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Treball Final de Grau

Fluid circulation in porous media (ANSYS®)

Simulació de la circulació de fluids en medi porós (ANSYS®)

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L’alegria de veure i entendre és el més perfecte do de la naturalesa.

Albert Einstein

Gràcies als meus tutors Alexandra i Joan per la seva ajuda en el seguiment d’aquest projecte i a tots els meus amics i família pel suport rebut.

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REPORT

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1. SUMMARY

A fluidized bed is defined as a process that consists of a bed of solid particles and a fluid flow to achieve a homogenous mixture between particles and fluid.

Actually, due to the increase of the computer's power, simulations based on microscopic balances are performed using with CFD (Computational Fluid Dynamics) software.

Therefore, with this tool, the behavior and the functioning of the simulated unit can be visualized and better understood. Consequently, in this project the simulation program ANSYS® is studied, considering the case study of a fluidized bed. It is going to analyze its behavior by the contours of volume fraction and its pressure drop. Eventually, the obtained results contribute to the understanding of how a fluidized bed works.

Keywords: fluidization, CFD, simulation

2. RESUM

Per visualitzar com es comporta un fluid en medi porós s'ha escollit una unitat molt útil en la indústria, llits fluïditzats. Aquets es defineixen com un procés en el qual tenim un llit de partícules sòlides i es fa passar un fluid per aconseguir una mescla homogènia entre les partícules i el fluid.

Actualment gràcies a la potència de càlcul dels ordinadors, es poden dur a terme simulacions mitjançant balanços microscòpics amb CFD (Computational Fluid Dynamics).

Per tant amb aquesta eina es podrà visualitzar el comportament i el funcionament de la unitat en qüestió.

En aquest projecte es durà a terme l'estudi de com funciona el programa de simulació ANSYS® mitjançant la simulació d'un llit fluïditzat. S'analitzarà el seu comportament extraient els perfils de fracció de volum del llit en qüestió i de la seva variació de pressió. A partir d'aquets resultats s'extrauran conclusions que ajudaran al lector a comprendre com funciona un llit fluïditzat.

Paraules clau: fluidització, CFD, simulació

3. INTRODUCTION

A fluidized bed is formed when a quantity of solid particles usually present in a holding vessel is placed under appropriate conditions to cause solid /fluid mixture to behave as a fluid. The resulting phenomenon is called fluidization. There are many uses of fluidized beds. A number of applications have become commercial successes; others are in the pilot-plant stage (Yu Che et al, 2015), and others in bench-scale stage (Depypere et al, 2004). Generally, the fluidized bed is used for gas-solids contacting.

Fluidized beds are found in many plant operations in chemical, pharmaceutical and mineral industries. Despite their widespread application, much of development and design of fluidized bed reactors has been empirical as the complex flow behavior of gas-solid flow in these systems makes flow modelling a challenging task.

Nowadays, there are numerous studies in literature related to the hydrodynamics of a two dimensional gas solid fluidized bed reactor using different methods of drag force and comparing together, (Taghipour et al,2005), (Deen et al, 2006). On the other hand, Depypere et al, (2004), have investigated the analysis of air distribution in fluidized equipment, because the features of a fluidized bed are highly dependent on the quality of fluidization resulting from the bubble characteristic of the fluidizing gas. Moreover, there are many uses of fluidized beds. Generally, are used for gas solid contacting and it has uses or special characteristics (Perry, 1999) such as:

I. Chemical reactions
    A. Catalytic
    B. Non-catalytic
        1. Homogeneous
        2. Heterogeneous

II. Physical contacting

A. Heat transfer

1. To and from fluidized bed
2. Between gases and solids
3. Temperature control
4. Between points in bed

B. Solids mixing

C. Gas mixing

D. Drying

1. Solids
2. Gases

E. Size enlargement

F. Size reduction

G. Classification

1. Removal of fines from solids
2. Removal of fines from gas

H. Adsorption-desorption

I. Heat treatment

J. Coating

Che et al (2015) conducted research about large-scale industrials bed reactors for polyethylene production, the prediction of the interactions between polymerization or the effects of the polymerization on the particle flow behaviors and particle size distributions. Considering all this, the influence of the drag model used on the behavior of the gas and solid phase is not clearly analyzed in literature. The drag model is one of the dominant forces between gas phase and the particles in a fluidized bed, it is defined as the resistance of the particles in the fluid environment. Therefore, the main objective of this project is the understanding of the behavior of a simple fluidized bed, comparing the results between the classical equations with the simulation results.

3.1. GENERAL CHARACTERISTICS OF A FLUIDIZED BED

Generally, this type of gas-solid operation, follows a particularly fluidization regimes depending on the gas velocity inlet.

In general, the behavior of gas-fluidized systems is considerably more complex than that of liquid-fluidized systems which exhibit a gradual transition from fixed bed to fluidized bed followed by particle transport, without a series of transition regions, and with bed expansion and pressure drop conforming reasonably closely to values calculated for ideal systems.

Part of the complication with gas–solid systems arises from the fact that the purely hydrodynamic forces acting on the particles are relatively small compared with frictional forces between particles, electrostatic forces and surface forces which play a much more dominant role when the particles are very fine. As the gas velocity in a fluidized bed is increased, the system tends to go through various stages:

1. Fixed bed in which the particles remain in contact each other and the structure of the bed remains stable until the velocity is increased to the point where the pressure drop is equal to the weight per unit area of the particles.
2. Particulate and regular predictable expansion over a limited range of gas velocities.
3. A bubbling region characterized by a high proportion of the gas passing through the bed as bubbles which cause rapid mixing in the dense particulate phase.
4. A turbulent chaotic region in which the gas bubbles tend to coalesce and lose their identity.
5. A region where the dominant pattern is one of vertically upward transport of particles, essentially gas–solids transport or pneumatic conveying. This condition, sometimes referred to as fast fluidization, lies outside the range of true fluidization.

So this scheme represents the different stages that, has explained in Figure 1.

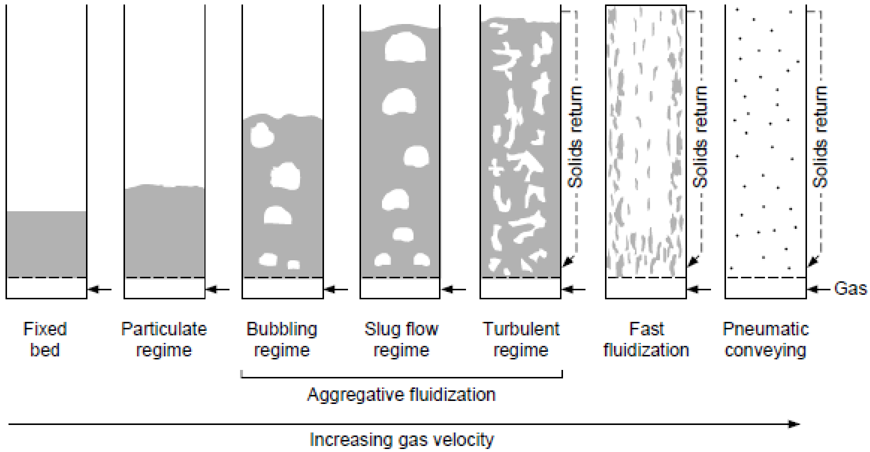

Figure 1. Schematic behavior of a fluidized bed (Perry, 1999)

Moreover, there are different types of solids called Geldart which are divided into four groups exhibiting different properties when fluidized with a gas (Chemical Engineering, 2002).

Table 1. Types of solid Geldart

Type	Typical size (µm)	Example of materials
Group A	30-100	Cracker catalyst
Group B	100-800	Sand
Group C	20	Flour, Fine silica
Group D	1000	Wheat, Metal shot

The use of the fluidization technique requires in almost all cases the employment of a fluidized bed system rather than an isolated piece of equipment. The major parts of a fluidized bed system are shown in Figure 2.

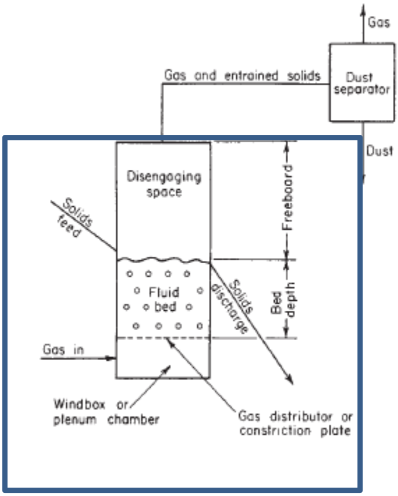

Figure 2. Schematic parts of a fluidized bed

Fluidization Vessel: The most common shape is a vertical cylinder. Just as for a vessel designed for boiling a liquid, space must be provided for vertical expansion of the solids and for disengaging splashed and entrained material.

