UNIVERSITI PUTRA MALAYSIA

PREDICTION OF ONSET FLUIDIZATION USING CRITICAL RAYLEIGH NUMBER

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To Dad and Mom

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The incipient instability in gas fluidized bed has not been fully understood despite extensive studies were conducted. A new transient theory was proposed by adopting the principles advanced by Tan and Thorpe (1992 and 1996) and Tan *et al.* (2003), and this was verified by computational fluid dynamic (CFD) simulations. The theory of instability in porous media has two functions. One involved the molecular diffusion of a microscopic mass flux in the gas phase with potential adverse density gradient, buoyancy convection in gas will occur, but the solid particles will stationary. If the solid particles were subjected to very high mass fluxes which is characterized by its high gas velocity such as those exceeding the minimum velocity of fluidization, then the buoyancy force of the particles will be overcome and the solids will be moved and fluidized almost instantaneously.

2D time dependent simulations were conducted using a CFD package - FLUENT for gas diffusion in porous media to observe buoyancy convection and also the incipient instability in fluidized bed, using various gas pairs, mass fluxes and particles sizes. The simulation conducted was validated and verified by comparison with the experimental data from literature. As a prelude to these studies, transient convection induced by gas diffusion in another gas was conducted, so as to understand fully the instability induced by mass diffusion. The simulated critical Rayleigh number were found to be 531 and 707 for top-down and bottom-up gas-gas diffusion respectively, which were very close to the theoretical value of 669 and 817. For transient buoyancy instability induced by gas diffusion in porous media, the average simulated critical Rayleigh number was found to be 26.7, which agreed very well with the theoretical value of 27.1. The simulated onset time of buoyancy convection were also found to be in good agreement with the predicted value. Incipient instability in fluidized bed is caused by fluid velocity higher than the minimum fluidization velocity, U_{mf}. The simulations of incipient instability showed that the bed behavior was dependent on the fluid velocity and the particle size and porosity. The incipient instability was preceded by the gas or pressure saturation of the interstices, induced a high momentum force due to the high mass flux which mobilized and lifted the particles once the critical Rayleigh number was exceeded. The simulated critical Rayleigh number was found to be 30.4, which agreed with the theoretical value of 27.1 for buoyancy instability in porous media. The simulated critical times of the incipient instability in fluidized bed were in good agreement with the predicted values and reported experiments in literature. The bed pressure drop, expansion ratio and void fraction after the fluidization were successfully simulated and were found to be in good agreement with experiments and theoretical values.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai keperluan ijazah Master Sains

THEORI DAN SIMULASI UNTUK KETAKSTABILAN INCIPIEN TURUS TERBENDALIR GAS-PEPEJAL

Oleh

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Ketakstabilan incipien dalam turus terbendalir gas masih belum difahami sepenuhnya walaupun banyak pengajian telah dijalankan. Satu theori transient baru dicadangkan dengan merujuk kepada dasar-dasar yang dimajukan oleh Tan dan Thorpe (1992 dan 1996) dan Tan *et al.* (2003), dan ini telah pun dikenal-pasti dengan simulasi komputasi bendalir dinamik (CFD). Theori ketakstabilan dalam poros media ini ada dua fungsi. Satu melibatkan resapan molekular yang disebabkan oleh flux jisim mikroskopik dalam fasa gas dengan kecerunan ketumpatan lawanan potensi, perolakan pengapungan akan berlaku dalam gas, tetapi butiran pepejal tetap tidak bergerak. Jikalau butiran pepajal itu dikenalkan kepada flux jisim yang sangat tinggi yang disifatkan oleh kelajuan gasnya yang tinggi seperti yang mana melebihi kelajuan pengbendaliran minimum, maka kuasa pengapungan butiran itu akan diatasi dan pepejal pun digerakkan dan dibendalirkan pada masa yang sangat singkat.

