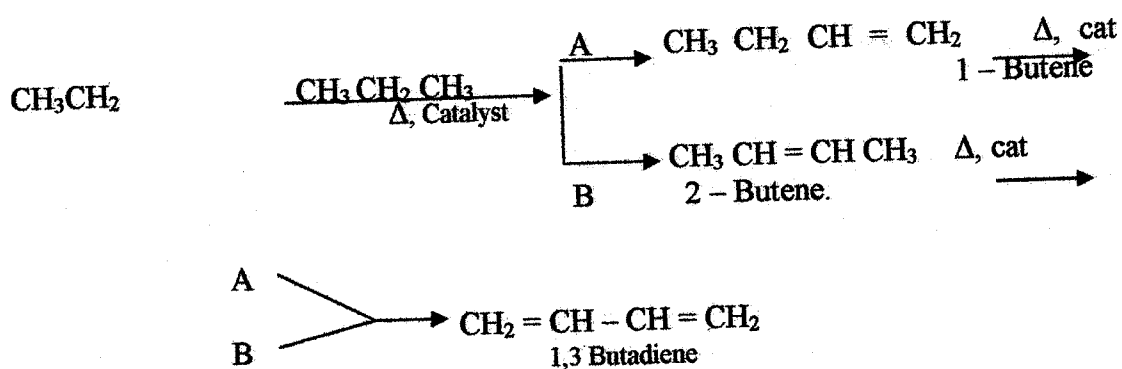
The mathematical model of catalytic fluidized bed reactor is thus written as follows;

Gas phase:

Mass balance; from laws of conservation of mass,

Input = Output + Accumulation + Disappearance

Thus,

{Rate of accumulation of reactant in gas phase} = {Rate into the reactor} − {Rate out

of reactor} + {Mass transfer rate between gas and particle}.

i.e

$$V \frac{\in \rho_g}{MP} \frac{dp}{dt} = \frac{q}{MP}(p_e - p) + a_v k_g V (p_p - p) \text{_____(3.1)}$$

where p = partial pressure of the reactant in the gas phase

p_e = partial pressure of the reactant at the entrance

p_p = partial pressure of the reactant in the particles

M = molecule weight of the reactant

P = Total Pressure

V = Volume of the bed

$\in$ = Void fraction of the bed

ρ_g = Density of the gas

q = gas mass flow rate

k_g = mass transfer coefficient

The gas phase energy balance is,

{Rate of thermal accumulation} = {sensible heat into reactor} – {sensible heat out

of   reactor} + {heat transfer rate between reactor wall and gas} + {heat transfer rate

between gas and particle}.

$$V \in \rho_g c_g \frac{dT}{dt} = q c_g (T_e - T) + \frac{V 2\pi r h_w}{\pi r^2}(T_w - T)$$

$$+ a_v h_g V (T_p - T) \qquad \text{-----------------(3.2)}$$

where T = gas phase temperature

T_p = particle temperature

T_e = inlet gas phase temperature

T_w = reactor wall temperature

c_g = heat capacity of the gas phase

h_w = heat transfer coefficient between the wall of the reactor and the gas

h_g = heat transfer coefficient between the gas and the catalyst

r = radius of the fluidized bed

Particles Mass Balance,

{Rate of mass Accumulation of reactants in particles} = {Rate into particle} – {Rate

out of particle} – {Reaction rate mechanism},

$$\alpha v p \frac{\rho_g}{MP} \frac{dp_p}{dt} = s_p k_g (p - p_{pl}) - v_p \alpha k p_p \qquad \text{-----------------(3.3)}$$

Where α = void fraction of the particles

vp = volume of each particle

s_p = area of a particle

k = reaction rate constant

The energy balance gives,

{Rate of heat Accumulation in particle} = {sensible heat into particle} − {sensible heat out of particle} + {Reaction mechanism},

$$v_p \rho_s c_s \frac{dT_p}{dt} = s_p h_g \left(T - T_p\right) + \left(-\Delta H\right) v_p \alpha k p_p \quad \text{----------(3.4)}$$