Bed: generally, bed heights are not less than 0.3 m or more than 15 m. Although the reactor is usually a vertical cylinder, there is no real limitation shape. The specific design features vary with operating conditions, available space and use. The lack of moving parts lends toward simple, clean design.

Freeboard: the freeboard or disengaging height is the distance between the top of the fluid bed and the gas exit, sometimes its identification is difficult in fast and transport units.

Gas distributor: it has a considerable effect on proper operation of fluidized bed. Basically there are two types: for use when the inlet gas contains solids and when the inlet gas is clean. The distributor is designed to prevent back flow of solids during normal operation, and in many cases it is designed to prevent back flow during shutdown.

3.2. CFD PROGRAMS

Computational fluid dynamics, usually abbreviated as CFD, is a branch of fluid mechanics that include the numerical method of solving the conservation of momentum equations, the conservation of mass and any other required equations. With the advent of increased computational capabilities computational fluid dynamics, CFD, is emerging as a very promising new tool in modeling hydrodynamics. While it is now a standard tool for single-phase flows, it is at the development stage for multiphase systems, such as fluidized beds (Taghipour, et al, 2005).

Predicting and controlling fluid flow is critical in optimizing the efficiency of many products and processes — the combustion of gases in an automobile engine, the movement of a chemical solution through pores in a shale gas formation, the complex passage of air through a jet engine turbine, and the transfer of heat among components of a printed circuit board, to name a few. ANSYS® CFD allows to model and simulate all fluid processes, assuring an optimal performance of the process studied before making the first prototype. Whether designing a particle transport system, an air bubble injection system, or predict erosion rates in pipes, ANSYS® CFD enable the optimization of the design by simulating complex phenomena like bubbly flows, slurries, fluidized beds, and more. This is possible due to the inclusion of a comprehensive set of capabilities for solving fluids particulate systems. The problems range from dilute to frictional flows. ANSYS® offers a full range of validated and proven physics supported by global experts in particulate flows (ANSYS®, 2015), thus enabling to accurately model the behavior of particulates and track millions of particles in an Eulerian phase model.

3.3. GOVERNING EQUATIONS

In this chapter, the main equations used to describe the behavior of a fluidized bed are presented. There are two different models: the classical, which represents macroscopic balances and the computational model, which is used by ANSYS® and is able to work with microscopic balances.

3.3.1 Classical model of fluidized beds

For a non-fluidized bed, the general expression of macroscopic energy balance is as following:

$$g(z_2 - z_1) + \frac{1}{2} \cdot ({v_2}^2 - {v_1}^2) + \int_1^2 \frac{dp}{\rho} + \sum F + W_s = 0 \tag{1}$$

In this case study, two terms of the equation (1) are considered: the sum of forces and the pressure drop, because all the others are negligible in a fixed bed due to their very low values. Therefore, Equation (1) becomes as following:

$$\frac{\Delta p}{\rho} + \sum F = 0 \tag{2}$$

The pressure drop (∆p) is calculated in the same manner as for a compressible fluid; as the temperature is the same in all the figure's nodes, the operation is at constant gas density. Otherwise, the sum of forces is defined as in the main equation used for granular flow (Ergun equation),

$$\sum F = \frac{150\ (1-\varepsilon)^2 \cdot v \cdot \mu \cdot L}{\varepsilon^3 \cdot dp^2 \cdot \rho} + \frac{1{,}75\ (1-\varepsilon) \cdot v^2 \cdot L}{\varepsilon^3 \cdot dp} \tag{3}$$

When the bed is fluidized, a mass balance of particles must be defined:

$$L \cdot \$ \cdot (1-\varepsilon) \cdot \rho_s = L_{mf} \cdot \$ \cdot \left(1-\varepsilon_{mf}\right) \cdot \rho_s = L_f \cdot \$ \cdot \left(1-\varepsilon_f\right) \cdot \rho_s \tag{4}$$

These equations of mass balance are supplemented by the macroscopic energy balance, which it is considering the pressure drop, the weight of fluid and the weight of particles. All these terms represent the sum of forces that is applied on a bed of particles and is equal to mass flow rate.

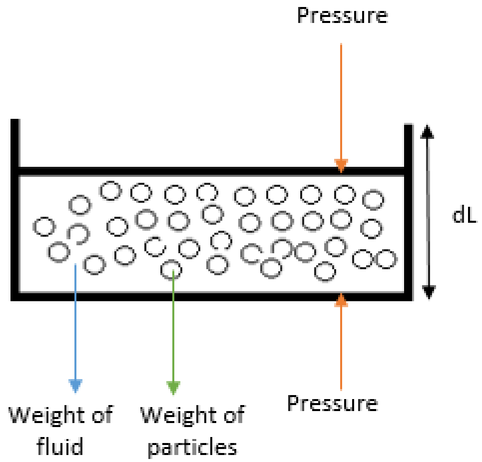

Figure 3. Forces that it is considering in a fluidized bed

$$-\$ \cdot dP - (\$ \cdot dL) \cdot \left(\varepsilon_f \cdot \rho_g \cdot g + \left(1 - \varepsilon_f\right) \cdot \rho_s \cdot g\right) = \$ \cdot v \cdot \rho_g \cdot dv \qquad (5)$$

When integrating between the bottom and the top of the bed particles, the following expression is obtained, representing the macroscopic energy balance

$$g \cdot L_f + \frac{\Delta v^2}{2} + \int_1^2 \frac{dP}{\rho_g} + g\left(1 - \varepsilon_f\right) \cdot \int_1^2 \frac{\rho_s - \rho_g}{\rho_g} dL = 0 \qquad (6)$$

Generally, it is simplified as:

$$\sum F = g\left(1 - \varepsilon_f\right) \cdot \frac{\rho_s - \rho_g}{\rho_g} L \qquad (7)$$

Consequently, the final expression of the macroscopic energy balance is the same as equation (2), in which the sum of forces is replaced by the expression in Equation (7):

$$\Delta P = -g\left(1-\varepsilon_f\right)\cdot\frac{\rho_s-\rho_g}{\rho_g}L\cdot\rho_g \tag{8}$$

Additionally, another important parameter to calculate is the minimum velocity of the fluidized bed. The minimum fluidization velocity of the gas is when the pressure drop in the bed is equal to the weight of the particles. When the velocity of the gas is too high, the particles move upwards until the top of the equipment is reached or, on the contrary, when the gas velocity is too small, the bed particles remain still.

Therefore, the minimum velocity of the fluidized bed is a relevant value that must be taking into account in the modelling of a fluidized bed.

The balance that takes into consideration the minimum velocity of the fluidized bed is presented in equation 9.

$$\frac{150\cdot(1-\varepsilon_{mf})}{{\varepsilon_{mf}}^3}\cdot Re_{mf}+\frac{1{,}75}{{\varepsilon_{mf}}^3}\cdot{Re_{mf}}^2=\frac{dp^3\cdot\rho_g\cdot\left(\rho_s-\rho_g\right)\cdot g}{\mu^2} \tag{9}$$

Where the first term on the left hand side of equation 9 is deduced by the Ergun equation (3) and represents the sum of forces acting on the system and this value is equal to Archimedes number which is used to determine the motion of fluids due to different densities.

$$Re_{mf}=\frac{v_{mf}\cdot dp\cdot\rho_g}{\mu} \tag{10}$$

On the other hand, when the force of resistance of the air with the particles is equal in magnitude and opposite in direction to the particles force of gravity then the terminal velocity is attained. This parameter is also very important.

Hence, the equations that allow the assessment of the terminal velocity are as follows:

$$v_t = \sqrt{\frac{4 \cdot g \cdot dp \cdot (\rho_s - \rho_g)}{3 \cdot \rho_g \cdot C_{fric}}} \tag{11}$$

where C_{fric} is the friction coefficient that depends on the Reynolds of particle, its shape.

$$\begin{gathered} Re_p = \frac{v_t \cdot dp \cdot \rho_g}{\mu} \\ Re_p > 1 \rightarrow Turbulent \\ Re_p < 1 \rightarrow Laminar \end{gathered} \tag{12}$$

Hence, when the system is laminar:

$$C_{fric} = 24/Re_p \tag{13}$$

and for a turbulent system:

$$C_{fric} = \left(\sqrt{0{,}4} + \sqrt{\frac{24}{Re_p}}\right)^2 \tag{14}$$

The terminal velocity is assessed following an iterative procedure, as the one described in Figure 4.