Simulasi 2D ketakmantapan telah dilakukan dengan menggunakan CFD- FLUENT untuk resapan gas dalam poros media untuk memperhatikan perolakan pengapungan dan juga untuk ketakstabilan insipien dalam turus terbendalir gas, dengan menggunakan bermacam-macam pasangan gas, flux jisim dan siaz butiran pepejal. Sebagai permulaan untuk pengajian ini, perolakan transien yang disebabkan oleh diffusi gas ke dalam gas lain telah dikaji, untuk memahami ketakstabilan yang disebabkan oleh diffusi gas dengan lebih jelas. Nombor Rayleigh kritikal daripada simulasi didapati bernilai 531 dan 707 masing-masing untuk bawah-keatas dan atas-kebawah resapan gas-gas, dimana ia adalah sangat dekat dengan nilai theori 669 dan 817 masing-masing. Untuk ketakstabilan pengapungan transien yang disebabkan oleh diffusi gas dalam poros media, purata nombor Rayleigh kritikal yang disimulasikan bernilai 26.7, dimana ia bersetuju dengan nilai theori 27.1. Masa permulaan perolakan pengapungan juga didapati bersetuju dengan nilai theori. Ketakstabilan incipien dalam turus terbendalir gas disebabkan oleh kelajuan bendalir yang lebih tinggi daripada kelajuan terbendalir minima, U_{mf}. Simulasi ketakstabilan insipien menunjukkan bahawa sifat turus itu adalah bergantung dengan kelajuan bendalir dan siaz butiran dan keruangan. Ketakstabilan insipien ini didahului oleh pengepuan ruang-ruang kosong dalam bed oleh gas, menyediakan satu kuasa momentum tinggi disebabkan oleh flux jisim besar dimana butiran pepejal itu akan digerakkan apabila nombor Rayleigh kritikal telah dilebihi. Nombor Rayleigh kritikal didapati bernilai 30.4, dimana bersetuju dengan nilai theori 27.1 dalam ketakstabian pengapungan dalam poros media. Masa simulasi kritikal untuk permulaan ketakstabilan adalah persetuju dengan nilai ramalan dan yang dilaporkan dalam gajian lain.

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Thank you!!

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NOMENCLATURE

$\tilde{a}_c$	dimensionless critical wavenumber
B_i	Biot number
c	concentration, kg/m^3
c_s	surface concentration, kg/m^3
C_D	drag function
d_s	diameter of the solid particle, m
D	diffusion coefficient, m^2/s
D_{eff}	effective diffusion coefficient, m^2/s
E	total energy, J
$\vec{F}_q$	external body force, N
$\vec{F}_{lift,q}$	lift force, N
$\vec{F}_{v,mq}$	virtual mass force, N
g	gravity acceleration, m/s^2
h	Height, m
h	heat transfer coefficient, $W/m^2.K$
j^o	constant mass flux, $kg/m^2.s$
k_{eff}	effective conductivity, W/m.K
K_e	Permeability, m^2
H_o	Initial bed height, m
H_{mf}	Height of the bed at minimum fluidization, m
H_f	Height of the fluidized bed, m
$\dot{m}_{pq}$	mass transfer from phase p^{th} to q^{th}, kg/s
p	pressure, Pa
$\vec{R}_{pq}$	interaction force between phases, N
Ra_c	Critical Rayleigh number
Re	Reynolds number
R_i	net rate of production of species i, kg/s
S_i	rate of creation of species i, kg/s
S_h	heat of chemical reaction, J
t	time, sec

t_c	critical time, sec
Δt	time step
U	velocity, m/s
U_{mf}	minimum fluidization velocity, m/s
z	diffusion depth, m
z_{max}	critical diffusion depth, m

Greek symbols

μ	Viscosity, Pa.s
ε	void fraction
ε_{mf}	void fraction of the fluidized bed at minimum fluidization
λ	wavelength, m
τ	tortuosity
ρ_s	density of the solid particle, kg/m^3
ρ_g	density of the gas, kg/m^3
$\vec{v}_q$	velocity of phase q, m/s
$\bar{\bar{\tau}}_q$	q^{th} phase stress-strain, Pa
τ_s	particulate relaxation time, sec
k_{sl}	exchange coefficient
$v_{r,s}$	terminal velocity correlation for the solid particle

CHAPTER 1

INTRODUCTION

Fluidized bed is one of the most common encounter operation units in chemical industry. Fluidized bed has been widely used in the process industries such as protein purification process, submerged oxidation, anaerobic wastewater treatment systems, hydro-carbon cracking and re-forming (Chase, 1994, Perry, 1997) to enhance the mass and heat transfer.