Where, c_s = heat capacity of the particles

$\left(-\Delta H\right)$ = heat of reaction

The model is simplified by introducing the following dimensionless groups:

$$A = \frac{\alpha v_p a_v}{\in s_p} \qquad\qquad C = \frac{\alpha_v c_s v_p \rho_s}{\in s_p c_g \rho_g}$$

$$F = \frac{\left(-\Delta H\right) kg}{hg} \qquad\qquad H_g = \frac{\alpha_v kgMPV}{q}$$

$$H_T = \frac{a_v h_g V}{q c_g} \qquad\qquad H_w = \frac{2 h_w V}{T c_g q}$$

$$K = \frac{\alpha v_p}{s_p k_g} \qquad\qquad \tau = \frac{qt}{\in \rho_g V}$$

and the fact that

$$\left(1 - \in\right) \frac{s_p}{v_p} = a_v \quad \text{----------(3.5)}$$

where a_v = interfacial area per unit volume.

The model of the fluidized bed therefore becomes,

Gas Phase   Mass balance: $\quad \dfrac{dp}{d\tau} = pe - p + H_g\left(p_p - p\right) \quad \text{----------(3.6)}$

Energy balance: $\quad \dfrac{dT}{d\tau} = Te - T + H_T\left(T_p - T\right) + H_w\left(T_w - T\right) \quad \text{-------(3.7)}$

Particles   Mass Balance: $\quad A\dfrac{dp_p}{d\tau} = -H_g K k p_p + H_g\left(p_p - p_p\right) \quad \text{----------(3.8)}$

Energy Balance: $\quad C\dfrac{dT_p}{d\tau} = H_T F K k p_p + H_T\left(T - T_p\right) \quad \text{--------(3.9)}$

The reaction rate constant obeys the Arrhenius temperature dependency

$$k = k_{0e}^{-\frac{\Delta E}{RT_p}} \qquad \text{---------------}(3.10)$$

where k_0 = the pre/exponential factor

ΔE = the activation ener

3.4 SIMULATION OF THE MODEL EQUATION

The model equation developed was simulated using matlab programming. The matlab files program and the command window instructions for running the program are shown.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
% SOLVES MATHEMATICAL MODEL OF CATALYTIC FLUIDIZED BED
%            REACTOR (CATALYTIC DEHYDROGENATION OF BUTANE TO
%            BUTADIENE)
%
% The differential equations are provided in reactor.m
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Initialize time
t = cputime;

% Integration time interval
TSPAN = [ 0 750 ];

% Initial conditions
Y0 = [ 0.1 600 0 690 ];

% Integrate using ode15s
[T,Y] = ode15s('model310',TSPAN,Y0(:));

% Print how long it took for the integration
time = cputime-t

% Plot the results
subplot(2,1,1), semilogx(T,Y(:,2),T,Y(:,4),'-.');
xlabel(' Time')
ylabel(' T, Tp')
legend(' T',' Tp')
title(' Dynamic Approach to Low Steady State')
subplot(2,1,2), semilogx(T,Y(:,1),T,Y(:,3),'-.');
xlabel(' Time')
ylabel(' P, Pp')
legend(' P',' Pp')
```

Function for solving the differential Equations

```
function ydot = reactor(t,y)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
% This function defines the catalytic reactor dynamics.
%
% Input variables:      t - time
%                       y - state column vector
%                           y(1) = P
%                           y(2) = T
%                           y(3) = Pp
%
```

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```
%
%
% Output variables:        ydot - state derivatives column vector
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Reaction rate constant

K = 6e-4*exp(20.7-15000/y(2));

ydot(1) = 0.1+320*y(3)-321*y(1);
ydot(2) = 1752+266.667*y(4)-269.267*y(2);
ydot(3) = 1866.8*(y(1)-(1+K)*y(3));
ydot(4) = 10369*K*y(3)+1.2964*(y(2)-y(4));

ydot = ydot(:);
```

