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Evaluation of Various Estimation Equations for Particle-Fluid Interaction Forces and Modeling of Heat Transfer between Particles for DEM Simulations

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EVALUATION OF VARIOUS ESTIMATION EQUATIONS FOR PARTICLE-FLUID INTERACTION FORCES AND MODELING OF HEAT TRANSFER BETWEEN PARTICLES FOR DEM SIMULATIONS

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論 文 内 容 の 要 旨

申請者氏名 AZRI BIN ALIAS

論文題目 EVALUATION OF VARIOUS ESTIMATION EQUATIONS FOR PARTICLE-FLUID INTERACTION FORCES AND MODELING OF HEAT TRANSFER BETWEEN PARTICLES FOR DEM SIMULATIONS

The gas-solid two-phase flow takes a very important role in various industries such as medicine manufacturing, food processing, and combustion or gasification of coal. Although these wide applications of the gas-solid two-phase flow have led to extensive researches, this phenomenon is very complicated and difficult to implement an experimental investigation of the flow characteristics. On the other hand, not only the abilities of computers, but also the numerical algorithms to solve the phenomena coupled of fluid and particles have been developed. As a result, numerical approaches have been introduced to design the powder processing industries.

The numerical simulations methods for two-phase flow are basically divided into three kinds of methods, which are the Two-Fluid Model (TFM), the Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD) coupling model that is simply called as the DEM, and the Direct Numerical Simulation (DNS). In the TFM, both gas phase and solid phase are treated as a fluid and solved by Eulerian method. The number of particles is not limited and it is also possible to analyze larger reactor relatively, as TFM can be incorporated into a lot of commercial code. However, the particle adherence and the applicability to simulate various small scale phenomena in powder industry problem are difficult.

On the other hand, in the DEM-CFD coupling model. The original DEM concept based was derived by Cundall and Strack in the field of geo-mechanics. DEM was developed by Tsuji et al. by incorporating the CFD into the DEM. To distinguish the DEM from the original, they referred it as DEM + CFD model, but as write above, we will simply expressed it as DEM. In the DEM, the motion of each particle is solved with Lagrangian method, and the motion equation for all particles needs to be solved. Accordingly, the computational time of the DEM depends on the number of particles, and the computational load caused by the large number of particles sometimes brings serious problem. In these two methods, some constitution equations for particle-gas interaction forces are also required. In addition, these two methods also cannot directly determine the small scale phenomena occurred around the particles such as drag, lift forces, viscous torque and also lubrication force.

In such small scale phenomena in fluidized bed, it would be a necessary to use other method such as the DNS. The DNS method does not basically require any constitution equations for the particle-gas interaction forces. So far, various methods for the DNS have been derived, e.g. the finite element method (FEM), the boundary-fitted coordinates systems (BFC), the volume of fraction method (VOF), and the Immersed

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CHAPTER 1

INTRODUCTION

1.1 Research background

Fluidization is commonly defined as *"the operation by which the fine solids are transformed into a fluid-like state through contact with a gas or liquid"* [1]. This process occurs when a fluid whether a liquid or gas is passed up through the granular material. When a fluid flow is introduced from the bottom of a bed of solid particles, the fluid will move upwards through the bed via the empty spaces between the solid particles. At low fluid velocities, an aerodynamic drag on each particle is also low, and thus the bed remains in a fixed state. By this time, the static bed is called as a fixed fluidized bed. By increasing the velocity of the fluid flow, the aerodynamic drag forces will begin to counteract the gravitational forces, causing the bed to expand in volume as the particles move away from each other.

As further increasing in the fluid velocity, it will reach a critical value at which the upward drag forces will exactly equal to the downward gravitational forces, causing the particles to become suspended within the bed. At this critical value (minimum fluidization velocity), the bed is said to be fluidized and will exhibit fluidic behavior. By further increasing fluid velocity, the bulk density of the bed will continue to decrease, and its fluidization becomes more violent, until the particles no longer form a bed and conveyed upwards by the fluid flow.