The instability of the gas-solid fluidized bed is a very complex mechanism. This is owing to the heterogeneous structure of the bed and the existence of the rising bubbles within the column. The occurrence of fluidization is dependent on the flow velocity, which must be in excess of the buoyancy force of the particles. This minimum fluidization velocity can only estimated roughly from experiments, which Grace (2000) show that the design of the fluidized bed is quite empirical. Many studies have been devoted to understand the instability of the gas fluidized bed. Theoretical frameworks to characterize the instability of the bed also had been proposed such as by Jackson (1963), Jackson and Anderson (1969) and Batchelor (1988), which were recently reviewed by Sundaseran (2003). Unfortunately, until now the origin of the instability is not well understood. This suggested that this instability of the fluidized bed shall be restudy from other new approach, such as the perturbation theory by Lord Rayleigh which is also looking into the instability of a system.

Buoyancy convection induced by heat or mass diffusion is a simple instability phenomenon owing to its nature physic. The onset of buoyancy convection is driven by the adverse density gradient (Rayleigh 1916). Lapwood (1948) examined the onset of convective instability in a homogenous porous media by conducting linear stability analysis (LSA). Lapwood (1948) provided a criteria, Rayleigh number to predict the onset time for the onset of convective instability in porous media. If a microscopic mass flux is subjected and hence induced a molecular diffusion to the porous media with potential adverse density gradient, buoyancy convection in the fluid phase will occur but the solid remain stationary. On the other hand if high mass fluxes with high fluid velocity is subjected to the porous media and overcome the buoyancy force of the solid particles, the particles will be mobilized almost instantaneously, which exactly what happen during the onset of fluidization. Due to the different driving force in the onset of fluidization compared with convective instability, hence the instability study by Lapwood is modified accordingly to be applicable in the onset of fluidization. This was done by incorporating U_{mf} function into the Lapwood (948) instability study. There has been a strong current in the instability studies induced by mass diffusion, but breakthrough was only achieved recently by Tan and Thorpe (1992, 1996) and Tan *et al.* (2003).

The research problem is to study the onset of incipient instability in fluidized bed by adopting the transient instability theory, which is a new approach in the study of fluidized bed instability. As discussed above, the onset of instability in porous media under high mass flux showed the same behavior of the incipient instability in fluidized bed. Hence, it is believed that the incipient instability in fluidized bed can be described by the transient instability theory concept to certain extends.

The objectives of this study are:

1. To develop and propose a theory to determine the onset of incipient instability in fluidized bed.
2. Verification of the theory by comparison with the literature experimental data.
3. Conduct simulation and verify the simulated result against literature experimental data for further discussion.

In order to achieve above objectives, the scope in this study were identified as follow:

1. The instability analysis in porous media conducted by Lapwood (1948) will be explored and exploited to investigate and predict the onset of the incipient instability in gas fluidized bed.
2. Transient instability in gas system induced by other gas diffusion will be studied as well, as the prelude to the porous media geometry and for better understanding of the transient instability induced by transient mass diffusion.
3. Verification of the transient instability theory for gas-solid fluidized bed by comparison of the prediction value with published experimental results.
4. 2D time dependent simulations will be conducted. The important parameters such as the onset time of instability, size of the convection plumes and bed pressure drop obtained in the simulations will be investigated.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

The mechanisms underlying the incipient fluidization are poorly understood, despite its importance in the various process industries. This is owing to the very complex particle-particle and particle-fluid interactions. Despite its difficulties, the instability of the fluidized bed has been studied extensively but its mechanisms remain to be explained. The occurrence of fluidization is dependent on the flow velocity, which must be in excess of the buoyancy force of the particles. There is no successful theory of fluidization for the prediction of the onset of instability. In this study, the incipient instability of fluidization is found to be related to mass diffusion in porous media.

Lapwood (1948) had conducted linear stability analysis (LSA) to study the thermal instability in porous medium induced by steady-state heat conduction, he assumed the porous media to be a homogenous fluid, which will move at the onset of instability. This is an analog for the buoyancy convection induced by transient mass diffusion in porous media, expect that the solid is impermeable to the gas. If a microscopic mass flux is used which induced molecular diffusion and adverse density gradient is encountered, buoyancy convection will happen in the porous media. If a very high mass flux which is characterized by its high velocity is subjected to the porous media, the particles may be mobilized and moved almost instantaneously, which is exactly observed in the gas fluidized bed. This suggested