CHAPTER FOUR

4.0   RESULTS AND DISCUSSION OF RESULTS

4.1   RESULTS

The results of the simulation of the catalytic fluidized bed reactor carried out are

presented below.
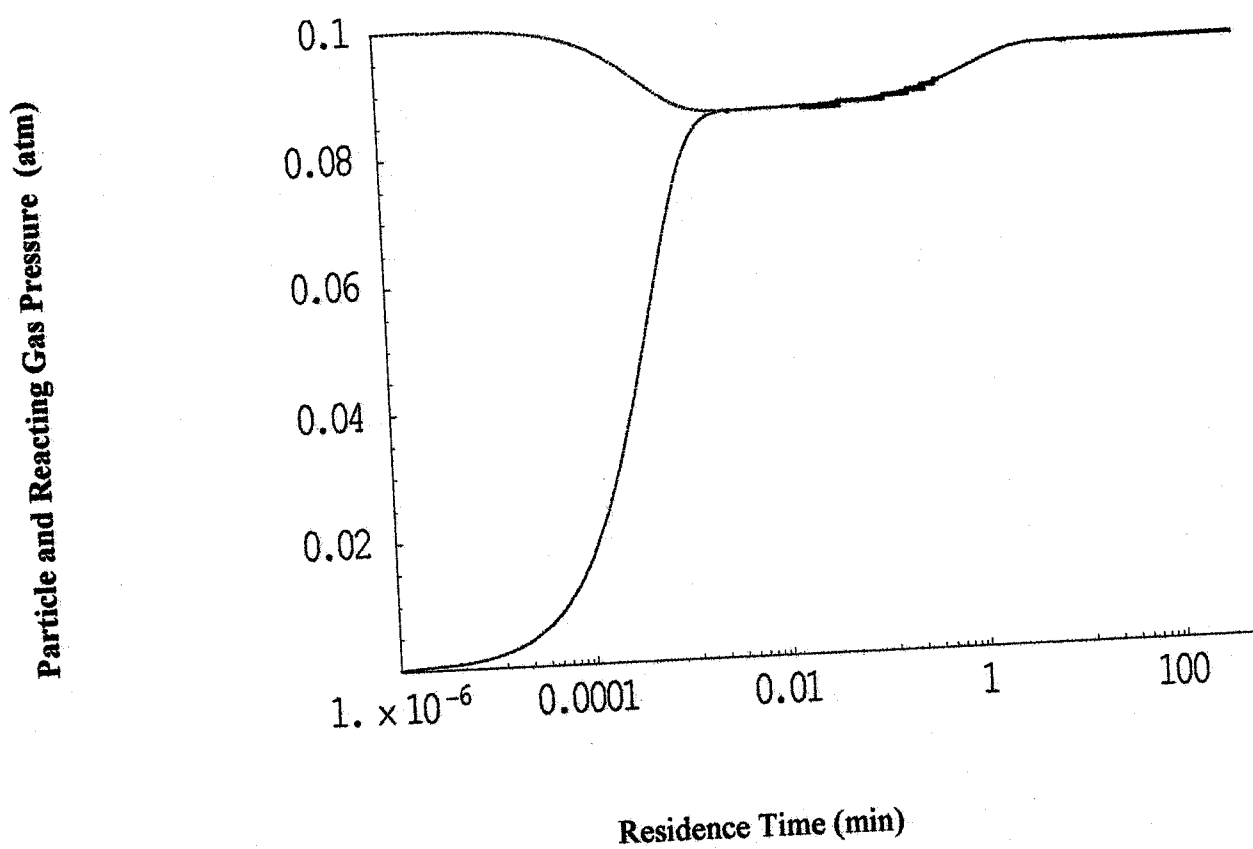
Figure 4.1 The Plot of Catalytic Particle and Reacting gas pressure against Time
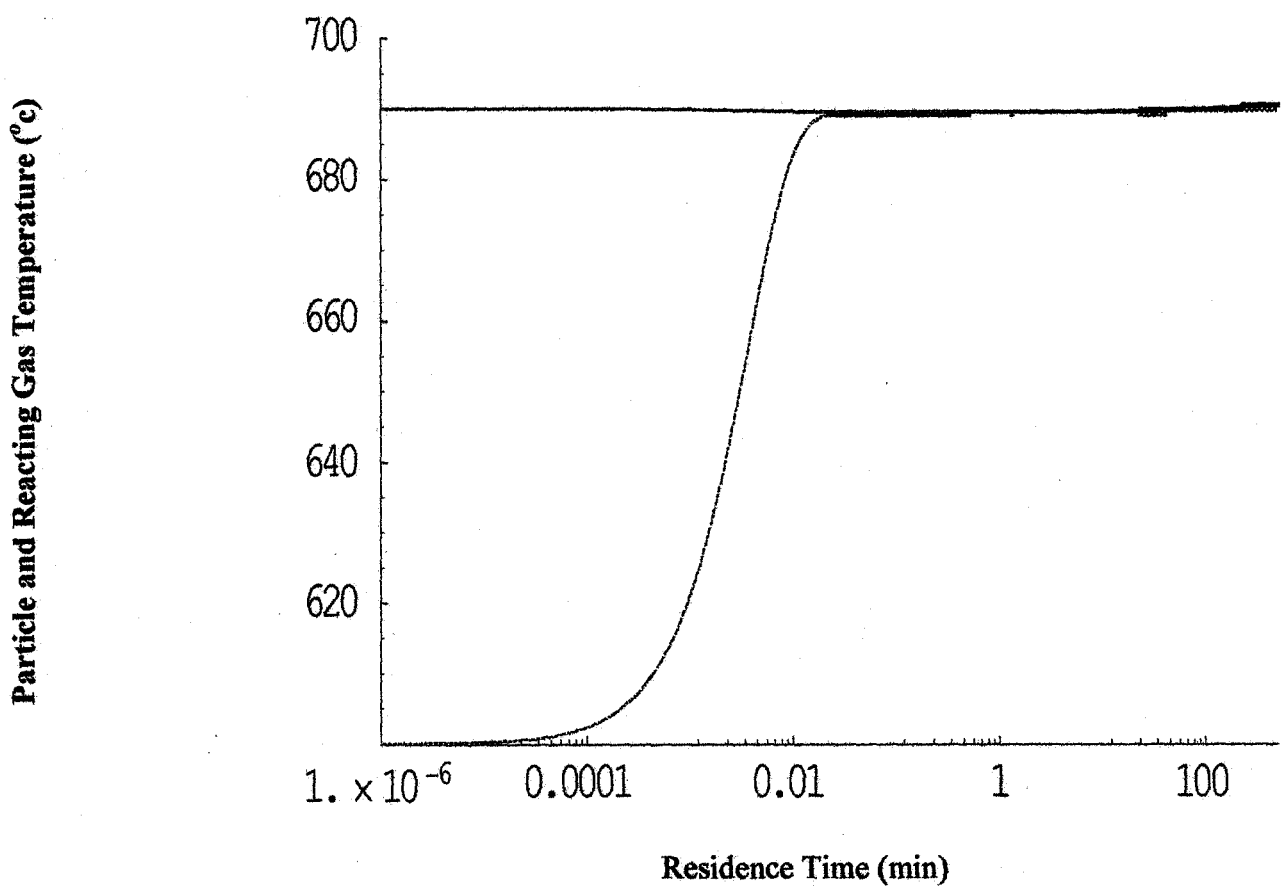
Figure 4.2 The Plot of Catalytic Particle and Reacting gas against Time