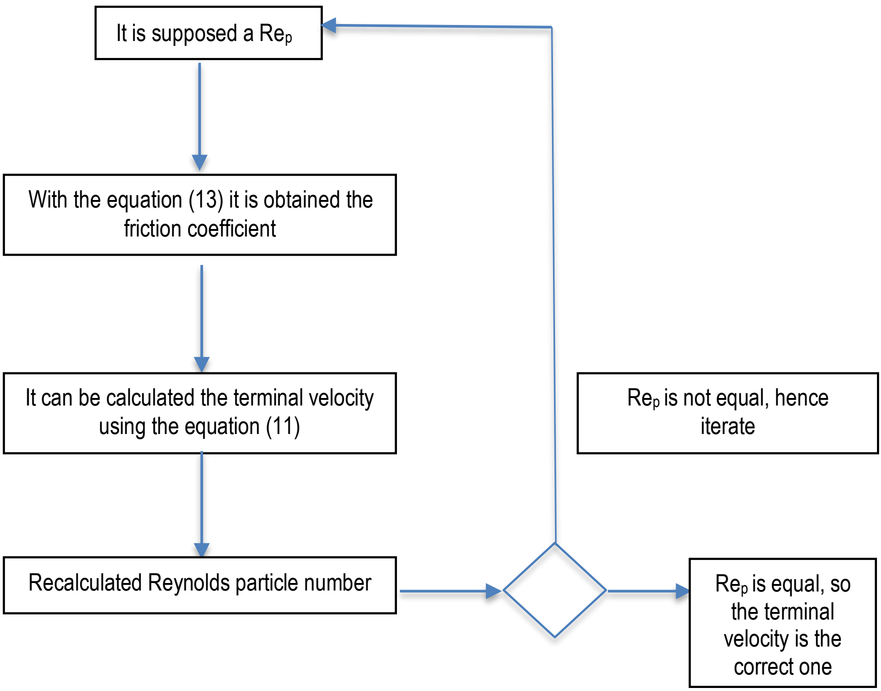

Figure 4. Iterative procedure

3.3.2. Computational model

As previously mentioned, ANSYS CFD is a software suit that spans the entire range of physics, providing access many fields of engineering simulation that a design process requires. ANSYS® Fluent is fully integrated into the ANSYS Workbench environment and represents a complete suite of models that capture the interplay between multiple fluid phases like gasses and liquids, dispersed particles and droplets, and free surfaces. In this work, ANSYS® Fluent is used to reproduce the simulation of a fluidized bed solving the governing equations of mass, momentum and energy conservation. A multifluid Eulerian model, which considers the conservation of mass and momentum for the gas and fluid phases, was applied. The kinetic theory of granular flow, which considers the conservation of solid fluctuation energy, was used for closure of the solids stress terms.

Mass conservation of gas and solid phase:

$$\frac{\partial}{\partial t} \cdot \left(\alpha_g \cdot \rho_g\right) + \nabla \cdot \left(\alpha_g \cdot \rho_g \cdot \overrightarrow{v_g}\right) = 0 \tag{15}$$

$$\frac{\partial}{\partial t} \cdot \left(\alpha_s \cdot \rho_s\right) + \nabla \cdot \left(\alpha_s \cdot \rho_s \cdot \overrightarrow{v_s}\right) = 0 \tag{16}$$

where $\alpha_g + \alpha_s$ =1 (17)

Momentum conservation equation in gas phase:

$$\frac{\partial}{\partial t} \cdot \left(\alpha_g \cdot \rho_g \cdot \overrightarrow{v_g}\right) + \nabla \cdot \left(\alpha_g \cdot \rho_g \cdot \overrightarrow{v_g}^2\right) = \tag{18}$$

$$-\alpha_g \cdot \nabla p + \nabla \cdot \overline{\tau_g} + \alpha_g \cdot \rho_g \cdot \vec{g} + K_{gs} \cdot \left(\overrightarrow{v_g} - \overrightarrow{v_s}\right)$$

where $\overline{\tau_g}$:

$$\overline{\tau_g} = \alpha_g \cdot \mu_g \cdot \left(\nabla \overrightarrow{v_g} + \nabla \overrightarrow{v_g^T}\right) \tag{19}$$

Momentum conservation equation in solid phase:

$$\frac{\partial}{\partial t} \cdot \left(\alpha_s \cdot \rho_s \cdot \overrightarrow{v_s}\right) + \nabla \cdot \left(\alpha_s \cdot \rho_s \cdot \overrightarrow{v_s}^2\right) = \tag{20}$$

$$-\alpha_s \cdot \nabla p - \nabla p_s + \nabla \cdot \overline{\tau_s} + \alpha_s \cdot \rho_s \cdot \vec{g} + K_{gs} \cdot \left(\overrightarrow{v_g} - \overrightarrow{v_s}\right)$$

where $\overline{\tau_s}$:

$$\overline{\tau_s} = \alpha_s \cdot \mu_s \cdot \left(\nabla\overrightarrow{v_s} + \nabla\overrightarrow{v_s^T} \right) + \alpha_s \cdot \left(\lambda_s - \frac{2}{3} \cdot \mu_s\right) \cdot \nabla \cdot \overrightarrow{v_s} \cdot \bar{I} \tag{21}$$

In the equation (18) and (20) the last term on the right hand side provides information related to the interaction force between the solid particles and gas. Hence there is a momentum exchange coefficient (K_{gs}) that depends on the type of drag function chosen, which is performed using the suitable equations describing each drag model. The solid- gas momentum exchange coefficient is shown in equation 22.

$$K_{sg} = \frac{\alpha_s \cdot \rho_s \cdot f}{\tau_r} \tag{22}$$

while the dimension of f depends on the type of exchange model chosen, τ_r representing the particle relaxation time. To understand its meaning, a particle initially with zero velocity is into a fluid of constant velocity. Because of the drag of the fluid on the particle, the particle will start moving and will be accelerated so that after a while the particle's velocity will be the same as the fluid velocity. Equation 23 defines the particle relaxation time

$$\tau_r = \frac{\rho_s \cdot {d_p}^2}{18 \cdot \mu \cdot g} \tag{23}$$

There are different drag models: Wen-yu, Syamlal-O'Brien and Gidaspow (Taghipour, 2005). In this case, Syamlal-O`Brien model is chosen, because all of them achived aproximately the same results (Tahgipour, 2005).

$$f = \frac{C_D \cdot Re_s \cdot \alpha_g}{24 \cdot {V_{r,s}}^2} \tag{24}$$

where C_D and $V_{r,s}$ are:

$$C_D = \left(0.63 + \frac{4.8}{\sqrt{\frac{Re_{r,s}}{V_{r,s}}}}\right)^2 \tag{25}$$

$$V_{r,s} = 0.5 \cdot \left(A - 0.06 \cdot Re_s + \sqrt{(0.06 \cdot Re_s)^2 + 0.12 \cdot Re_s \cdot (2 \cdot B - A) + A^2}\right) \tag{26}$$

with

$$A = \alpha_g^{4.14}, \quad B = 0.8 \cdot \alpha_g^{1.28} \quad for \quad \alpha_g \leq 0.85$$
$$A = \alpha_g^{4.14}, \quad B = \alpha_g^{2.65} \quad for \quad \alpha_g > 0.85$$

Solid pressure is used for granular flow in a compressible regime, the equation contains two different terms: a kinetic term and a particle collision term (Eq. 27).

$$p_s = \alpha_s \cdot \rho_s \cdot \theta_s + 2 \cdot \rho_s \cdot (1 + e_{ss}) \cdot {\alpha_s}^2 \cdot g_{0,ss} \cdot \theta_s \tag{27}$$

On the other hand, the solid stress tensor, $\overline{\overline{\tau_s}}$, contains shear and bulk viscosities generated by particle momentum exchange during collision and translation. Also a frictional and kinetic viscosity is included. Hence the solid stress tensor is defined as:

$$\mu_s = \mu_{s,col} + \mu_{s,kin} + \mu_{s,fric} \tag{28}$$

Every term of the equation (28) are different models that are considered depending on the process to simulate. Moreover, ANSYS® Fluent takes into account the granular temperature which is proportional to the kinetic energy of particles' random motion.

Equations above mentioned, describe the computational model of the fluidized beds.

