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CFD Simulations of a Square-Based Spouted Bed Reactor and Validation with Experimental Tests Using Rice Straw as Feedstock

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The present work aims to develop a model to simulate the fluid dynamic behavior of processes related to the exploitation of biomass as energy source by means of gasification. In particular, the attention has been focused on a spouted bed reactor with a square base using rice straw as feedstock.
Spouted Bed reactors are attracting particular attention for their use in gasification processes. In these devices, the gas is introduced through a single nozzle at the center of the base and, as a result, a particular fluid dynamic pattern is followed which results in an enhanced solid circulation movement increasing therefore the mass and energy transfer rates.
A Computational Fluid Dynamic (CFD) modeling technique was used to simulate the previously described fluid flow. The Eulerian-Eulerian method was applied to predict the gas-solid flow behavior and the kinetic theory of granular flow was incorporated within the method as closure equation. The gas and particle dynamics were investigated through the simulation of different operational regimes by varying the gas flow rate at the inlet and the amount of initial solids in the initial bed of particles.
The obtained model was validated through experimental activities on a square based-reactor with a pyramidal bottom. Air was used as the gas phase and the particles were a mixture of rice straw and silica. The fluid dynamic parameters (minimum spouting velocity, Ums and pressure drop along the bed of particles, ΔP) of the system were recorded for each case and compared with the values provided by the developed model.
The resulting model will be used to optimize the fluid dynamic parameters defining the process and it will lead to an improvement of the gas-solid mass transfer and the minimisation of the energy requirements of the system.

1. Introduction

The first spouted bed was developed in 1954 as an alternative method for drying moist wheat particles with fluidized bed reactors, as they presented serious slugging problems (Gishler, 1983). Nowadays they are widely applied in various physical operations such as gasification, drying, coating and granulation (San José et al., 2010). A Spouted Bed Reactor is a device where gas (or occasionally liquid) is injected vertically upwards through a single central orifice into a bed of solid particles. If the flow rate of the fluid is sufficient and the bed depth is less than the ‘‘maximum spouted bed depth’’, the central jet breaks through the upper surface, resulting in a characteristic flow pattern known as spouting. Three regions can be distinguished in a spouted bed reactor: a dilute central jet, called “spout”, in which particles are entrained, a peripheral annular region called "annulus" and a “fountain “region above the bed surface where entrained particles ascend centrally and then return less centrally due to gravity forces to land on the bed surface. In the annulus, fluid percolates outwards and upwards, counter-current to the movement of the particles (Epstein and Grace, 2011). The

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overall bed thereby becomes a composite of a dilute phase central core with upward moving solids entrained by a concurrent flow of fluid and a dense phase annular region with counter-current percolation of the fluid. A systematic cyclic pattern of solid movement is established with effective contact between the gas and the solids. The vessel forming a spouted bed is usually a circular cylinder, but sometimes it may have a square section. To enhance the solid motion and eliminate dead spaces at the bottom of the vessel, it is very common to use a diverging conical (or pyramidal) base (Altzibar et al., 2013).

Simulation activities are used to model the fluid behaviour of Spouted Bed reactors in order to design the equipment as precisely as possible. A deep study in spouted beds using appropriate multiphase models must be performed in order to understand what it is actually happening inside the fluidized bed. Computational fluid dynamic (CFD) modelling has become a powerful tool for understanding dense gas–solid systems thanks to the development of the computing power, the advance of numerical algorithms, and the deeper understanding of multiphase flow phenomena in the recent years.

