SIMULATIONS OF CATALYTIC OZONE DECOMPOSITION REACTION IN FLUIDIZED BED

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DEDICATION

To my Father and Mother, my Dear Wife and Son, whose prayers

always afforded me the power to accomplish this work.

And my supportive lecturer, Assoc. Prof Dr Kahar bin Osman for his guidance

through the whole process for this project.

To all I dedicate this work with great respect and love

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All praise to Allah SWT, the Most gracious and Most Merciful, Who has created the mankind with knowledge, wisdom and power. Being the best creation of Allah, one still has to depend on other for many aspects directly and indirectly. This is, however, not and exception that during the course of study the author received so much help, cooperation and encouragement that need to duly acknowledgement.

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ABSTRACT

The accuracy in predicting the ozone decompositions is influenced by correctly predicting the solid particle hydrodynamics. In this study, computational fluid dynamics modelling of catalytic ozone decomposition reactions is used to study the performance of a fluidized bed reactor that uses sand silica particles as catalyst. The Eularian-Eularian method with kinetic theory of granular flow in two-dimensional is used to solve the gas-solids flow in the fluidized bed reactor. Turbulence model is applied in two phase's reaction while considering the effect of the specularity coefficient and particle wall restitution coefficient wall to predict the hydrodynamic of solid particle distribution inside the chamber. The numerical results under different operating conditions are compared with the similar studies for the solids volume fraction, solids velocity and ozone concentrations in the radial and axial directions to validate the generality of the proposed CFD model. In conclusion, the ozone concentration decreases with the decrease in the superficial gas velocity and vice versa while the particle size also plays a major role on the reaction contributed by the contact surface area between two phases

ABSTRAK

Di dalam menentukan ketepatan penguraian ozon, pemahaman mendalam terhadap kesan hidrodinamik partikel halus amatlah diperlukan. Di dalam kajian ini, satu model dinamik bendalir berkomputer direka bagi memodelkan tindakbalas penguraian ozon dalam mengkaji pencapaian reaktor *fluidize bed* terhadap kesan kelajuan udara yang disuntik dan diameter partikel halus tersebut. Kaedah *Eulerian-Eulerian* digunakan bersama-sama dengan teori aliran serbuk pepejal dalam menyelesaikan permasalahan aliran gas dan pepejal secara 2 dimensi. Model *turbulence* dikenakan dalam menyelesaikan tindakbalas dua fasa di sambil mengambil kira kesan pekali *specularity* dan pekali perendam dinding partikel dalam menduga pergerakan serbuk pepejal di dalam camber. Keputusan pengiraan berdasarkan parameter yang berbeza dibandingkan dengan kajian serupa oleh penulis lain untuk membuktikan model yang dibentuk tepat. Secara kesimpulannya, penguraian ozon berkurang dengan pengurangan halaju udara yang disuntik dan saiz partikel yang besar.

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A_p	particle surface area per unit volume, m
C_{O3}	ozone concentration, ppm
C_μ	turbulence constant, dimensionless
$C_{1\varepsilon}$	turbulence constant, dimensionless
$C_{2\varepsilon}$	turbulence constant, dimensionless
$C_{3\varepsilon}$	turbulence constant, dimensionless
D	mess diffusion coefficient, dimensionless
d	diameter, m
e	restitution coefficient, dimensionless
G_s	solids circulation rate, $kg/m^2 \cdot s^{-1}$
g	gravity, m/s^2
$g_{s,0}$	radial distribution function, dimensionless
I	unit matrix, dimensionless
K	interphase exchange coefficient, $kg/m^3 \cdot s^{-1}$
K	turbulence kinetic energy, m^2/s^2
k_r	reaction rate constant, s^{-1}
$k_{\theta s}$	diffusion coefficient of energy, $kg/m \cdot s^{-1}$
p	pressure, Pa
q	Collision energy, kg/s^{-3}
R	radius of the riser, m
r	radial coordinate, m
Re	Reynolds number, dimensionless
Sct	turbulent Schmidt number, dimensionless
t	time, s
v	velocity, m/s
x	axial coordinate, m
Y	species concentration, dimensionless

Greek symbols

α	volume fraction, dimensionless
γ	collision dissipation of energy, $kg/m\cdot s^{-3}$
ε	turbulence dissipation rate, m^2/s^3
θ	granular temperature, m^2/s^2
λ	bulk viscosity, $kg/m\cdot s^{-1}$
μ	viscosity, $kg/m\cdot s^{-1}$
ρ	density, kg/m^3
τ	stress tensor, Pa
Φ	energy exchange coefficient, $kg/m\cdot s\text{-}^{3}$
φ	specularity coefficient, dimensionless

Subscripts

g	gas phase
s	solids phase
m	molecular
t	turbulence
w	wall

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CHAPTER 1

INTRODUCTION

1.1. Introduction

Fluidized bed is a reactor built on the fluidization phenomenon between solid and gas particles, which can be applied to a range of multiphase chemical reactions. In a gas-solids fluidized bed, gas is injected through granular solid particles at an adequate velocity to fluidize the particles to make it flow as a fluid. Depending on the velocity, the solid particle will perform phenomenon such as bubbling fluidization, slugging fluidization, turbulent fluidization, circulating fluidization and dilute phase conveying regimes. A fluidization operated under sufficient gas velocity in the bubbling flow regime is a BFB, which is the subject of the study here.