4. OBJECTIVES

The main objective of this project is to simulate a fluidized bed. The fundamental problem encountered in modeling hydrodynamics of a gas–solid fluidized bed is the motion of two phases where the interface is unknown and transient, and the interaction is understood only for a limited range of conditions. To solve this, CFD is an emerging tool that is capable of dealing with this kind of systems.

One of the aims of this project is to learn how ANSYS® Fluent works simulating the behavior of a fluidized bed between the gas phase and the solid phase and how the particles interact.

The results of the simulation are then discussed and compared to the results obtained by applying the classical model of fluidized beds. Moreover, this work also studies the influence of some variables such as the velocity inlet and the size of the particle on the system behaviour.

5. MATERIAL, METHODS AND SETTINGS

5.1 MATERIAL

In this project, it is used the program called ANSYS®, this enables to predict with confidence the real world. Industry leaders use ANSYS® to create complete virtual prototypes of complex products and systems – comprised of mechanical, electronics and embedded software components – which incorporate all the physical phenomena that exist in real-world environments.

Predicting and controlling fluid flow is critical in optimizing the efficiency of many products and processes, ANSYS® CFD (Computational Fluid Dynamics Software) solutions give it the power to model and simulate all fluid processes, hence it can have confidence that the product will perform optimally before the first prototype.

The simulation is performed with ANSYS® Fluent package that is a powerful computational fluid dynamics (CFD) software tool available, empowering it to go further and faster as it optimizes the product performance. Fluent includes well-validated physical modeling capabilities to deliver fast, accurate results across the widest range of CFD and multiphysics applications.

Due to this, ANSYS® Fluent simulation program is used as the main tool to perform the analysis of a specific Chemical Engineering study, in this case the behavior of a fluidized bed.

5.2 METHODS

ANSYS® follow different steps in order to effectuate the simulation correctly, which are:

1. Preprocessing

- Geometry: it consists of drawing the physical bounds of the problem defined.
- Mesh: the surface occupied by the fluid is divided into discrete cells. The mesh can be uniform or non-uniform.
- Define the physical model: this involves specifying the fluid behavior and the properties at the boundary conditions. For transient problems, the initial conditions are also defined.

2. The simulation is started and the equations are solved iteratively as a steady-state or transient condition.

3. Post processor: allows the analysis and visualization of the obtained solution.

5.2.2 Preprocessing

5.2.2.1 Design modeler

The Design modeler application is designed to be used as a geometry editor of existing CAD models or to generate a geometry from scratch. This tool is a parametric feature-based solid modeler designed so that one can intuitively and quickly begin drawing sketches, modeling 3D parts, or uploading 3D CAD models for engineering analysis preprocessing. The Design Modeler application interface is similar to that most of other feature-based modelers. The program displays menu bars along the top of a screen and features two basic modes of operation: 2D and 3D.

In the beginning, the mode (2D or 3D is chosen. Before starting a new model in the Design Modeler application, three mutually perpendicular planes are displayed, corresponding to the three mutually perpendiculars planes in the Cartesian coordinate system.

The features shown in the Tree Outline list all of the operations used to create a model. A Sketch is always required at the start of creating a new model. The sketch is defined on a plane.

Only a single sketch can be worked, therefore this sketch is the" active sketch". The draw toolbox is displayed by default when you enter the Sketching mode. It is used to draw in 2D edges and applied dimensions and constrains.

The following tools have been used to provide the fluidized bed geometry in the Design Modeler application:

- Line: it is an option inside the draw toolbox in Sketching Toolboxes that permitted to draw a line using the cursor to indicate a start and the end of the line.
- Dimensions: let us indicate the dimensions of the lines drawn in the previous step.
- Generate: to update the model after any number of changes in the model's features or sketch/plane dimensions or changes in design parameters.
- Surface from Sketches: allows the creation of surface bodies using sketches as their boundary. This option is located in the Concept menu, and has two operations: Add material and Add frozen. In this case Add material is chosen to create material and merge it with the active bodies in the model.
- Named sections: allows the creation of named selections that can be transferred to the ANSYS® meshing application. Selections are performed through an Apply/Cancel property called Geometry in the details view of ANSYS® Design Modeler.

5.2.2.2. Mesh

Meshing is an integral part of the computer aided engineering simulation process. The mesh influences the accuracy, convergence and speed of the solution.

The partial differential equations that governs fluid flow and heat transfer are not usually amenable to analytical solutions, except for very simple cases. Therefore, in order to analyze fluid flows, flow domains are split into smaller subdomains (made up of geometric primitives like hexahedral and tetrahedral in 3D, and quadrilaterals and triangles in 2D) and discretized governing equations are solved inside each of these portions of the domain. Typically, one of three methods is used to solve the approximate version of the system of equations: finite volumes, finite elements, or finite differences. Care must be taken to ensure proper continuity of solution across the common interfaces between two subdomains, so that the approximate solutions inside various portions can be put together to give a complete picture of fluid flow in the entire domain.

Each of these portions of the domain are known as elements or cells, and the collection of all elements is known as mesh or grid. At the time the geometry is generated, is imported to the next step or sequence of the simulation, creating the mesh. This part of the project is produced by the Meshing module of ANSYS®.

Mesh generation is one of the most critical aspects of engineering simulation. Too many cells may result in long solver runs, and too few may lead to inaccurate results. ANSYS® Meshing technology provides a means to balance these requirements and obtain the right mesh for each simulation in the most automated way possible. The quality of the meshing would determinate the quality of the simulation.

The default mesh controls that ANSYS® program uses may produce a mesh that is adequate for the model. In this case is do not need to specify any mesh controls. Mesh controls allows to establish different factors such as the element shape, midsize node placement and the element size used in meshing.

The mesh is set up according to the following features:

- Physics Preference: allows to establish how Workbench will perform meshing based on the physics of the analysis type specified. Available options are: Mechanical, Electromagnetic, CFD and Explicit. The value of the Physics Preference options sets the default for various meshing controls.
- The sizing group let control these options:
    - Use Advanced size function provides greater control over sizing functions.
    - Relevance Center: sets gauge of the relevance slider control in the default group. Options are Coarse, Medium and Fine.
    - Element size: let you specify the element size used for the entire model. This size will be used for all edge, face and body meshing.
    - Smoothing: attempts to improve element quality by moving locations of nodes with respect to surrounding nodes and elements.
    - The Low, Medium or High option controls the number of smoothing iterations along the threshold metric where the mesher starts smoothing.

5.2.2.3 Physical model

Once the mesh has been properly designed, the physical model must be selected, considering that the physical model defines the type of simulation to perform.

ANSYS® Fluent software contains the broad physical modeling capabilities needed to model flow, turbulence, heat transfer, and reactions for industrial applications ranging from air flow over an aircraft wing to combustion in a furnace, from bubble columns to oil platforms, from blood flow to semiconductor manufacturing, and from clean room design to wastewater treatment plants. Special models that give the software the ability to model in-cylinder combustion, aeroacoustics, turbomachinery, and multiphase systems have broadened its reach.

The following paragraphs present the characteristics chosen particularly in this project.

Basic Capabilities Modeling:

- Steady and transient flows: the time dependence of the flow characteristics can be specified as either steady or transient. Steady state simulations are those whose characteristics do not change with time and whose steady conditions are assumed to have been reached in a long interval time. On the other side, transient simulations require real time information to determinate the time interval at which CFD-solver calculates the flow field.
- Laminar mode: laminar flow is governed by the unsteady Navier –Stokes equations. The laminar option does not apply a turbulence model to simulation and is only appropriate in the flow, which it has generally Re < 1000.
- Turbulent model K-epsilon:

  -The **RNG**-based - turbulence model is derived from the instantaneous Navier-Stokes equations, using a mathematical technique called “renormalization group” (RNG) methods. The RNG model has an additional term in its equation

  that improves the accuracy for rapidly strained flows and enhancing accuracy for swirling flows.

- **The realizable** - model contains an alternative formulation for the turbulent viscosity. A modified transport equation for the dissipation rate, ε, has been derived from an exact equation for the transport of the mean-square vorticity fluctuation. The term “realizable” means that the model satisfies certain mathematical constraints on the Reynolds stresses, consistent with the physics of turbulent flows.

Selecting the model:

- Multiphase flow: is a flow in which more than one fluid is present such as particles and air.
- Eulerian-Eulerian model: is one of the two main multiphase models that has been implanted in CFD. Within this model, certain interphase transfer terms used in momentum, heat and other interphase transfer models, can be modeled using either the Particle Model, the Mixture model or the Free Surface Model.