When fluidization occured, a bed of solid particles will behave as a fluid, like a liquid or gas. The bed will conform to the volume of the chamber, its surface remaining perpendicular to gravity; objects with a lower density than the bed density will float on its surface, blobbing up and down if pushed downwards, while objects with a higher density sink to the bottom of the bed. These fluidic behavior allows the particles to be transported like a fluid, channeled through pipes and holes in machines. Thus, there is no need in requiring the mechanical transport (e.g. conveyer belt).

Fluidized beds are known for their high heat and mass transfer coefficients, due to the high surface area-to-volume ratio of fine particles. Fluidized beds are used in a wide variety of industrial processes such cracking and reforming of hydrocarbons, reaction, drying, mixing, granulation, gasification of coal, coating, heating and cooling as well as garbage burning process. An example of an industrial application of fluidized beds is circulating fluidized bed boiler type as shown in Figure 1.1 [2] and also the incinerator shown in Figure 1.2 [2].

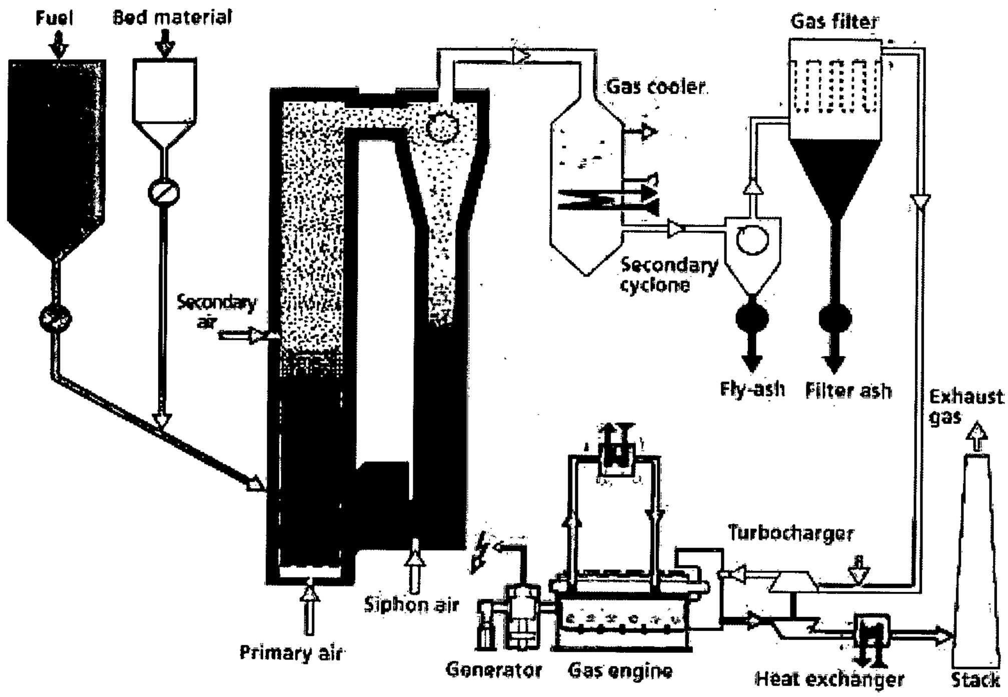

Figure 1.1: Example of circulating fluidized bed boiler type [2]