Figure 1: Experimental system

Currently, there are two main CFD approaches: the Eulerian-Eulerian approach (two fluid model, TFM), and the Eulerian-Lagrangian (discrete element method, DEM) approach. In the Eulerian-Eulerian approach, the fluid and particulate phases are treated mathematically as interpenetrating continua. Several studies (Wang et al., 2006) have shown that this approach is capable of predicting gas-solids behaviour in spouted beds with high accuracy. In this approach, volume fractions of the overlapping phases are assumed to be continuous functions of space and time, with their sum always equal to one. The conservation equations have similar structure for each phase. Owing to the continuum description of the particle phase, two-fluid models require additional closure laws to describe particle–particle and particle–fluid interactions. In the Eulerian-Lagrangian approach, the fluid phase is treated as a continuum medium by solving the time-averaged Navier-Stokes equations, whereas the dispersed phase is solved by tracking a large number of individual particles through the computed flow field, not requiring additional closure equations (Cundall and Strack, 1979). The dispersed phase can exchange momentum, mass, and energy with the fluid phase, and interphase forces couples the two phases. However, it is much more computationally demanding, especially as the number of particles simulated becomes large.

2. Experimental

In a previous work (Moliner et al., 2014), low temperature essays were performed in a square-based spouted bed reactor using rice straw as feedstock and silica as inert bed material to characterize the fluid dynamic behaviour of the system in terms of pressure drop and height of the fountain. An air compressor, a flow meter and a conical spouted bed reactor compose the system. A half section device with a Plexiglas wall was used in order to better evaluate the fluid dynamic phenomena occurring inside the reactor. As proven elsewhere (Rovero et al, 1985) the wall did not add extra effects and the results obtained with this device are taken as valid to describe the behaviour of the whole reactor. The inlet distributor consists on a single orifice placed in the center of the base of the reactor. Rice straw was chopped and considered as a cylinder with constant diameter and an average length of 1 cm. Different percentages of rice straw (0 % v/v, 10 % v/v) were tested for the present work. The effect of the height of the bed was assessed with values set at 25, 35 and 45 cm for each experiment. Figure 1 shows the experimental system.

3. Model equations

In the present work, the TFM approach is adopted to model the complex gas–solid flow in a Spouted Bed reactor. The full Eulerian-Eulerian approach includes conservation equations of mass and momentum for each phase; closure equations, which requires a proper description of interfacial forces, solid stress, and turbulence phenomena of the phases; meshing of the domain, discretization of equations, and finally, solution algorithms.

3.1 Conservation equations of mass and momentum

The volume fraction balance equation is:

$$\sum_{q=1}^{n} \alpha_q = 0 \tag{1}$$

where α_q is the volume fraction of the phase *q* (*q* = *g, s, r* where *g* is air, *s* is silica and *r* is rice)
The mass conservation equation for phase *q* is:

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right) + \nabla\left(\alpha_q \rho_q \vec{v}_q\right) \tag{2}$$

where ρ_q and v_q are density and velocity of phase *q* respectively
The momentum conservation equation for phase *q* is:

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q \vec{v}_q\right) + \nabla\left(\alpha_q \rho_q \vec{v}_q \vec{v}_q\right) = -\alpha_q \nabla P + \nabla \tau_q + \sum_{p=1}^{n} \vec{R}_{pq} + \alpha_q \rho_q \times \left(\vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{vm,q}\right) \tag{3}$$

where *P* is the fluid pressure, τ_q is the Reynolds stress tensor, R_{pq} is the interaction force between phases, F_q is the external body force, $F_{lift,q}$ is the lift force and $F_{vm,q}$ is the virtual mass force.
The drag model chosen for defining the interaction silica-air and interaction rice-air is Huilin and Gidaspow (2003) model. This model uses the Ergun (1952) equation for dense phase calculations and the Wen and Yu (1966) equation for the case of dilute phases.