Boundary conditions: The boundary conditions produce different solutions for a given geometry and set of physical models. Hence, boundary conditions determine to a large extent the characteristics of a solution. Therefore, it is important to set boundary conditions that accurately reflect the real situation to obtain accurate results. The boundary types available in Fluent are classified as follows:

- Flow inlet and exit boundaries: pressure inlet, mass flow inlet, inlet vent, intake fan, pressure outlet, pressure far-field, outflow and exhaust fan.
- Wall, repeating and pole boundaries: wall, symmetry, periodic and axis.
- Internal cell zones: fluid and solid.
- Internal face boundaries: fan, radiator, porous jump, wall and interior.

Adapt region: allows to mark or refine cells inside or outside a specific region defined by text or mouse input. ANSYS® contain different shapes of particle that define the adapt region:

- Hex/Quad: define a hexahedral region in 3D or a rectangular region in 2D.
- Sphere/Circle: defines a spherical region in 3D or in a circular region in 2D
- Cylinder: defines a cylindrical region in 3D or a rectangular region in 2D.

5.3 SETTINGS

5.3.1 Fluidized bed parameters

First, the configurations and the dimensions of the studied system are chosen. Generally, bed heights are not less than 0.3 m and not more than 15 m. Although the fluidized bed is usually a vertical cylinder, there is no real limitation on shape. The specific design features vary with operating conditions available, space and use. So to represent the behavior of the particles in fluidized bed values are chosen inside the commonly range values. (PERRY,1999)

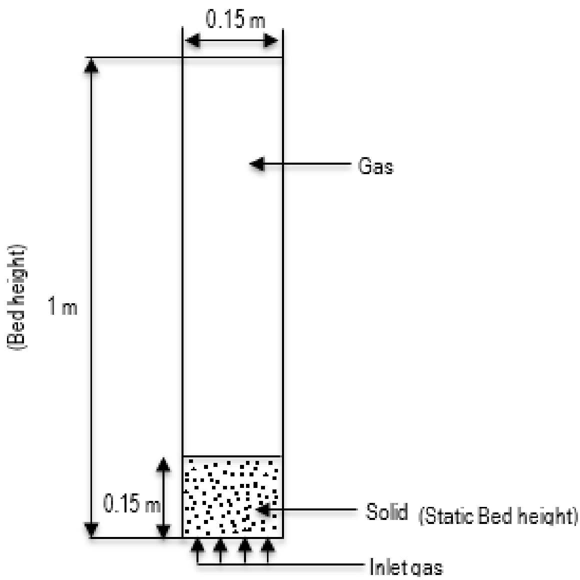

Figure 5. Schematic drawing of a fluidized bed

In this case the specified dimensions of the fluidization bed and the initial conditions are shown in Table 2:

Table 2: Initial conditions

Description	Value	Comment
Bed height	1m	Fixed value
Bed diameter	0.28 m	Fixed value
Static bed height	0.15 m	Fixed value
Gas density	1.2 kg/m3	Air
Particle density	2,600 kg/m3	Sand

5.3.2. Geometry

With the ANSYS® DesignModeler tool, the geometry of the fluidized bed is reproduced, following the steps explained in section 5.2.2.1.

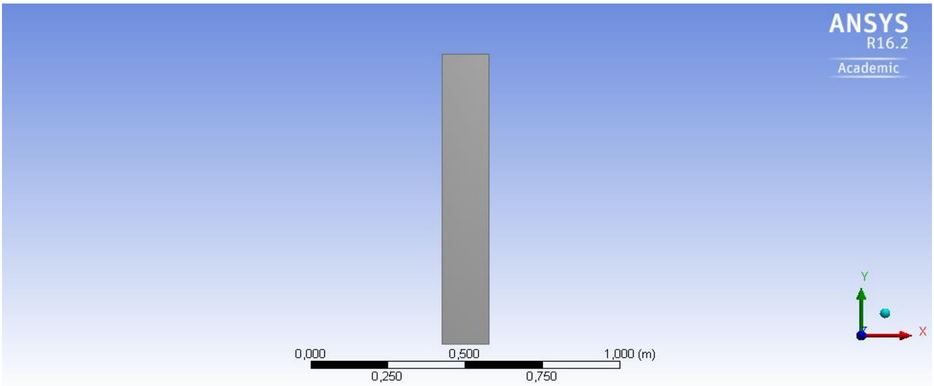

Figure 6. Geometry

5.3.3. Mesh

The next step is to mesh the geometry previously defined. The mesh parameters are chosen in order to achieve the optimum quality that allow to reliably simulate the system behaviour Therefore, the specific parameters are as following:

- Physics Preference: CFD
- Use Advanced size function: In this case the default option is selected: Use Advanced size function, which is On: Curvature.
- Relevance Center: fine
- Element size: 0.009 m
- Smoothing: high

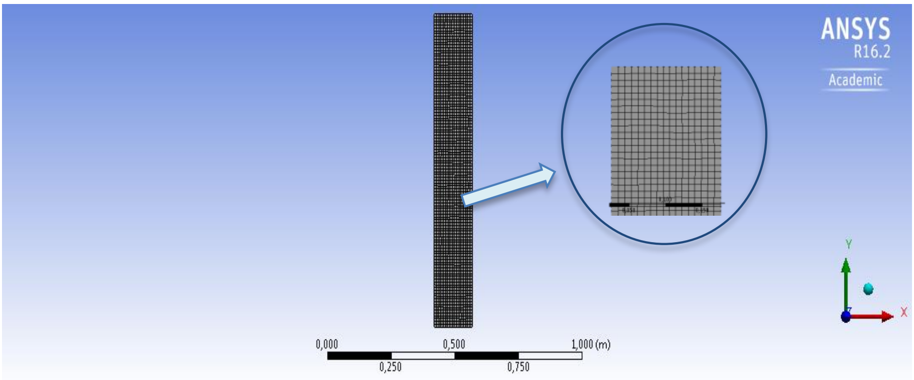

Figure 7. Geometry

5.3.4. Fluent Settings

It is the last step before running the calculation. Consequently, in this stage, the materials, boundary conditions and the region that determine the fixed bed are set up.

- Materials: it is necessary to define the gas flow as *air* in normal conditions and the solid with a specific density.
- Phases: the phases in the system are defined: the gas as a primary phase and solid as a secondary phase. At this point, it is necessary to indicate that the bed is constituted by granular solid and specify the diameter of the solid particles.
- Boundary Conditions: Fluent recognizes the boundary conditions from the Named Sections exported from the geometry and meshing stages. So, in the inlet, the gas velocity according to Y axis is indicated. Otherwise the outlet boundary condition has to be select as an outflow.
- Operation conditions: gravitational acceleration in the Y direction is enabled and specific operating density is set as 1.2 kg/m^3.
- Solution:
    - At this point, the adapt region is selected, indicating that the maximum value of X is 0.15 m and the maximum value of Y is also 0.15 m.
    - Update solution initialization
- Phase interaction: this tab is used to define the drag force chosen, that it is Syamlal O'brien Model.
- Run calculation: Table 2 provides the specifications used for running the simulation, allowing to reach a converged solution of this transient system.

Table 3. Specification of the run calculation

Description	Value	Comment
Time steps	0.001 s	Specified
Maximum number of iterations	20	Specified
Convergence criteria	10^{-3}	Specified

6. RESULTS AND DISCUSSION

One of the aims of this project is to simulate the behavior of a fluidized bed considering a gas phase and a solid phase and the interactions occurring among the particles in the system.

This chapter is divided into three blocks:

1. The comparison between the minimum fluidization velocities obtained from the simulation and the one assessed using the classical model. Additionally, the influence of the particles diameter on the minimum fluidization velocity is studied.
2. How the fluidized bed had been expanded.
3. The molecular behavior of the fluidized bed in all its stages when the particle diameter is 0.0002 m and 0.05 m. These diameters are chosen as representative values of extreme conditions.

6.1 MINIMUM FLUIDIZATION VELOCITY

First of all, it is known that there is a relation between de pressure drop of the bed and the main velocity of flow. Generally, fluidization is considered to begin at the gas velocity at which the weight of the solids gravitational force exerted on the particles equals the drag on the particles from the rising gas. When the gas velocity is increased to a sufficiently high value, however, the drag on an individual particle surpass the gravitational force on the particle, and the particle will be entrained in a gas and carried out of the bed. The point at which the drag on an individual particle is about to exceed the gravitational force exerted on it is called the maximum fluidization velocity.

