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C. Cadile
CNRS, Aix Marseille Université, France

F. Topin
CNRS, Aix Marseille Université, France

L. Tadrist
CNRS, Aix Marseille Université, France

EULER-LAGRANGE/DEM SIMULATION OF SHALLOW DENSE FLUIDIZED BED DYNAMIC AND APPLICATION TO WOOD GASIFICATION

C.Cadile, F.Topin, L.Tadrist
IUSTI UMR 7343, CNRS, Aix Marseille Université 5 rue Enrico Fermi,13453 Marseille cedex 13, France
CNIM, ZI de Brégaillon, 83500 La Seyne-sur-Mer, France
T : (+33)4 91 10 69 37 ; E : ccadile@polytech.univ-mrs.fr

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ABSTRACT
We present an unsteady Euler-Lagrange 3D method of shallow dense fluidized bed dynamic for an application to the simulation of wood gasification in a bubbling fluidized bed. The gas phase is modeled as a continuum using 3D Navier-Stokes equations and the solid phase is modeled by a Discrete Element Method (DEM) using a soft-sphere approach for the particle collision dynamic. The model is validated using previous experimental results carried out in the laboratory.

INTRODUCTION
Considering the depletion of fossil resources and environmental problems caused by their consumption, the use of alternative energy sources is essential to continue to meet global energy needs while preserving the environment.
Gasification is a thermochemical treatment that converts a fuel carbonaceous solid in hydrogen and carbon monoxide gases. It has significantly been developed since the interwar period, with a worldwide of 70 GWth capacity installed in 2010 (1). Current biomass gasification systems use fixed, fluidized or circulating bed reactors, and pulverized fuel burners. Despite the long tradition of utilizing the combustible fuel gas from wood gasification, there still is a lack of detailed scientific knowledge about the complex interactions between the chemical reactions and the hydrodynamic of fluidized beds. The transition to an industrial scale encounters technological difficulties. The objective of this work is to achieve a more detailed understanding of a dense fluidized bed behavior during gasification by numerical approach.
The problematic of our study is the coupling, including heat transfer (conduction, convection, radiation), fluidized bed hydrodynamics, and chemical reactions. Nowadays, most of studies discuss about 0D, 1D and 2D results, which is reflecting the complexity of this subject. So, we can find in the literature different ways to approach the system. For example, pure chemists will agree to develop a model of complex chemical gasification mechanisms, depending on the atomic composition of biomass, with primary and secondary, even tertiary cracking tar reactions. But, a major simplification of the fluidized bed is made: it can be modeled as a porous medium effective fixed bed or as an equivalent system with two-phase bubbling bed (bubble and emulsion) in one direction or two directions (2 - 5). Finally, these studies present an important discard between experimental and numerical data. So, a more detailed hydrodynamic model is necessary to describe all the phenomena. In this perspective, we can use different approach

like Euler, Lagrange, DPM, DEM (6 - 8). In our case, we chose to use a DEM-Euler model for the simulation of dense fluidized bed, which seems like a good compromise between purely Lagrangian method and the Eulerian method. Indeed, the discrete element method (DEM) is similar to DPM method, ie particles are grouped into parcels, whose the position is tracking like a single representative particle. In addition, despite the development of computer technology, including commercial, research and open source CFD tools, the modeling of dense bed gasifier in 3D is almost nonexistent in the literature. In this way, we will present some results obtained with a 3D validation made from the experimental results of Sierra (9) and a feasibility study based on data from the Oevermann et al. article (8). For this, we use a CFD tool named Fluent_v14.

Nomenclature

v,u : velocity (m/s)
$\dot{m}$: mass flow rate (kg/m^3.s)
P : pressure (Pa)
g : gravitational acceleration (m/s^2)
F_D : drag force (N/kg)
d : diameter (m)
C_D :drag coefficient (dimensionless)
S : surface (m^2)
K : momentum exchange term (N/m^3)
k : stiffness coefficient (N/m)
i : unit vector
f : frequency of bed dynamics (Hz)
$\hat{f}$: renormalized frequency (dimensionless)

greek letters

α : volume fraction (dimensionless)
ρ: density of qth eulerian phase (kg/m^3)
μ : shear viscosity (kg/m.s)
δ : damping coefficient (N/m.s)

Subscripts

q : qth eulerian phase
p : pth particle phase
DPM : Discrete Phase Moldel
1,2 : particle number
f : fluid

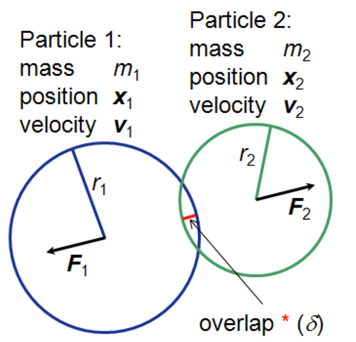
MATHEMATICAL MODELING

Continuous phase

The gas phase is considered as a continuous phase, which can interpenetrate and interact with other Eulerian phases. This model is usually governed by the Navier Stokes 3D equations (10) with a finite volume approach. The Morsi & Alexander (11) drag law is used for this case.