$$\beta_{Ergun} = 150\frac{\left(1-\alpha_g\right)^2 \mu_g}{\alpha_g^2 d_p^2} + 1.75\frac{\left(1-\alpha_g\right)\rho_g}{d_p}|\vec{v}-\vec{u}| \qquad \alpha_g < 0.8 \tag{4}$$

$$\beta_{Wen-Yu} = \frac{3}{4}\frac{\left(1-\alpha_g\right)}{d_p}\rho_g C_D \alpha_g^{-2.65}\left|\vec{u}_g - \vec{u}_s\right| \qquad \alpha_g \geq 0.8 \tag{5}$$

where μ_g is the air viscosity, d_p is the particle diameter, *v* is the particle velocity, *u* is the gas velocity and the drag coefficient C_D is defined as:

$$C_D = \begin{cases} \dfrac{24}{\alpha_g Re_p}\left[1 + 0.15\left(\alpha_g Re_p\right)^{0.687}\right] & Re_p < 1000 \\ 0.44 & Re_p \geq 1000 \end{cases} \tag{6}$$

$$Re_p = \frac{\rho_g |\vec{v}-\vec{u}| d_p}{\mu_g} \tag{7}$$

where α_g is the gas volume fraction and ρ_g is the gas density.
To avoid the discontinuity of the two equations, a switch function is introduced in this model to give a rapid transition from one regime to the other one:

$$\varphi_{gk} = \frac{arctg\left[150 \times 1.75\left(0.2 - \left(1-\alpha_g\right)\right)\right]}{\pi} + 0.5 \tag{8}$$

Thus, the fluid-particle interaction coefficient can be expressed as:

$$\beta = \left(1 - \varphi_{gk}\right)\beta_{Ergun} + \varphi_{gk}\beta_{Wen-Yu} \tag{9}$$

The drag model chosen for the interaction silica-rice is Syamlal-O'Brien-Symmetric (Syamal, 1987). In this model, the silica-rice exchange coefficient has the following form:

$$K_{sr} = \frac{3(1+e_{sr})\left(\frac{\pi}{2} + C_{fr,sr}\frac{\pi}{8}\right)\alpha_s \rho_s \alpha_r \rho_r (d_s + d_r)^2 g_{0,sr}}{2\pi(\rho_s d_s^2 + \rho_r d_r^2)}|\vec{v}_s - \vec{v}_r| \tag{10}$$

where e_{sr} is the coefficient of restitution and $C_{fr,sr}$ is the coefficient of friction between the silica and rice phases.

3.2 Kinetic theory of granular flow

The kinetic theory of granular flow is analogous to the kinetic theory of gases. The fluctuations that occur in the solid particle phase were modeled using the kinetic theory of granular flow to account for inelastic collisions between the particles. In this model, this theory is applied for silica and rice. In the following equations, the symbol *k* is used to indicate phases *k* (*k = s, r* where *s* is silica and *r* is rice).
The transport equation for the turbulent fluctuating energy of the phase *k*, also called granular temperature is:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\alpha_k\rho_k\theta_k)+\nabla(\alpha_k\rho_k\theta_k\vec{v}_k)\right]=\left(-P_k\cdot\vec{I}+\tau_k\right):\nabla\vec{v}_k+\nabla\left(h_{\theta_k}\nabla\theta_k\right)-\gamma\theta_k+\phi_{gk} \tag{11}$$

where θ_k is the granular temperature, $(-P_k\ I + \tau_k):div(v_k)$ is the generation of energy by the solid stress tensor, $h_{\theta k}div(\theta_k)$ is the diffusion of energy, $\gamma\theta_k$ is the collisional dissipation of energy and ϕ_{gk} is the energy exchange between fluid and *k* phase.
Granular flows can be classified into two distinct flow regimes: a rapidly shearing regime, in which stresses arise because of collisional or translational transfer of momentum, and a plastic or slowly shearing regime, in which stresses arise because of friction among particles in contact (Campbell 2006). Closure of the solid phase momentum equation requires a description of the solid phase stress that depends on the magnitude of the particle velocity fluctuations. The granular temperature conservative equation of Lun et al. (1984) expresses the kinetic solid pressure as:

$$P_k=\alpha_k\rho_k\theta_k\left[1+2g_{0,kk}\alpha_k(1+e_{kk})\right] \tag{12}$$

where e_{kk} is the coefficient of restitution of particles and $g_{0,kk}$ is the radial distribution function.
Lun et al. (1984) defines the solid bulk viscosity as:

$$\lambda_k=\frac{4}{3}\alpha_k^2\rho_k d_p g_{0,kk}(1+e_{kk})\sqrt{\frac{\theta_k}{\pi}} \tag{13}$$

and Ding and Gidaspow (1990) express the solid shear viscosity as:

$$\mu_k=\frac{3}{5}\lambda_k+\frac{10\rho_k d_p\sqrt{\pi\theta_k}}{90(1+e_{kk})g_{0,kk}}\left[1+\frac{4}{5}g_{0,kk}\alpha_k(1+e_{kk})\right]^2 \tag{14}$$

3.3 Turbulence model

The dispersed turbulence model is the appropriate model when the concentrations of the secondary phases are low or when using the granular model. Fluctuating quantities of the secondary phases can be given in terms of the mean characteristics of the primary phase and the ratio of the particle relaxation time and eddy-particle interaction time. The model is applicable when there is clearly one primary continuous phase and the rest are dispersed dilute secondary phases (Launder and Spaulding,1972). Therefore, the dispersed turbulence model is adopted in this study, where the standard k–ε model is used to obtain the turbulence predictions for the gas phase.

4. Simulation procedure

The commercial CFD simulation package FLUENT® is used to simulate the hydrodynamics of the spouted bed. The set of governing equations are solved by a finite control volume technique. The pressure–velocity coupling is obtained using the SIMPLE algorithm. The physical and numerical parameters of the experimental run and the inputs for the computer run are presented in Table 1.

5. Results and discussion

The output variables height of the fountain and pressure drop were studied and compared with the experimental results. Table 2 shows the comparison for the different amount of initial solid with 0% of rice straw while Table 3 gathers the equivalent results for the case of an initial bed of solids containing 10% of rice straw.

Table 1: Physical and numerical parameters of the runs

Description	Experimental run	Computer run
Solids density (kg/m^3)	2,600	2,600
Rice straw density (kg/m^3)	238	238
Gas density (kg/m^3)	1.225	1.225
Diameter of the spout gas inlet (cm)	2.5	2.5
Diameter of the bed (cm)	20	20
Vessel height (cm)	200	200
Particle solids diameter (cm)	0.141	0.141
Particle rice straw diameter	0.4÷1	0.8
Minimum spouting velocity U_{ms} (m/s)	0.44-0.56-0.625	0.44-0.56-0.625

Table 2: Fountain height and pressure drop for different heights of initial solids with 0 % v/v of rice straw

Parameter	Height initial solids	Experimental result	Simulation result	Error %
Fountain height (cm)	25 cm	49.5	50.6	+ 2.22
Fountain height (cm)	35 cm	64.0	64.8	+ 1.25
Fountain height (cm)	45 cm	77.7	81.4	+ 4.76
Pressure drop (Pa)	25 cm	196.1	775.7	+ 295.77
Pressure drop (Pa)	35 cm	980.6	1212.5	+ 23.64
Pressure drop (Pa)	45 cm	1,931.7	2,157.4	+ 11.72

Results in table were obtained by setting 0.85 the coefficient of restitution among the silica particles. The inlet gas velocity is set as $u_{x,0}$ = 0 and $u_{y,0} = \sigma U_{ms}$ where σ is the geometric factor in the numerical model set as 40.764.

Table 3: Fountain height and pressure drop for different heights of initial solids with 10 % v/v of rice straw

Parameter	Height initial solids	Experimental result	Simulation result	Error %
Fountain height (cm)	25 cm	78.0	79.9	+ 2.43
Fountain height (cm)	35 cm	93.0	93.4	+ 0.43
Fountain height (cm)	45 cm	107.0	102.4	- 4.30
Pressure drop (Pa)	25 cm	294.2	894.3	+ 203.97
Pressure drop (Pa)	35 cm	784.5	1324.3	+ 68.67
Pressure drop (Pa)	45 cm	2,392.7	2,559.36	+ 6.96