To comprehend the characteristics of gas-solids reaction in fluidized bed reactor, catalytic ozone decomposition reaction is often applied as a model reaction. Bolland and Nicolai (2007), Snider and Banarjee (2009), Li et al (2013) have done extensively study on ozone decomposition in recent years. During the fluidization, the ozone decomposition process into diatomic oxygen involves very low concentration of the ozone so that the ozone temperature and density variations produced by the reaction in the reactor can be neglected. In addition, ozone decomposition reaction has a certainly measurable first-order reaction rate at ambient temperature. Furthermore, ozone detection technology is effective using equally simple methods (Syamlal and O'Brien, 2003). Hence, the advantages make ozone decomposition widely used for the characterization of gas-solids contacting in fluidized bed reactors.

Although experiments are generally considered as more accurate, most experiments are expensive and difficult to measure the fluidization process with details. Thus, CFD is considered relatively economical method compared to actual experiments in fluidized bed application. CFD is a subtopic of fluid mechanics that uses algorithms and numerical methods for fluid flow analysis. High performance computers are the tool to execute the calculations required in the numerical methods. With the high pace of technology development of computers, certain characteristic like turbulence can be easily obtained using CFD methods. Furthermore, CFD tools provide additional comprehensive data profile without disturbing the flow via internal probes (Ranade, 2002). Significantly, CFD only required less time compared with experimental methods.

1.2. Research Background

Because of an extensive use of fluidized bed reactors, their modelling is of interest to describe the complex hydrodynamic behaviour and to ensure the design and scale up of a new efficient reactor. Fluidized bed reactors have been widely used in both catalytic and non-catalytic gas–solid reactions. The ozone decomposition reaction was chosen by many researchers to study the chemical reactor behaviour of fluidized bed due to the modest of this study to predict hydrodynamic characteristic of fluidized bed reactor. Quyang and Potter, (1993) and Schoenfelder et al. (1996) are examples who have conducted experiment on ozone decomposition to study hydrodynamic characteristic of fluidized bed.

This study on fluidized bed reactor is based on pilot scale of bubbling fluidized bed gasifier (BFBG) at TNB Research Sdn Bhd. All setup and parameters used in this study basically based on the pilot scale reactor, as figure 1.1. However certain issues and problem related to hydrodynamic characteristic still arises in that reactor. Hence, failure to identify the efficient design and optimization of fluidized bed reactor was due to the lack of knowledge about the flow behaviour of fluidization.

Therefore, the aim of this work was to develop hydrodynamics model to describe the behaviour of fluidized bed reactor with ozone decomposition reaction by using the Eulerain-Eulerian method and kinetic theory of granular flow, emphasizing on effect of particle size and superficial velocity.

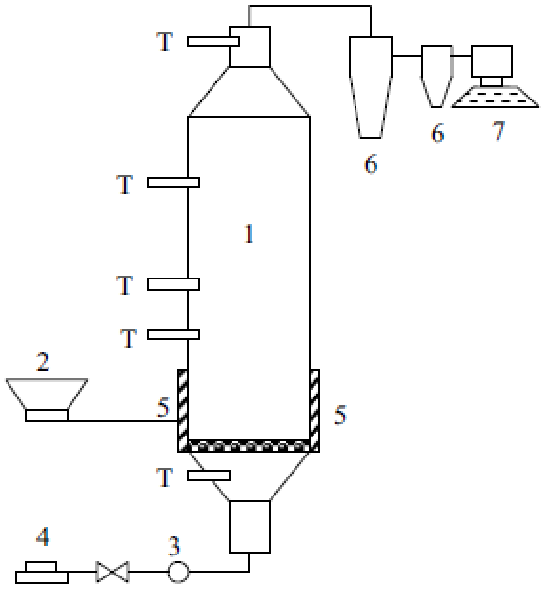

Figure 1. A schematic diagram of the experimental system consists of seven main parts: (1) fluidized bed gasifier, (2) screw-feeder, (3) steam generator, (4) air-blower, (5) electric heaters, (6) cyclones (7) gas analysis and (T) thermocouples.

Figure 1.1: Schematic Diagram of laboratory scale of Fluidized Bed Gasifier at TNBR Research Sdn. Bhd.

1.3. Research Objective

The objective of this study is to develop a CFD model for catalytic ozone decomposition in a fluidized bed reactor using the Eulerain-Eulerian method and kinetic theory of granular flow emphasizing on effect of particle size and superficial velocity.