Discrete Phase

The DEM approach differs from the DPM in the following ways: The mass used in the calculations of the DEM is that collisions of the entire parcel, not just the single representative of that particle. The biomass particles will be considered as a discrete phase averaged component, governed by the following conservation equations:



* not to scale, greatly exaggerated

Fig. 1: Particles represented by softs spheres

$$\frac{\partial}{\partial t}(\alpha_p\rho_p) + \nabla.(\alpha_p\rho_p\overrightarrow{v_p}) = \sum_{p=1}^{n}(\dot{m_{qp}} - \dot{m_{qp}})$$

$$\frac{\partial}{\partial t}(\alpha_p\rho_p\overrightarrow{v_p}) + +\nabla.(\alpha_p\rho_p\overrightarrow{v_p}\overrightarrow{v_p}) =$$
$$-\alpha_p\nabla P + \nabla.\left(\alpha_p\mu_p\left(\nabla\overrightarrow{v_p} + \nabla\overrightarrow{v_p}^T\right)\right) + \alpha_p\rho_p\vec{g} +$$
$$\sum_{q=1}^{n}(\dot{m}_{qp}\,\overrightarrow{v_{qp}} - \overrightarrow{v_{pq}}\dot{m}_{pq} + \overrightarrow{K_{qp}}(v_q - v_p)) + K_{DPM}(\overrightarrow{v_{DPM}} - \overrightarrow{v_p})$$

The DEM implementation is based on the work of Cundall and Strack (12), and accounts for the forces, resulting from the collision of particles (the so-called “soft sphere” method). The forces from the particle collisions are determined by the deformation, which is measured by an overlap.

$$F_1 = (k\delta + \gamma(\overrightarrow{v_{12}}.\overrightarrow{\iota_{12}}))\overrightarrow{\iota_{12}} \qquad \& \qquad \overrightarrow{F_2} = -\overrightarrow{F_1}$$

In the resolution of above equations, it keeps track of the heat, mass, and momentum gained or lost by the particle stream that follows the trajectory. These quantities can be incorporated in the subsequent continuous phase calculations. Thus, while the continuous phase always impacts the discrete phase, the effect of the discrete phase trajectories is incorporated on the continuum. Alternately solving the discrete and continuous phase equations accomplish this two-way coupling until the solutions in both phases have stopped changing. This interphase exchange of heat, mass, and momentum from the particle to the continuous phase is depicted qualitatively.

MODEL DEVELOPMENT: DISCUSSION & RESULTS

PART 1: Dynamic study of shallow dense fluidized bed

Description

The objective of this study is to characterize the unsteady dynamics of a dense bed, and, through this, to be able to validate the simulation tool. If we refer to the literature, the techniques mostly used to validate hydrodynamics of fluidized bed are instantaneous and/or local averaged values (in space and/or time). In fact, we can find, for comparison experiments/numeric, concentration profiles (voidage), velocity profiles on section (13), or measuring the height of bed expansion (14 - 15), or by following the speed of a bubble in the bed (15).

In addition, the majority of these tests have ever been made to support the consistency of the results predicted