Results in table were obtained by setting a value of 0.85 to the coefficient of restitution among the silica particles and a value of 0.3 for the case of silica and rice straw particles and among rice straw particles. The inlet gas velocity was set as $u_{x,0}$ = 0 and $u_{y,0} = h\sigma U_{ms}$ where σ is the geometric factor and *h is* the velocity correction coefficient in the numerical model with a value of 0.636. The diameter of the solid particles was set as ωd_s where d_s is the diameter of the solid particle and ω is the diameter correction coefficient set as 0.313.
The precise determination of the height of the fountain allows the identification of the main zone of the spouted Bed Reactor because in it occurs the main transfers of mass and energy. Moreover, it also permits the optimisation of the initial amount of solid and the velocity of the gas at the inlet in order to minimize the energy requirements of the system. However, the model does not provide good values for the predicted pressure drop especially in the cases with low height of initial solid. This error may be due to interference of the edge of the probe in the experimental measurement because the probe was located in the intern of the bed at 20 cm from the bottom. A potential solution is to change the position of the probe in the intern of the bed. In addition, an upgraded 3D model of the Spouted Bed Reactor might be necessary in order to obtain a better prediction of the pressure drop. The graphic simulation results are shown in Figure 2.

6. Conclusions

In this work, through the combination of experimental data and a numerical model, the fluid dynamic behaviour of a Spouted Bed Reactor was studied. The obtained data show that the model approximates with good results the height of the fountain in all cases with a maximum error of less than 5 %. This result allows identifying in advance the region where the fountain will develop, which is very important because in it takes place bulk transfers between gas and solids. However, this model does not provide, with the same precision, the predicted values of pressure drop. It is likely to be necessary an upgrading of the experimental apparatus and a setup of the 3D model of the SBR to obtain a correct prediction of the pressure drop. The calibration of the model for pressure drop is left for a future study.

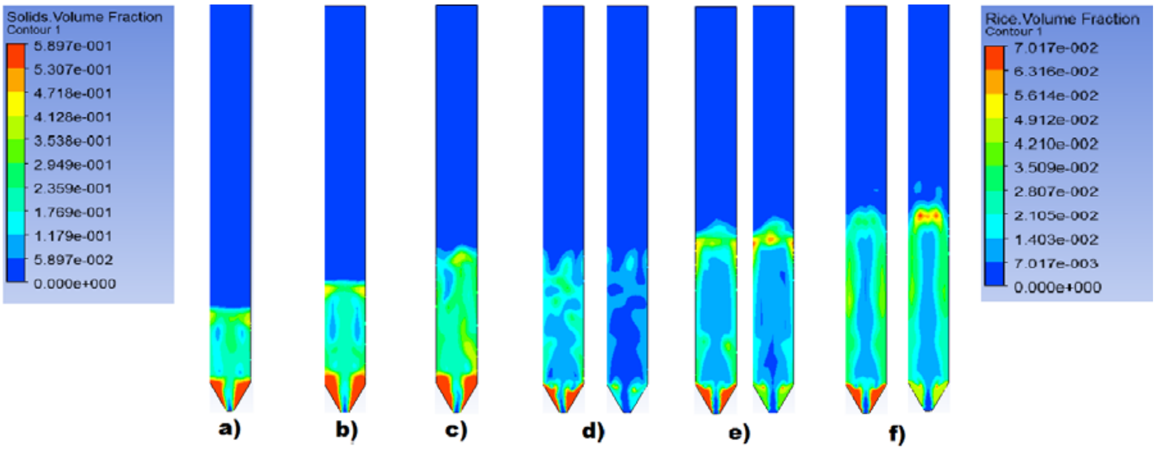

Figure 2: Volume fraction for different heights of initial solids with 0 % v/v of rice straw: a) 25 cm, b) 35 cm, c) 45 cm and with 10 % v/v of rice straw (on the right of the figures): d) 25 cm, e) 35 cm f) 45 cm

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