Hence it studied the minimum fluidization velocity of the present fluidized bed. Then, it is compared with the classical model. Different values of velocity are required and extract the pressure drop from the simulation results. Consequently, representing the pressure drop versus the main velocity, the behaviour in Figure 7 provides the main stages followed in the bed fluidization, identifying the point where the minimum fluidization velocity is achieved.

As the minimum fluidization velocity is an important parameter in characterizing a fluidized bed, the influence of the particle diameter on the value of the minimum fluidization velocity is studied.

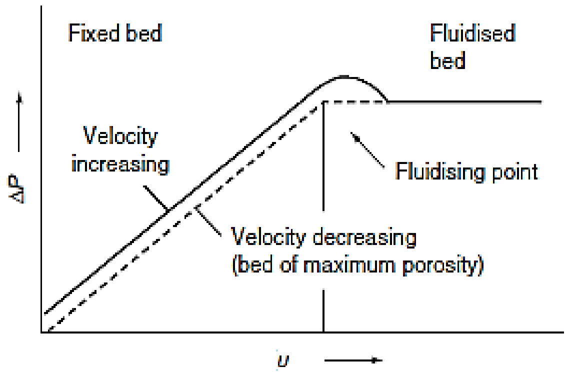

Figure 8. Stages of bed fluidization, Minimum fluiditzation Velocity.
(Perry,1999)

6.1.1. Particle diameter d = 0.0003 m

Initially a particle diameter of 0.0003 m is considered. Table 3 provides the results of pressure drop values function of the velocity inlet.

Table 3. Results of the pressure drop depending on the velocity inlet when diameter is 0.0003 m *(*minimum fluidization velocity)*

Velocity(m/s)	Pressure drop (Pa)
0.05	1,962.1
0.10	2,049.2
0.15	2,075.0
0.20	2,076.3
0.23	2,093.5
0.25*	2,124.1
0.30	2,111.2
0.35	2,105.9
0.40	2,097.4
0.45	2,109.2

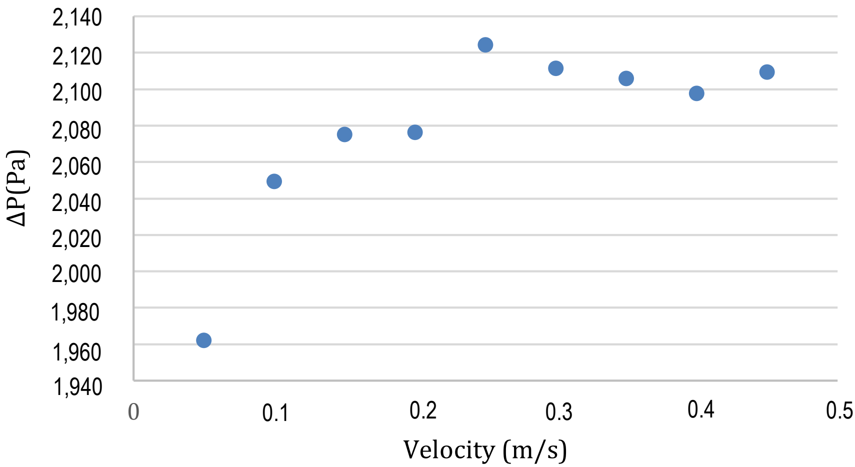

Figure 9. Dependence of ΔP vs velocity inlet, d = 0.0003 m

It is shown in Figure 8 that the bed begins to be fluidized when the velocity is 0.25 m/s, for this reason this velocity is called the minimum fluidization velocity It is appreciated a gradual increase of pressure drop that indicates the bed is starting to be fluidized, and when the velocity of 0.25 m/s is reached, the pressure drop maintains around a constant value of 2,105-2,124 Pa, so there are not any important fluctuations.

Table 4 provides the results obtained from the simulation of the fluidized bed in ANSYS® Fluent to the ones calculated using the classical model equations. The values provided in Table 4 illustrate that the simulation results and the classical model results are practically the same.

Table 4. ANSYS® simulation results versus classical models

	Velocity	**Pressure drop**
Classical	0.25 m/s	2,101.1
Simulation	0.25 m/s	2,124.1
Error	-	1%

6.1.2. Particle diameter d = 0.0002 m

The same procedure as described in section 6.1.1 is applied to study the influence of the particle diameter on the minimum fluidization velocity. In this case, the particle diameter considered is of 0.0002 m Table 5 provides the variation of the pressure drop function of initial velocity input:

Table 5. Results of the pressure drop depending on the velocity inlet when the diameter is 0.0002. *(*minimum fluidization velocity)*

Velocity(m/s)	Pressure drop (Pa)
0.01	2,031.8
0.05	2,071.2
0.1	2,081.6
0.13	2,085,2
0.15	2,095.9
0.20*	2,130.7
0.25	2,121.9
0.30	2,111.2
0.35	2,113.4
0.40	2,113.1

Table 6 provides the results obtained from the simulation of the fluidized bed in ANSYS® Fluent to the ones calculated using the classical model equations. The values provided in Table 6 illustrate, as in the previous case, that the simulation results and the classical model results are practically the same.

Table 6. ANSYS® simulation results versus classical

	Velocity	Pressure drop
Classical	0.13 m/s	2,101.1
Simulation	0.15m/s	2,130.7
Error	35%	1%

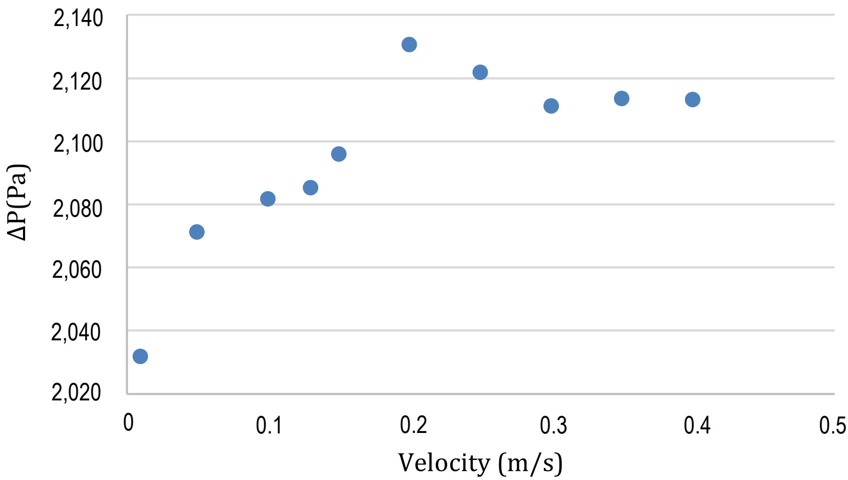

Figure 10. Dependence of ΔP vs velocity inlet, d=0.0002 m

Theoretically when all the parameters of the bed are the same and the only change in the system is related to the diameter of the particles, the minimum fluidization velocity changes in function of the particles diameter. Therefore, when the diameter is lower, the minimum fluidization velocity decrease too because the particles take up less volume and their weight is lower, so the bed is faster fluidized. Analyzing the results obtained so far, the behaviour of the fluidized bed is consistent from this point of view. Therefore, comparing the minimum velocity of fluidization when the particle diameter is 0.0003 m and 0.0002 m, it can observe that are V_{mf} = 0.25 m/s and V_{mf} = 0.20 m/s, respectively.

6.2 BED EXPANSION

When a bed is fluidized, the initial height of the bed tends to increase due to the expansion of the particles. At this point, the bed of particles with diameter 0.0002 m is chosen in order to provide the visualization of the bed expansion.

