A Numerical Model of Rice Husk Combustion in Bubbling Fluidized Bed

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Abstract: *Fluidized bed reactors have attracted significant interest in recent times due to their ability to ensure high combustion efficiency at low reactor temperatures, along with impressive heat retention capacity in the bed. Generally, combustion in the fluidized bed is very complicated and the effect of certain parameters like temperature on the hydrodynamic properties of the reactor have not been fully understood.*

To address this, Computational fluid dynamics is employed in modelling the homogeneous combustion of rice husk feed stock in order to observe the turbulent reaction temperature and specie concentration within the fluidized bed. The study adopts the Eulerian-Eulerian and finite rate/ eddy dissipation reaction models to predict the combustion behavior of the solid fuel within the reactor, using ANSYS computational software.

Simulation results indicate that combustion in the bed begins at a point close to the fuel exit, with the reaction model predicting much higher reactor temperatures when compared with Magnussen's eddy dissipation combustion model.

Keywords: *Combustion; Fluidized; Biomass; Numerical; hydrodynamics*

1. Introduction

Thermochemical processes for solid fuel conversion have been explored for centuries. These methods have become more sophisticated in an attempt to improve conversion efficiency, as well as address the environmental aspects associated with solid fuel combustion. Coal for example has been widely utilized in power generation, often with unique handling and combustion problems. In recent decades, conversion technologies have migrated from the conventional fixed-bed reactors, to the moving bed, and eventually fluidized bed combustion and gasification. In fact, the combustion of solid fuels in pressurized fluidized bed boilers has been identified as the blueprint of modern power plant engineering [1]

The theory governing the design characteristics and behavior of fluidized bed has been well documented throughout literature. However, studies of the numerical model of the combustion process is of vital importance in understanding the reactor hydrodynamics and the mechanisms that govern the formation of some species, which are otherwise harmful to the fluidization process. These reaction models provide information regarding the intrinsic properties of the reactor including bed temperature distribution, specie concentration, physical-chemical properties characterization gradient and other factors leading towards process optimization [2].

Numerical solution of thermochemical conversion of coal in circulating fluidized bed boilers could be characterized by high oxygen and low carbon dioxide (CO2) concentrations along the dense bed region, with a near-constant temperature distribution of 950oC across the reactor height [3]. CO2 concentration gradient is an important factor in determining the combustion quality of reactors, due to its tendency to reduce soot volume fraction [4]. However, practical use of fluidized beds in solid fuel combustion must also contend with the level of alkali salts and chlorides present in most biomass and coal samples. These impurities could lead to significant levels of deposits on reactor walls, quite often causing bed agglomeration and sintering, thereby leading to reactor shut down [5]. Experimental studies of pollution characteristics in fluidized bed of sand particles hinted a possible role for computational methods in improving the ash quality during rice husk combustion [6]. Temperature plays a major role in pollution control in fluidized beds. Nitrogen oxide (NOx) formation and ash melting are suppressed at low temperature values, thereby mitigating environmental pollution while preventing the formation of agglomerates [7]. Comparison of numerical study of the temperature profile in coal fired grate boilers, with experimental tests, shows good agreement in-terms of the temperature distribution across the reactor cross section [8]. The authors concluded that soot modelling could also provide further insight into certain properties of the combustion gases which could impact on reactor temperature.

Hence, the present study focuses on the numerical investigation of specie distribution in a bubbling fluidized bed reactor during the combustion of rice husk. The computational domain consists of a bed diameter of 255 mm and an overall height of 700 mm, with a feeding section located at 127 mm from the bed. A plenum chamber of 100mm height is also introduced at the bottom of the fluid bed.