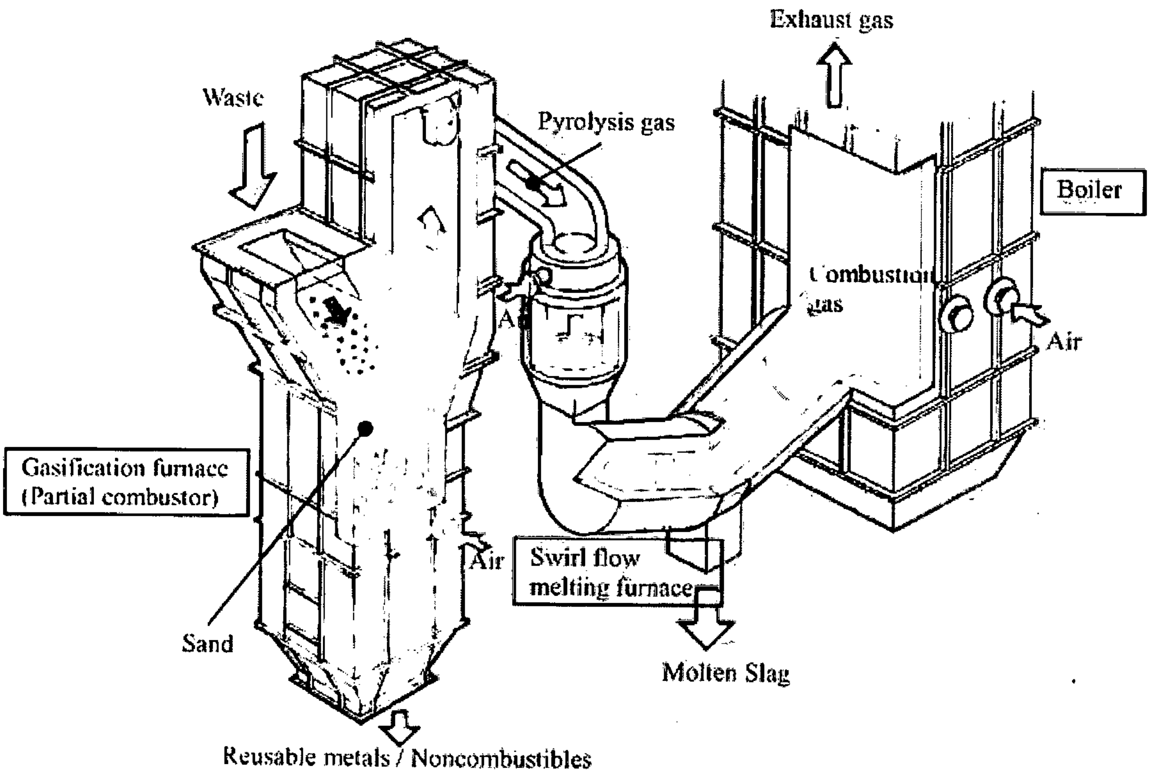

Figure 1.2: Example of the incinerator [2]

The phenomena in fluidization can be classified into a few group such as explained before. These group in fluidized bed can be called fixed bed, homogeneous fluidized bed, bubbling fluidized bed and also turbulant fluidized bed as shown in Figure 1.3.

Firstly, the explanation of fixed bed in fluidization. When a fluid of gas or liquid flow were injected from the bottom at a low rate of a bed made by solid particles, and the fluid were just pass through the void spaces of the bed without disturbing the movement of the bed it is called a fixed bed.

On the other hand, when pressure drop or the force acting on the solid particles, the fluid flowing through the bed equals or exceeds the weight of the particles bed, the fixed bed expended and the solids particle behave like a liquid behavior. This behaviour of the particles bed we called homogeneous fluidized bed. When the flow rates exceeds the minimum velocity of fluid, the solid particles bed expands and bubble seem to be appearing in the bed, it is called a bubbling fluidized bed.