Table 7. Results of the bed expansion

Velocity(m/s)	H/H0
0.10	0.067
0.15	0.20
0.20	0.40
0.25	0.53
0.3	0.67
0.35	0.86

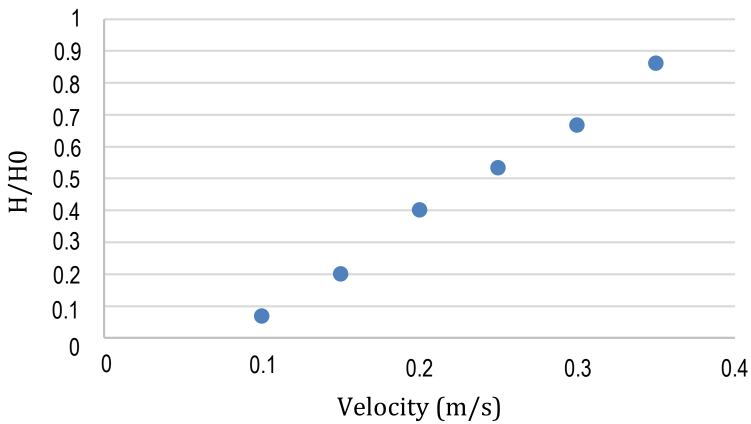

Figure 10. Bed expansion: representation of H/H0 vs velocity

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It is illustrated in Figure 10 that the expansion of the bed increases due to the rising of the velocity of the gas. It can appreciate that the values tend to follow a linear adjustment. Therefore, it is confirmed that effectively the bed expand its height compared to the initial one

6.3 BEHAVIOR OF A FLUIDIZED BED

The visualization of the microscopic behavior of a fluidized bed for different superficial velocities is performed using the case study of particles bed of 0.0002 m particle size. Following the simulation procedure detailed in Chapter 5, the evolution of the fluidized bed can be followed, capturing images of the system status in different times of the process of fluidization.

First, it is chosen one of the velocities for which the bed is not yet fluidized.

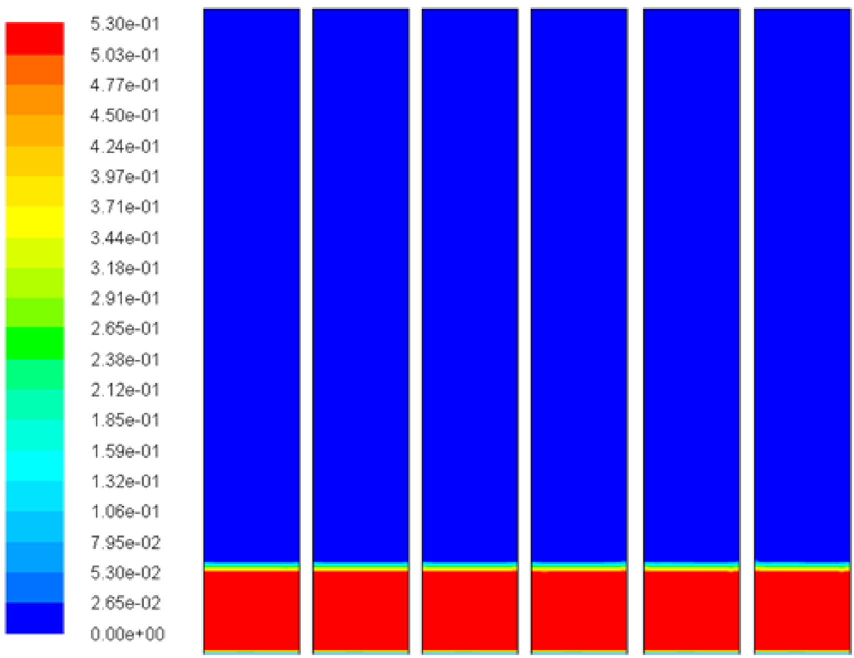

Figure 11. Contours of volume fraction with 0.01 m/s (0.45s; 0.55s; 0.65s; 0.75s; 0.90s; 1,00s)

Figure 11 illustrates that the bed expansion is not appreciable as the velocity is not high enough to sweep along the particles.

On the other hand, the system behavior can be reproduced starting from a velocity value of 0.15 m/s for which the bed is starting to be fluidized.

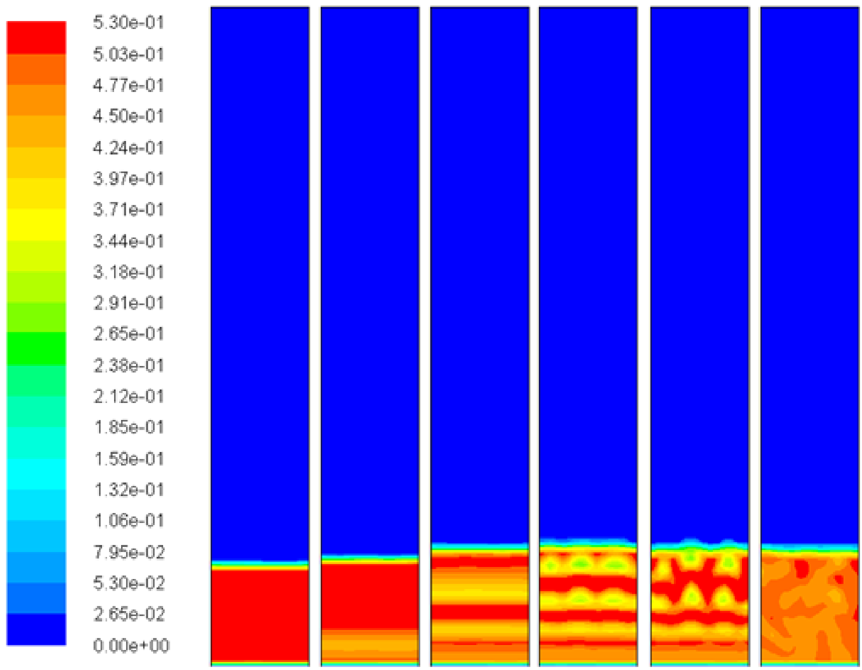

Figure 12. Contours of volume fraction with 0.15 m/s (0.01s; 0.20s; 0.50s; 0.90s; 1.08; 2.00s)

The beginning of the fluidization is illustrated in Figure 12, in which the movement of the particles can be perceived it can be appreciate some movements of the particles and how it behave at the beginning.

The same procedure is applied starting from a velocity value for which the bed is fluidized and had achieved the minimum fluidization the bed. The system behaviour in this case is illustrated in Figure 13.

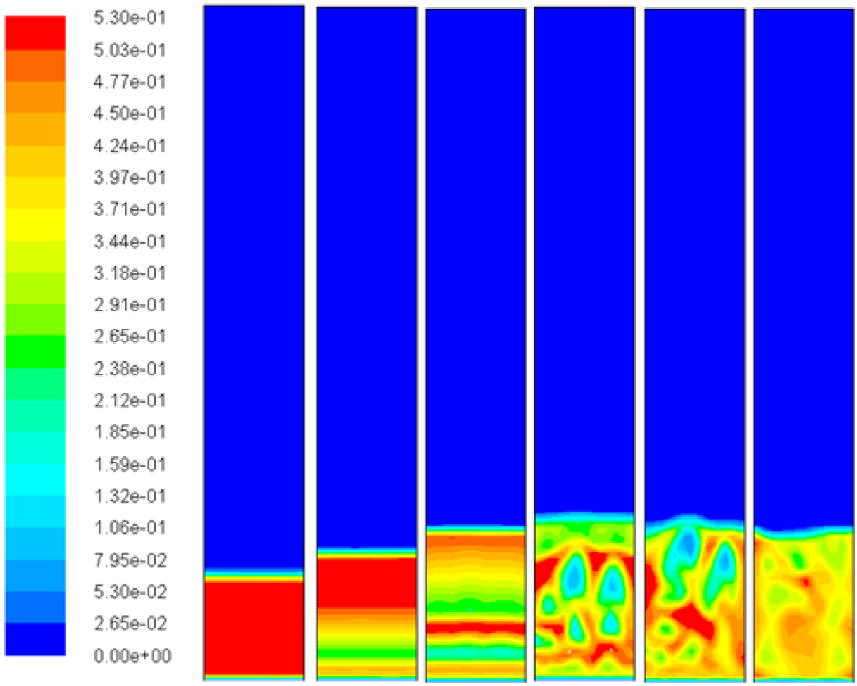

Figure 13. Contours of volume fraction with 0.25 m/s (0.02s; 0.25 s; 0.50 s;0.80 s;0.90 s; 1.70s)

It is appreciated that in both Figures 12 and 13, the system behaves in a similar way, several stages being observed in the system evolution. Firstly, the particles go up gradually, however as the time passes it is perceived that the region of particulate fluidization usually form gas bubbles. Thus, the bubbling region is an important feature of beds operating at gas velocities in excess of the minimum fluidizing velocity. The formation of bubbles in a fluidized bed, including measurement of their size, the conditions under which they will coalesce with one another, and their rate of rise in the bed has been still investigated.

When the gas flowrate is increased to a level at which the bubbles become very large and unstable, the bubbles tend to lose their identity and the flow pattern changes to a chaotic form without well-defined regions of high and low concentrations of particles. This is commonly described as the turbulent region.