2. Numerical model

In this study, the combustion process of rice husk samples in a bubbling fluidized bed reactor is simulated using ANSYS computational software. The reactor, in its basic form, is a

prototype used in the experimental works of Ghaly et al. [11], where bed pressure variation with various distributor grid shapes and inclination was studied. The reactor geometry is presented in Figure 1

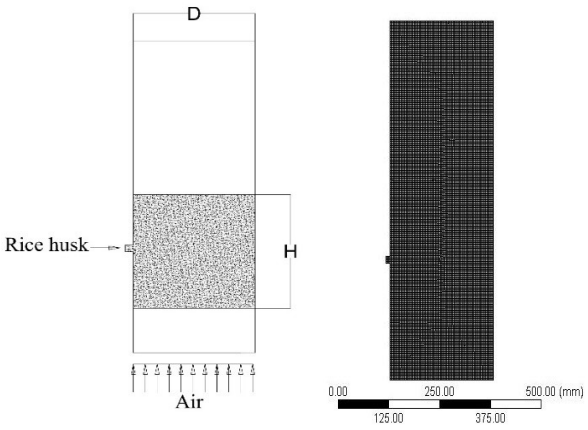

Fig.1. Reactor schematic and computational domain

The approach concerns an initial stage in which the hydrodynamics of the reactor column is modeled during cold fluidization, before simulating the biomass combustion process. The Eulerian two-fluid and finite rate/eddy dissipation models are used for the hydrodynamics and combustion processes respectively. The overall simulation process is therefore decoupled to account for computational time and model simplicity.

The idea is to perform a holistic system validation, in preparation for a more comprehensive study, which could involve the use of a more complex distributor grid design, and the observation of salient bed parameters, together with their impact on the combustion process within the reactor.

Hydrodynamic model. The hydrodynamic properties of the reactor are simulated using the Eulerian – Eulerian (two fluid) model, where both the solid bed particles and fluidizing gas are treated as a single continuum [12]. The model provides a relatively shorter computational time, while allowing enough stability to ensure reliable predictions of certain quantities of interest, including void fraction of sand, pressure and temperature [12], [13]. The Navier Stokes equations for continuity and momentum are given by equations (1) and (3) respectively.

$$\frac{\partial(\alpha_l \rho_l)}{\partial t} + \nabla.(\alpha_l \rho_l u_l) = \sum(\dot{m}_{kl} - \dot{m}_{lk}) \tag{1}$$

Where $\dot{m}_{lk}$ is the mass flow rate between phases k and l. Similarly, the gas – solid interaction triggers the transfer of multiple species or fines, as given by the transport equation (2)

$$\frac{\partial(\alpha_l \rho_l Y_{il})}{\partial t} + \nabla.(\alpha_l \rho_l u_l Y_{il}) = \sum\left(\dot{m}_{ij}^{lk} - \dot{m}_{ji}^{kl}\right) \tag{2}$$

Y_{il} is the mass fraction of specie i in phase l. The corresponding momentum Navier Stokes equation is given by

$$\frac{\partial(\alpha_g \rho_g u_g)}{\partial t} + \nabla.(\alpha_g \rho_g u_g u_g) = -\alpha_g \nabla P + \nabla.\bar{\bar{\tau}}_g + \alpha_g \rho_g g + \sum\left(R_{sg} + \dot{m}_{sg} u_{sg} - \dot{m}_{gs} u_{gs}\right) \tag{3}$$

Where g and s denote the gas and solid phases respectively.

The force exerted on the solid particles by the fluidizing gas is of considerable importance to avoid defluidization. Several drag models including the Syamlal O Brien, Wen-yu, Morsi-Alexander and Gidaspow model among others, have been used to model the fluidized bed with varying degrees of success under different modeling conditions [14]–[17]. However, the Gidaspow model (equation 4), represents a very reliable means of predicting the drag force since it combines the Wen-yu and Ergun equations [14].

$$K_{gs} = \begin{cases} K_{gs}\ (Wen\ Yu), & \alpha_g > 0.8 \\ K_{gs}\ (\ Ergun), & \alpha_g \leq 0.8 \end{cases} \tag{4}$$

The corresponding Wen-yu model is given as

$$K_{gs} = \frac{3}{4}\frac{\alpha_g \rho_g (1 - \alpha_g)}{d_s}.C_D.\left|\vec{V}_s - \vec{V}_g\right|\alpha_g^{-2.65} \tag{5}$$

The hydrodynamics of the reactor places significant emphasis on the pressure drop across the distributor grid. For a bubbling regime, the pressure drop across the bed is related to the fluidization velocity as given by the ergun equation [10].