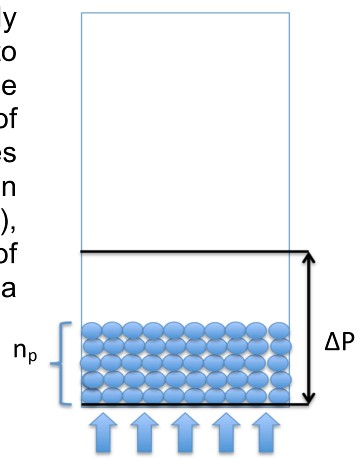


Fig.3: Schematic representation of fluidisation modeling

by Fluent (16 - 18). In the last paper (18) is presented a comparative study between three CFD software (OpenFoam, Mfix and Fluent). Finally, Fluent and Mfix seem to agree on the overall bed behavior for several configurations, and have a good agreement with experimental data. It should be noted that all these simulations have been studied in 2D, and mostly in euler-euler.
The main originality of our work is the study in euler-Lagrange/DEM 3D and we use an unsteady approach to characterize the bed dynamic behavior.
For that, we relie on experiments conducted by Sierra (9), which consisted on the characterization of shallow dense fluidized beds behavior. He measured the pressure loss at the gas inlet, reflecting an oscillatiory signal in which appears a periodicity traduced by a dynamic frequency (Hz) (see Fig.3). To characterize the bed behavior, we can vary the following parameters: the particle diameter, the density of particles, the number of particles layers and the fluid velocity inlet. In his experiments, Sierra has developped a dispenser able to homogenize the air flow over the inlet surface of the reactor. Hence, the apparent axisymmetry, as shown in (image.1), enables to restrict the domain to simulate for several hundreds of thousands particles. In view to simplify the system (without any approximation) and an optimum precision, we have chosen to work in pure Lagrangian (ie one particle by parcel) to validate the numerical tool used here.


Image 1: photography of the shallow fluidized bed surface for copper beads: 170 µm, n_p=10 (9)

Table of the reference case study:

Geometry	Unit	Value
Length*Width*Height	m	0,01*0,01*0,06
Mesh	m	0,005
Air		
Density	kg/m^3	1,225
Temperature	K	298,15
Viscosity	kg/(m.s)	$1,7894.10^{-5}$
Velocity inlet	m/s	1,3 ; 1,5 ; 1,7 ; 1,9 ; 2 ; 2,5 ; 3
Particles		
Density	kg/m^3	8802
Temperature	K	298,15
Particle diameter	µm	170
Parcel diameter	µm	170
N_p		17,20,25,30,40

Results & Discusssion

We encountered some numerical difficulties with no pressure signal when we approach the experimental values of gas velocity inlet. As a result, We have increased the fluidisation velocity to u_f = 1,3 m/s. To illustrate it are presented two pressure oscillatory signals obtained for two different cases, one experimental and one by simulation (see Fig.4):

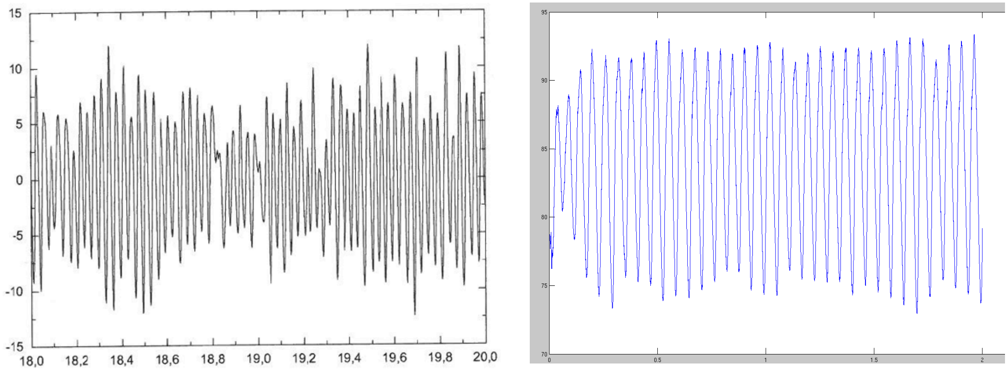


Fig.4: On the left, numerical pressure signal for n_p=12 & u_f=1,3m/s ; On the right, Experimental pressure signal for n_p=7 & u_f=0,13m/s

More specifically, we studied the influence of the particles layers number with the same fluidization velocity on frequency. The principle of using a renormalized frequency is to highlight a constitutive shallow fluidized beds. Like Basbakov et al. (1986) has done : $\hat{f} = \pi \left(\frac{h_{cp}}{g}\right)^{1/2} f$

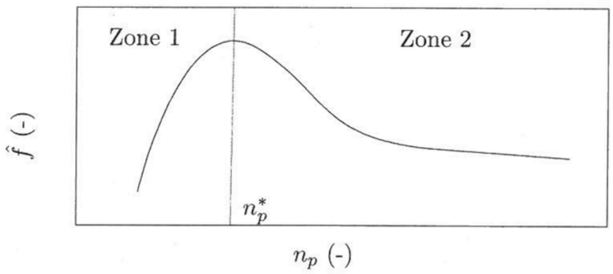


Fig.5: renormalized frequency evolution over n_p

However, the work of Sierra has demonstrated that this relationship was not as obvious: one can observe two regimes of behavior depending on the number of layers n_p, separed by a characteristic height of transition, which we denote n_p*(see Fig.5).

We can see that the behavior described by the observations of Sierra is well predicted by Fluent where the value of n_p* is almost the same (see Fig.6).