Table 4.1: Simulated Fluid and Particle Temperature against Time

Time (min)	Tf(^{o}C)	Tp(^{o}C)
0	600	690
1	689.411	689.562
5	689.425	689.577
10	689.452	689.605
21	689.513	689.666
32	689.563	689.716
42	689.609	689.763
52	689.653	689.807

Table 4.2 Experimental Fluid and Particle temperature against time

Time (min)	Tf(^{o}C)	Tp(^{o}C)
0	600	690
1	699.4975	686.4393
5	699.5122	687.4541
10	699.5393	687.4815
21	699.6002	687.5429
32	699.65	687.5933
42	699.6964	687.6401
52	699.7401	687.6842

Table 4.3: Coefficient of Determination between Experimental and Simulated

Results

	Value

MATHEMATICAL MODELING AND DYNAMIC SIMULATION

OF CATALYTIC FLUIDIZED BED REACTOR

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MINNA,

A PROJECT SUBMITTED IN PARTIAL FULFILLMENT OF THE

REQUIREMENTS FOR THE AWARD OF BACHELOR OF ENGINEERING

(B.ENG) IN CHEMICAL ENGINEERING, IN THE SCHOOL OF

ENGINEERING AND ENGINEERING TECHNOLOGY,

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from 600 to 605°C within the residence time of 0.0001 min. the catalytic particle temperature increased sharply from 605°C to 690°C within the residence time of 0.0001 - 0.01 min where it reached a stable temperature of 690°C for the next 100 mins.