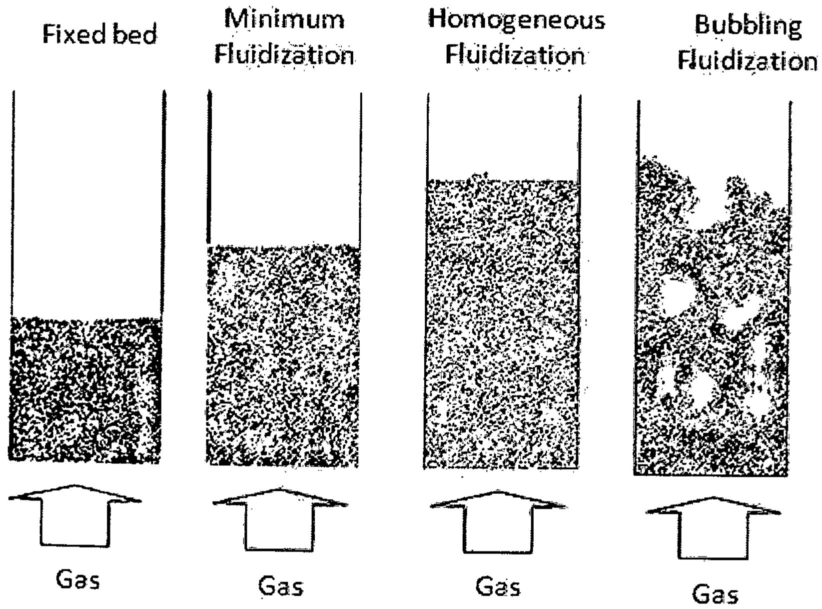

Figure 1.3: Classification of fluidized state with increased gas velocity

1.2 Application of fluidized bed in industrial

As we all know, there are a lot of applications of fluidization not only for the circulating fluidized bed (CFB) boiler and also incinerator but also in the gasoline refining as a catalyst and in the medicine manufacturing as granular and coating. The fluidized bed technology also was being applied mineral and metallurgical process.

Fluidized bed combustion (FBC) is the major application for the fluidization technology mainly used for power plants. Fluidized beds suspend solid fuels on upward-blowing jets of air during the combustion process. The result is a turbulent mixing of gas and solids. The tumbling action, much like a bubbling fluid, provides more effective chemical reactions and heat transfer. There is a rapid increase of FBC in combustors. The reasons are because of a lot of choice in respect of fuels in general, not only the possibility of using fuels which are difficult to burn using other technologies, is an important advantage of FBC. The second reason is which it has become increasingly important is because of the possibility of achieving, during combustion, a low emission of nitric oxides and the possibility of removing sulfur in a simple manner by using limestone as bed material. FBC were able to control pollutant emissions without external emission controls. The technology burns fuel at temperatures of 750-900°C well below the threshold where nitrogen oxides form at approximately 1400°C.

One of the new applicapable process is chemical looping combustion (CLC) [3] that are new application of fluidization technology which has not been yet commercialized. To reduce the potential effect of global warming, it is very important to sequestrate the carbon dioxide that was generated by fuel combustion such as in the power station. Gas nitrogen is mostly produce in regular combustion with air which prevents the economical sequestration. Chemical looping uses a metal oxide as a solid oxygen carrier. Metal oxide particles replace air to react with a solid, liquid or gaseous fuel in combustion, producing solid metal particles from the reduction of the metal oxides and a mixture of carbon dioxide and water vapor which is the major products of combustion reaction. The water vapor then was condensed, leaving pure carbon dioxide which can be sequestered.

As for the solid metal particles are circulated to another fluidized bed where they react with air, producing heat and regenerating metal oxide particles that are re-circulated to the fluidized bed combustor as shown in Figure 1.4 [4] below.

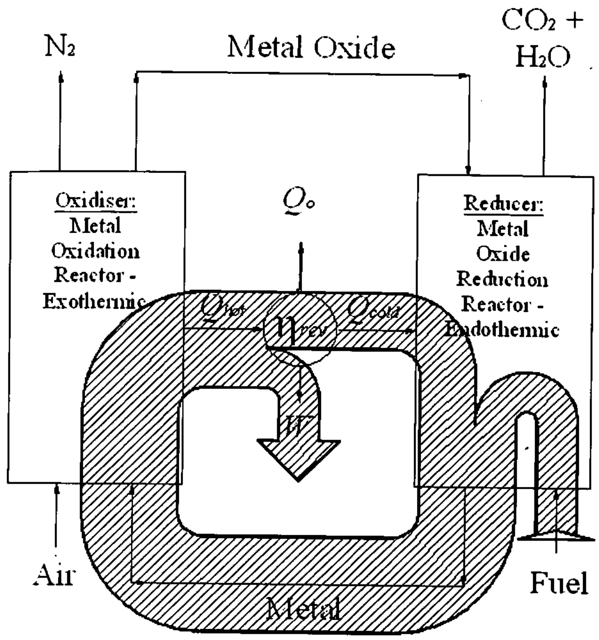

Figure 1.4: Sankey diagram of energy fluxes in a reversible CLC system [4]

1.3 Motivation and research purpose

1.3.1 Analysis on small scale phenomenon

As we all know, Discrete Element Method (DEM) is a very useful tool to analyze a fluidized bed for various powder processes also possible to incorporate problem–factors in the level of particle size. DEM is also used to investigate the hydrodynamic behavior of gas–solid interactions. However, in spite of the fact that DEM can be applied to problem pertaining to cohesion, heat transfer and chemical reaction, it is impossible to use DEM for dealing with phenomena whose scale is smaller than the particle size, such as the heat transfer between the colliding particles, the effect of drag, lubrication, and lift forces.