The beginning of turbulent fluidization appears to be independent of bed height, or height at the minimum fluidization velocity, if this condition is sufficiently well defined. It is deduced that there is a strong influence by the bed diameter which imposes a maximum on the size of the bubble which can form.

In contrast, the behavior of the bed is studied when the inlet velocity takes the maximum velocity or the terminal velocity that in this case is v_t = 1.35 m/s. Generally, when the particles achieved the maximum fluidization velocity tends to get around of the bed. Moreover, it can be observed in Figure 14 that particles behave differently as before. In this case, it is analyzed that the particles go up until the space interstices between them increases, and consequently the velocity decreases due to the particles separation. Hence, the particles go down again when losing the maximum fluidization velocity.

In addition, also it can be observed that when the terminal velocity is applied to the bed, the particles go up until the end of the unit. So, it can’t be possible because it is a closed system and anything has to go out. It is observed the effect of the wall friction because the particles are submitted by the stress tensor which makes their flow difficult, therefore remaining on the walls of the bed.

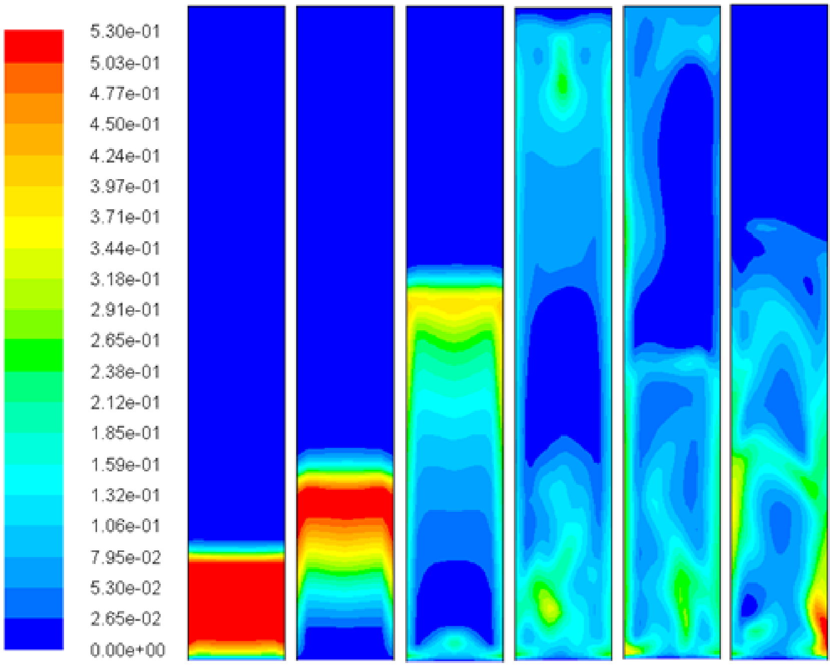

Figure 14. Contours of volume fraction with 1.35 m/s (0.02s; 0.16s; 0.50 s; 1.25 s; 1.80 s; 2.43 s)

When considering the same fluidized bed and changing the particle diameter as a bigger value of 0.05 m it can be observed in Figure 15, that the behavior of the bed is totally different as before. A velocity of v = 14 m/s is chosen because it represents the minimum fluidization velocity when the particles diameter is 0.05m. In this case, due to the dimensions of the particle, the bed begins to be fluidized near the walls. This type of regime is called annular flow as to the particles are bigger and the air find it easier to pass next to the walls of the bed rather than through the interstices of the bed particles. So as the time passes, at the same time that the particles move from the walls to the center axis of the bed, also have been expanded and created an oscillatory movement. This movement is due to the axial velocity because when the bed has expanded the particles are going to be more separated and the axial velocity tends to decrease, causing the particles to fall down again.

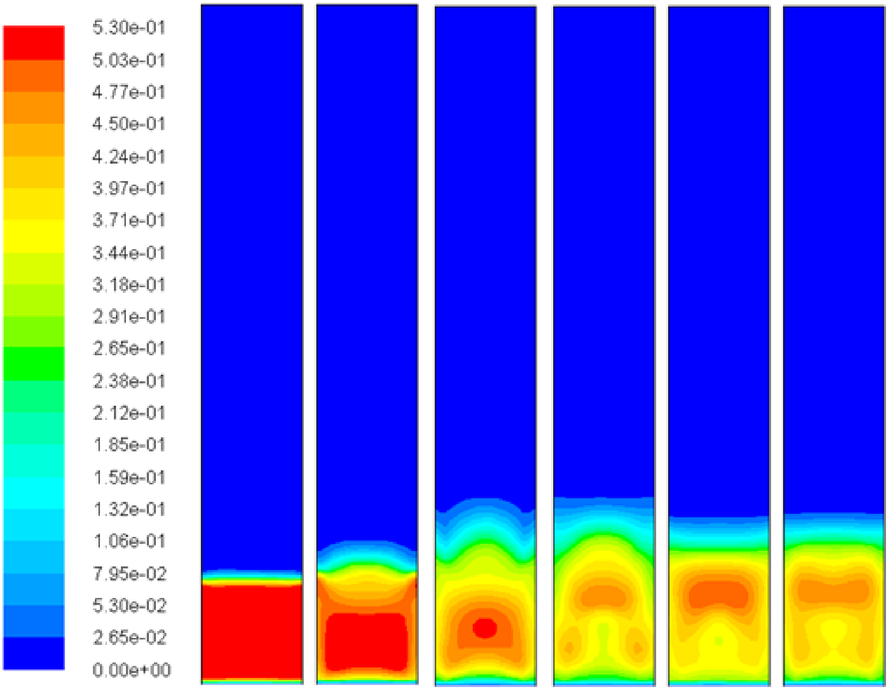

Figure 15. Contours of volume fraction with 14 m/s (0.01s; 0.04 s; 0.11 s; 0.27 s; 0.61s; 1.14 s)

Finally, it is concluded that depending on the size of the particle, the behavior of the fluidized bed changes. Moreover, CFD software allows the visualization of these different manners in which the fluidized bed works function of the initial conditions, at microscopic level. All these different profiles cannot be experimentally seen as the magnitude of the changes are not perceived by the human eyes.

7. CONCLUSIONS

The main aim of this project is to examine the influence of different parameters on the operation of fluidized beds by Computational Fluid Dynamics (CFD) software (ANSYS ®). The obtained results are contrasted to the ones provided from classical methods, which proved to be similar and proving the consistency of the simulation with reality.

Analyzing the simulation results, it is concluded that:

- The progress of the fluidization of the bed can be viewed providing details that until now they were not easily obtained. The different stages of fluidization process can be clearly identified. When the terminal velocity is reached, it is observed that the particle motion in the top of the bed is of lifting and lowering in a cyclic way.
- Correct outcomes are obtained when the dependence of the minimum fluidization velocity on particle diameter is analyzed: the minimum fluidization velocity increases when particle diameter decreases.
- Plug flow is normally accepted as model flow in fixed and fluidized beds; however, this profile is not reliable known today. With CFD analysis we can obtain a more realistic flow model. Simulations show that when the sizes of the particles are relatively large in comparison to bed diameter, flow in the central core region is much lower than the flow in the annular wall region of the bed. This corresponds to differences on volume fraction of these regions.
- One of the main advantages of the CFD simulations is that we can see the effect on performance when change any process variable without the need for experiments.

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9. ACRONYMS

ε= voidage, dimensionless

dp = particle diameter, m

μ= viscosity, kg/m·s

L = high of the bed particles, m

v= velocity, m/s

ρ = solid density, kg/m^3

ρ= gas density, kg/m^3

$= surface area, m^2

Re= Reynolds, dimensionless

α= volume fraction, dimensionless

Kgs = gas/solid momentum exchange coefficient, dimensionless

τ = stress tensor, dimensionless

λ = bulk viscosity, kg/m·s

f= specific parameter of the drag function

τ_r= particle relaxation time, dimensionless

C_D =drag coefficient, dimensionless

$V_{r,s}$ = terminal velocity, m/s

p = pressure, Pa

Θ = granular temperature, m^2 /s^2

e_{ss} =restitution coefficient, dimensionless

$g0_{,ss}$ = radial distribution coefficient, dimensionless

$\mu_{s,col}$= collision viscosity, kg/ m·s

$\mu_{s,kin}$ = kinetic viscosity, kg/ m·s

$\mu_{s,fric}$ = friction viscosity, kg/ m·s

Cfric= friction coefficient

Subscripts:

s= solid

g= gas

mf = minimum fluidization

f =fluidized

p=particle

t = terminal