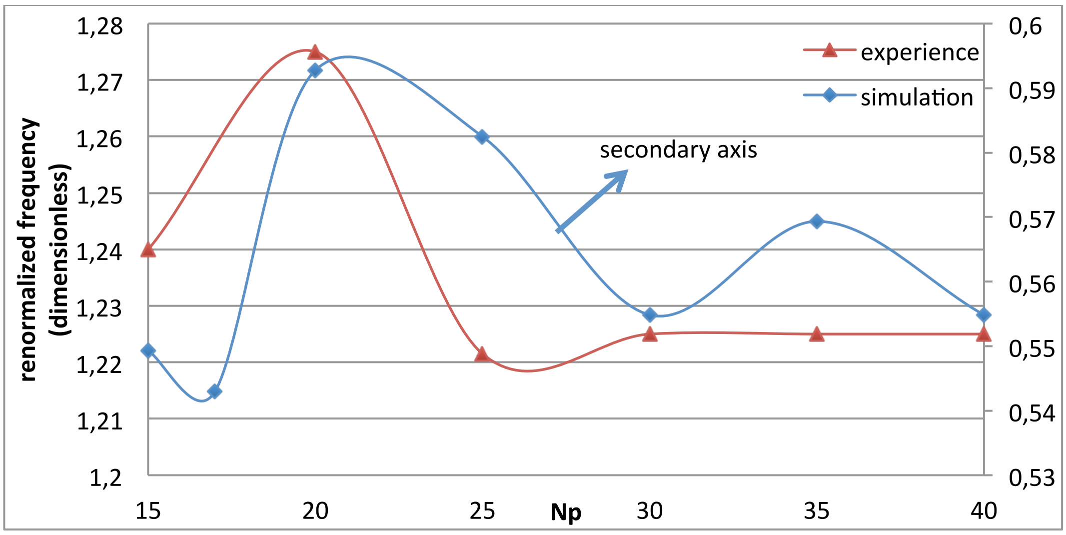


Fig.6: comparison between simulation (u_f = 1,3m/s) and experience (u_f = 0,13 m/s)

We can also check the evolution of frequency with the bed fluidization velocity (see Fig.7). We can observe that the curves follow the same evolution with the decrease of frequency increasing the inlet velocity, and we have a similar behavior with the increase of height bed.

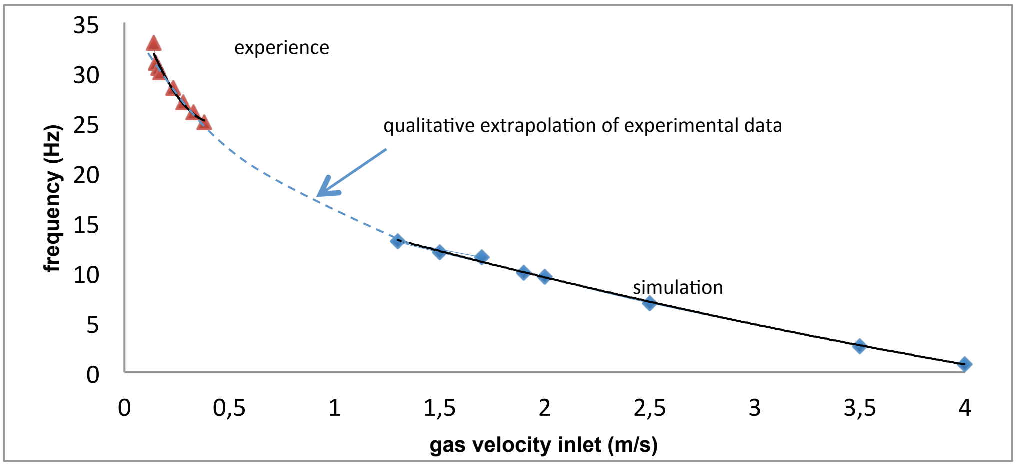


Fig.7: frequency over u_f for n_p=20

To conclude this section, after analyzing the literature, we have used an innovative method for the validation of CFD software because of the 3D, euler-lagrange/DEM approach and an unsteady characterization of the bed dynamics. After a thorough study of the pressure signals, we observed that the obtained curves are in good agreement with the experimental results of Sierra, which leads us to believe that with more investigation, we can have quantitative validations.