$$\frac{\Delta P}{H} = 150\frac{(1-\varepsilon)^2}{\varepsilon^3}\frac{\mu u}{(\phi d_p)^2} + 1.75\frac{(1-\varepsilon)}{\varepsilon^3}\frac{\rho_g u^2}{\phi d_p} \tag{6}$$

Furthermore, the distributor pressure is related to the bed pressure drop as follows [11].

$$\Delta P_D / \Delta P_B = 0.01 + 0.2\left[1 - exp\left(-0.5\frac{D}{H_{mf}}\right)\right] \tag{7}$$

Various particles have been categorized as group A, B, C and D by Geldart in 1973, based on the particle diameter and density. While this classification helps to identify suitable materials for fluidization, the Reynold's and Archimedes number strongly influence fluidization quality by defining suitable limits for the minimum fluidization velocity. Hence, for small particles where the Reynold's number is less than 20,

$$U_{mf} = \frac{(\emptyset_s d_p)^2(\rho_s - \rho_g)\varepsilon^3 g}{150\mu(1-\varepsilon)} \tag{8}$$

Similarly, for large particles with Reynold's number greater than 20,

$$U_{mf} = \left[\frac{(\emptyset_s d_p)^2(\rho_s - \rho_g)\varepsilon^3 g}{1.75\,\rho_g}\right]^{1/2} \quad (9)$$

The void fraction of the bed is another parameter that could be used to study fluidization quality. High particle density and initial bed height adversely affect fluidization velocity, and consequently, bed voidage. Equation (10) relates the volume fraction of bubbles with the gas and bubble velocities in a typical fluidized bed reactor.

$$\boldsymbol{\varepsilon_b} = \frac{U - U_{mf}}{u_b - U_{mf}(1+\alpha)} \quad (10)$$

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Reaction model The reaction model involves the chemical kinetics governing rice husk combustion, along with the release of heat. Biomass, like coal, could be defined by its rank, which is characterized by the amount of volatile matter and/or fixed carbon content. In combustion models, feed samples are represented as small entities typically in the order of a few microns in size, so that respective particle are considered pseudo homogeneous [18]. The primary step in solid fuel combustion is the drying process, which is accompanied by the vaporization of moisture within the fuel sample in the case of wet combustion, until the devolatalization temperature is reached [3]. Shortly after the devolatalization, char formation and subsequently, char or volatile combustion takes place. The two-step kinetic devolatalization of rice husk, which is similar to that of coal, is as follows [18].

$$Rice\ husk + Heat \overset{k_1}{\rightarrow} Volatile\ 1 + Residue\ 1 \quad (11)$$

$$Rice\ husk + Heat \overset{k_2}{\rightarrow} Volatile\ 2 + Residue\ 2 \quad (12)$$

$$\frac{dx_{rice\ husk}}{dt} = -k_1 x_{rice\ husk} - k_2 x_{rice\ husk} \quad (13)$$

$$k_1 = A_1\, exp\left(-{E_1'}/{RT}\right) \quad (14)$$

$$k_2 = A_2\, exp\left(-{E_2'}/{RT}\right) \quad (15)$$

Assuming the single particle combustion analysis is valid for every fuel particle, the mass combustion rate for various chemical species could be represented follows [3].

$$\frac{dC_{O_2}}{dz} = \tau_g\left[\frac{1}{2}\sum_i R_1, i\xi - \frac{1}{2}R_2(1-\varepsilon_s)\right] \quad (16)$$

$$\frac{dC_{CO}}{dz} = \tau_g\left[\sum_i R_1, i\xi + 2\sum_i R_3\xi - R_2(1-\varepsilon_s)\right] \quad (17)$$

$$\frac{dC_{CO_2}}{dz} = \tau_g\left[\sum_i R_3, i\xi + R_2(1-\varepsilon_s)\right] \quad (18)$$

The combustion of the fuel sample could be achieved using the finite rate, eddy dissipation or probability density function models. The finite rate model predicts the reaction rate by using the reaction kinetic expression to compute the source terms during specie transport. The overall reaction source term R, for several species can be computed using equation (19) [19].