1.4. Problem Statement

Very few works have been reported in the literature on the combination between detailed hydrodynamic modelling and chemical reactions in fluidized bed systems. Because of a wide use of fluidized bed reactors, their modelling is of interest to describe the complex hydrodynamic behaviour and to ensure the design and scale up of a new efficient reactor plus verification of reactor models.

In the search to find the best operating parameter for simulation of solid-gas interaction, various experimental need to be done. Due to cost constraint, CFD is the practical way in predicting the hydrodynamic behaviour of fluidized bed reactor with ozone decomposition reaction by using the Eulerain-Eulerian method and kinetic theory of granular flow emphasizing on effect of particle size and superficial velocity. Any modification on the reactor dimension, varying the feed rate of superficial velocity and bed particle size can be done without jeopardizes the pilot scale reactor.

1.5. Research Hypothesis

To improve the performance of fluidized bed reactors, the operating parameters, such as particle size and superficial velocity plays a major role in affecting the characteristic of the fluidized bed reactor. From previous study by Kong (2012), these variables did influence fluidized bed performance. Lower size of solid particles will increase the decomposition of ozone while lower velocity will decrease the ozone decomposition. Hence further study on effect of solid particle size and superficial velocity towards the performance of fluidized bed by considering all variables used by other authors are necessary.

1.6. Scope of Research

The scope of this project is

i. To develop a CFD simulation using Fluent to demonstrate the effect of different size of bed particles.
ii. To develop a CFD simulation using Fluent to demonstrate the effect of different size of superficial velocity.
iii. To develop a CFD simulation using Eulerian-Eulerian method and kinetic theory of granular flow.

1.7. Theoretical Framework

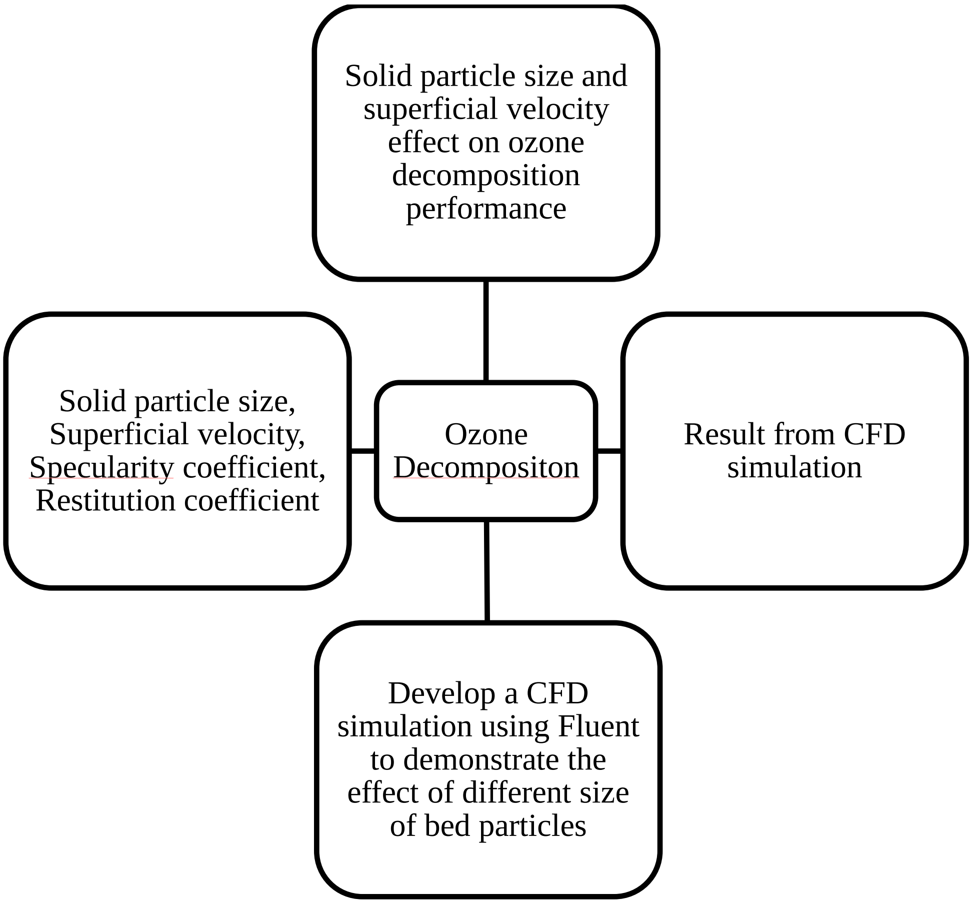

Figure 1: Mind mapping of theoretical of Framework

1.8. Organization of Proposal

This proposal consists of 6 chapters starting with chapter one which explains the background of the study follows by chapter two which discusses on the relevant literature reviews.

The most significant chapter will be chapter three that details on the research methodology to be exercised. Chapter four presents the results obtained from the simulations done and further discussion on the results.

Chapter 5 is dedicated for conclusion of the study and recommendations on future improvements for this study. This proposal will have the reference list post chapter 5 prior to appendixes

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