In DEM, there is for fluid and also particle motion equations. However, to make a more perfect simulation constitution, several equation are still needed. Some of the example are the equations for particle–fluid interaction force, such as drag, lift force and viscous torque. The heat transfer between the particles are also needed to incorporate with DEM.

In order to examine and clarify the small scale phenomena occured in fluidized bed, we had utilized and experiments and also using a direct numerical simulations, such as IBM in this study.

CHAPTER 2

INTRODUCTION OF DISCRETE ELEMENT METHOD (DEM)

2.1 Introduction

With the improvements in computer performance in recent years, numerical simulation has been utilized in many various fields. In these present years, personal computer that cost around 10-20 thousand yen also has reached a commercial software are also available at the level 3D single phase flow heat computational fluid dynamics (CFD). The information such as the trouble factors, new process development that can reduce the risk that and also potential that cannot be obtained from the experiments can be easily obtained using the numerical simulations has become indispensable in industrial tools. This situation for the fluidized bed field also has no exception. One of the numerical method for solid-gas two phase flow with mixed powder that is DEM, were also become a mainstream in fluidized bed simulations.

2.2 Discrete Element Method

2.2.1 DEM in various numerical analysis method for solid-gas two-phase flow

The type and various of numerical analysis method for solid-gas two-phase flow is shown in Table 2.1.

Two-Fluid Model (TFM) for powder is a Euler basic (which treats the same way as a fluid), the number of particles is not limited and it is possible to analyze larger reactor relatively, this can be incorporated into a lot of commercial code. However, it is shown as "'low"' in table 2.1, because in powder industry problem, the particles adherence and the

Table 2.1: Numerical analysis method for solid-gas two-phase flow

	Fluid	Powder	Appicability	Computer load
Two-Fluid Model (TFM)	Euler	Euler	Low	Low
DSMC	Euler	Lagrange	Medium	Medium
DEM	Euler	Lagrange	Medium ∽ high	Medium ∽ high
DNS	Euler	Boundary	High	High

applicability to simulate various phenomena is difficult and also need to take into account.

In Direct Simulation Monte Carlo (DSMC), by representing one particle in the pack of particles, is a method that simulates stochastically collisions of the particles and it is effective for most systems that have a lot of particles. Tanaka *et al.* [5] have succeeded to simulate cluster formation in the riser of the circulating fluidized bed using this technique. It is an effective method for simulation of the circulating fluidized bed, however similar to TFM, the deposition of the particles is considered difficult.

The original DEM concept based was derived by Cundall and Strack [6] in the field of geo-mechanics. Discrete element method (Discrete Element Method, DEM) was developed by Tsuji *et al.* [7] by incorporating the Computer Fluid Dynamics (CFD) into the DEM. To distinguish the DEM from the original, they referred it as DEM + CFD model, but here we just assumed it to be simply expressed as DEM. In order to calculate the contact force of the particles (impact force), this approach has an advantage as the particles adhesion can be easily considered. However, there are also disadvantages in the DEM, such as the computation time is relatively long because of the need to reduce the time step of the calculation, and also the need to continue the calculation of the contact force with respect to all the contacting particles in the collision process.

However, due to advances in computer performance even a hundred thousand of particles can be calculated in 2D calculations, and it is also possible for a 3D calculation for a numbers of particles.It is believed that the benefits of DEM and the easiness of incorporating the reaction, heat transfer and particle adhesion, it seems researchers using DEM is also increased.

Finally, the Direct Numerical Simulation (DNS), is a method by providing computational mesh (grid) around the powder solved as boundary condition for the powder surface, and if necessary the calculation of the powder portion (for example, stress and also temperature field calculation). This technique predefined models to be used can be reduced and the accuracy of the information obtained the highest between the other methods, however, for this simulations the computer load is the greatest. For the present calculations, a need to limit the analysis region at a certion area, and it is used for the basic reserach. From the above points, numerical simulation of the fluidized bed, DEM is the mostly will be the mainstream for now.