Table 4.1 shows the result of the simulated result for the fluid and catalytic partcle temperature.

Table 4.2 shows the results of the experimental result for the fluid and particle temperature.

Table 4.3 shows the statistical precision analysis of the comparison of the simulated result to the experimental results for both the fluid and catalytic particle temperatures. The correlation coefficient (coefficient of determination) value obtained for comparison between the simulated and experimental fluid temperature was 0.9999. This shows that there is a remarkable agreement between the two results. The correlation coefficient (coefficient of determination) value obtained for comparison between the simulated and experimental results for catalytic particle temperature was 0.889. This shows that there is a remarkable agreement between the two results.

Table 4.4 shows the statistical precision analysis of the model equation results. The R-Square (coefficient of determination) value obtained was 99.69%, which is high suggesting that the relationship between the predictor and response variables is linear. The R-Square value of 99.69% implies that only 99.69% of the variability in the output could be captured and explained by this model. The adjusted R-Square (adjusted coefficient of determination) value obtained was 99.69%, which is high suggesting that the relationship between the predictor and response variables is linear. The adjusted R-Square value of 99.69% implies that only 99.69% of the variability in the output could be captured and explained by the model equation results. Table 4.1 shows that variation in the closeness of the results of the model equation to that of experiment is 0.0082952. The low value of the variance shows that there is closeness between the two results and the model equations developed is accurate.

there is closeness between the two results and the model equations developed is accurate.

CHAPTER FIVE

5.0   CONCLUSSION AND RECOMMENDATION

5.1   CONCLUSSION

From the simulation result obtained, it was observed that there is a remarkable agreement between the experimental result and the simulation result of the model equation developed for catalytic cracking of butane to butadiene.

The simulation results show that fluidization is achieved between the catalytic particle and the reacting gas.

5.2   RECOMMENDATION

Based on the analysis carried out the followings have been recommended:

1.   The model should be simulated using other software packages.

2.   The effect of other design parameters on fluidization can also be investigated

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APPENDIX

Table A.1: The Catalytic particle and reacting gas partial pressures and temperatures

against time using Matlab

Time (min)	P (atm)	T(°C)	Pp(atm)	Tp(°C)
0	0.1	600	0	690
0	0.0999	600.0428	0.0003	689.9998
0	0.0999	600.0856	0.0007	689.9996
0	0.0998	600.1284	0.001	689.9994
0	0.0995	600.379	0.0029	689.9982
0	0.0992	600.629	0.0047	689.997
0	0.0989	600.8783	0.0065	689.9958
0	0.0986	601.1268	0.0083	689.9946
0.0001	0.0976	601.9915	0.0142	689.9904
0.0001	0.0966	602.8478	0.0197	689.9863
0.0002	0.0958	603.6957	0.0247	689.9822
0.0002	0.095	604.5352	0.0293	689.9781
0.0003	0.093	606.8665	0.0406	689.9669
0.0004	0.0915	609.1338	0.0496	689.9559
0.0005	0.0903	611.3388	0.0568	689.9453
0.0006	0.0893	613.4832	0.0626	689.935
0.0007	0.0885	615.5687	0.0672	689.9249
0.0009	0.0876	618.4566	0.0722	689.911
0.001	0.087	621.2315	0.0758	689.8976
0.0011	0.0866	623.8979	0.0784	689.8847
0.0013	0.0862	626.4601	0.0803	689.8724
0.0014	0.086	628.922	0.0817	689.8605
0.0017	0.0858	632.4732	0.0831	689.8433
0.0019	0.0856	635.8159	0.084	689.8272
0.0021	0.0855	638.9624	0.0845	689.812
0.0023	0.0855	641.9242	0.0849	689.7977
0.0026	0.0854	644.7122	0.0851	689.7843
0.0029	0.0854	649.1251	0.0852	689.763
0.0033	0.0854	653.1022	0.0853	689.7438
0.0037	0.0854	656.6869	0.0854	689.7264
0.0041	0.0854	659.9177	0.0854	689.7108
0.0045	0.0854	662.8297	0.0854	689.6968
0.0057	0.0854	670.5108	0.0854	689.6597
0.007	0.0854	675.9964	0.0854	689.6331
0.0082	0.0855	679.8868	0.0854	689.6143
0.0094	0.0855	682.6448	0.0854	689.601
0.0118	0.0855	685.7645	0.0855	689.5858
0.0141	0.0855	687.4003	0.0855	689.5779
0.0165	0.0855	688.3212	0.0855	689.5734