PART 2 : Qualitative study of a biomass gasification model: Example 3D Description

In this section, we focus particularly on the concept of coupling, including heat transfer, chemical reactions and hydrodynamics. For this, we referred to a case described by Oevermann et al. (8). It is a dense fluidized bed of inert particles wherein the particles are injected at the bottom of the bed and gas inlet is composed of air & steam. In this paper (8), Oevermann et al. try to represent a dense fluidized bed gasifier experience by a CFD tool called OpenFoam. In addition, they have used the DEM approach. For saving time and CPU memory, they developed a simplified 2D model. Here, we want to develop a 3D model with one particle by parcel for the two classes of particles (inert and reactive). The inert are made of charcoal with 3mm diameter at a temperature of 1050 K, biomass is composed of wood with a density of 585 kg/m^3 and 4mm in diameter. The bed is fluidized with a gas velocity (air) entering at 0.25 m/s with a temperature of 670K, and, the feed will be introduced with a rate of 0.105 kg/s at 423K, and, because of wood preheat, there is also a rate of water vapor at 0.079 m/s with the same temperature. We impose a constant temperature of 600K for walls.

It should be noted than, by application of Ergun law, the minimum fluidization velocity for this configuration is around 0.32 m/s, whereas we impose only 0.25

m/s, which corresponds to a quasi-static bed in terms of fluidization. For more information about the details of the model used in this simulation, we invite you to look directly at the article (8). The aim of this work is to compare our results to those from Oevemann et al. and check the results simulated in Fluent.

Results & Discusssion
We started with a quasi-2D, with 2 layers of particles in depth, and height of bed twice smaller than Oevermann et al.. The Observation of the first few seconds gave consistent results :

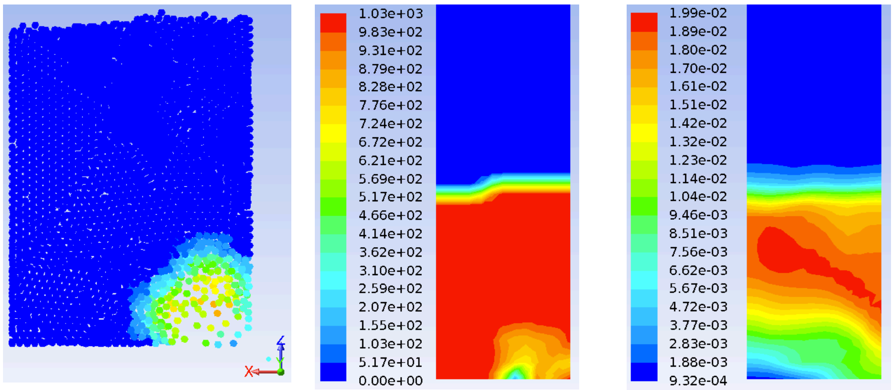


Fig.9: On the left, Char apparition and gassing by pyrolysis; in the middle, temperature (K) of particles; On the right, mole fraction of CO

We see the particles devolatilize, pyrolyze (see Fig.9: with the appearance (pyrolysis) and disparition (gasification) of the carbon) with emitted gases, which create a pocket inside the bed, as described in (8). So, the consistency of the results is in respect with the reactivity of biomass particles to their temperature: when particles come into contact with the hot dense bed, it begins to react . The complexity of subject resides on the diversity of parameters which can affect the behavior of particles: creation of gas, reduction of mass and diameter, and the interactions with dynamics of bed. Now that we have good agreement in reactivity of particles and bed behavior, the next step will be to develop simulations for a system at a higher scale, and compare it with available experimental data in (8).

CONCLUSION
We have presented an innovative unsteady Euler-Lagrange 3D method for the validation of shallow dense bed dynamics and the beginning of 3D study for the simulation of wood gasification in a dense fluidized bed.
The hydrodynamic validation method consists to observe the variation of pressure under a shallow fluidized bed, which normally presents an oscillating movement at a given frequency. This frequency depends on gas velocity, particle diameter and number of particles layers in the bed, as it was demonstrated by the experiments of Sierra (9) and confimed by our simulations. This method is innovative because of it's an unsteady description, which allows to obtain the "dynamic" of bed instead of local averaged variables described in most studies of the literature. By comparison of our simulated results with experimental Sierra

data, we observed the same curves trend, which reassures us in our choice for Fluent.
In the second part of this work, we have developed a model of biomass gasification in bubbling fluidized bed based on a case developed by Oevermann et al. (8). The purpose of this study was to obtain an element of comparison involving the coupling of heat transfer, mass, reagents and hydrodynamics. The results are in good agreement in comparison with (8): we have a mass transfer with the apparition of "gas pockets" around the feed injection, and heat exchange seemed consistent for activation of chemical reactions.
For the future, we suggest to develop a bigger 3D case and to complete the model for the hydrodynamic approach in order to obtain quantitative results.

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