0.0188	0.0855	688.8452	0.0855	689.5709
0.0212	0.0856	689.1256	0.0855	689.5695
0.0266	0.0856	689.4084	0.0856	689.5681
0.032	0.0856	689.4333	0.0856	689.5679
0.0375	0.0857	689.4168	0.0857	689.5679
0.0429	0.0857	689.4108	0.0857	689.5679
0.0971	0.0861	689.4144	0.0861	689.5672
0.1514	0.0865	689.4149	0.0864	689.5667
0.2056	0.0868	689.4144	0.0868	689.5662
0.5594	0.0887	689.412	0.0887	689.5637
0.9132	0.0901	689.4105	0.0901	689.5623
1.267	0.0911	689.4101	0.0911	689.5618
1.6208	0.0919	689.4103	0.0919	689.562
2.276	0.0927	689.412	0.0927	689.5638
2.9313	0.0932	689.4147	0.0931	689.5666
3.5865	0.0934	689.4181	0.0934	689.5699
4.2418	0.0936	689.4216	0.0936	689.5735
4.897	0.0937	689.4252	0.0936	689.5771
6.115	0.0937	689.432	0.0937	689.5839
7.333	0.0937	689.4387	0.0937	689.5908
8.5509	0.0937	689.4456	0.0937	689.5977
9.7689	0.0937	689.4523	0.0937	689.6045
10.9869	0.0937	689.459	0.0937	689.6112
21.3396	0.0937	689.5132	0.0937	689.6659
31.6924	0.0937	689.563	0.0937	689.7163
42.0451	0.0937	689.6094	0.0937	689.7631
52.3979	0.0937	689.6531	0.0937	689.8072
127.3979	0.0937	689.8754	0.0936	690.0317
202.3979	0.0936	690.0189	0.0936	690.1766
277.3979	0.0936	690.1121	0.0936	690.2707
352.3979	0.0936	690.1727	0.0936	690.3319
427.3979	0.0936	690.2122	0.0936	690.3717
502.3979	0.0936	690.2378	0.0936	690.3976
577.3979	0.0936	690.2545	0.0936	690.4145
652.3979	0.0936	690.2653	0.0936	690.4254
727.3979	0.0936	690.2724	0.0936	690.4325
750	0.0936	690.2741	0.0936	690.4343

Table 4.3: Coefficient of Determination between Experimental and Simulated Results

Correlation Coefficient	Value
Fluid Temperature	0.99999996
Particle Temperature	0.88995358

Table 4.4: Statistical Precision Analysis of the model Eqation simulation Results to the experimental Results.

Statistical Precision Coefficients	Values
R^2	0.9968905
R^2adj	0.9964665
Rmsd	0.0164305
Variance	0.0082952

4.2   DISCUSSION OF RESULTS

Matlab has been used for simulating the model equation developed for fluidization of catalytic cracking of butane. And the results of the simulation was compared to that obtained from experiment.

Matlab has been chosen over the traditional approach of writing program in Fortran, Pascal and others because the algorithm of Matlab is based on mathematics compared to the traditional programming languages that are abstract.

Figure 4.1 shows the plot of the particle and reacting gas partial pressure against time. At time of 0.008 min, the reacting gas partial pressure and the particle partial pressure attained same fluidized pressure of 0.08 atm. The particle and reacting gas pressure were fluctuating between the residence time of 0.008 - 10 min. the partial pressure of the particle and reacting gas remain const ant at 0.09 atm within the residence time of 10 – 100 mins.

Figure 4.2 shows the plot of catalytic particle and reacting gas temperature against residence time. The catalytic particle has a fluctuating temperature while the reacting gas has a constant temperature. The catalytic particle temperature increased

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