$$R_i = M_\omega, i \sum_{r=1}^{N_R} \hat{R}_i, r \quad (19)$$

Where M_ω, i is the molecular weight of specie i.
The molecular rate for the creation of a specie is

$$\hat{R}_i, r = \Gamma\left(\upsilon_{i,r}'' - \upsilon_{i,r}'\right)\left(k_{f,r}\prod_{j=1}^{N_r}\left[C_{j,r}\right]^{\eta_{j,r}'} - k_{b,r}\prod_{j=1}^{N_r}\left[C_{j,r}\right]^{\eta_{j,r}''}\right) \quad (20)$$

This finite rate model is more computationally expensive than the less demanding eddy- dissipation model, where reactions are controlled by the rate of turbulence. The eddy-dissipation combustion for a single step reaction is given by [20].

$$fuel + r_j oxidizer \longrightarrow (1 + r_j) products \quad (21)$$

The reaction rate R_a is obtained from the Arrhenius expression [21].

$$R_a = Da\left(\frac{\rho Y_f}{W_f}\right)^{r_f}\left(\frac{\rho Y_o}{W_o}\right)^{r_o} exp\left[-Ze\left(\frac{1}{T} - \frac{1}{T_F}\right)\right] \quad (22)$$

Hence equation (21) becomes

$$r_f W_f R_a + r_o W_o R_a \longrightarrow 2r_p W_p R_a \quad (23)$$

For eddy dissipation modeling, the reaction rate R_{edm} is expressed as

$$R_{edm} = A\frac{\bar{\epsilon}}{\bar{k}}\rho min\left(r_f Y_f, r_o Y_o, B r_p Y_p\right) \quad (24)$$

Where k is the turbulence kinetic energy.

3. Simulation results and discussion

A mesh independence study has been carried out for the computational domain, focusing on the bed voidage parameter as shown in Figure 2. Various grid element sizes ranging from 16 mm, 14 mm, 12 mm, 5mm and 1mm were tested. The value of the void fraction parameter is barely affected beyond an elemental size of 5mm, and consequently, a size of 4mm was used in this simulation to balance computational time with result accuracy.

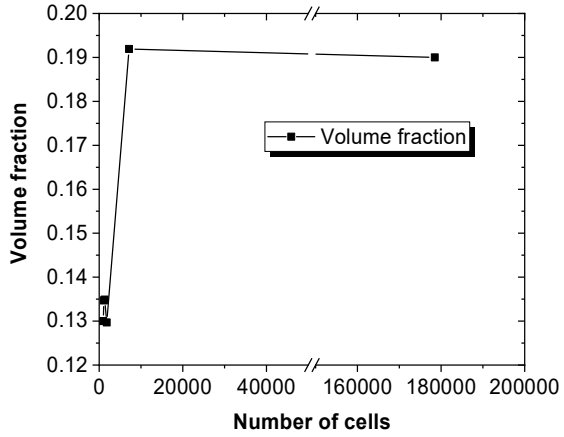

Fig. 2. Mesh independence test

The gidaspow drag model is used to simulate the fluidization process, with sand particles selected as the bed material. Figure 3 shows the 2-dimensional fluidization for an aspect ratio of 1, at a fluidization velocity of 7.35 cm/s.

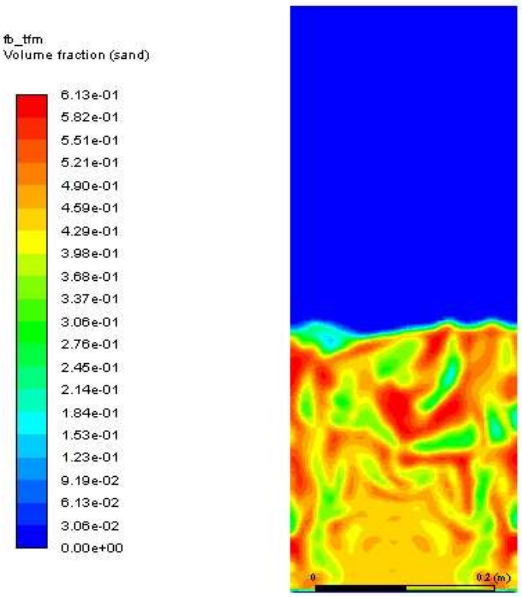

Fig. 3. Contours of two-fluid modeling of the fluidized bed at t = 0.0625s

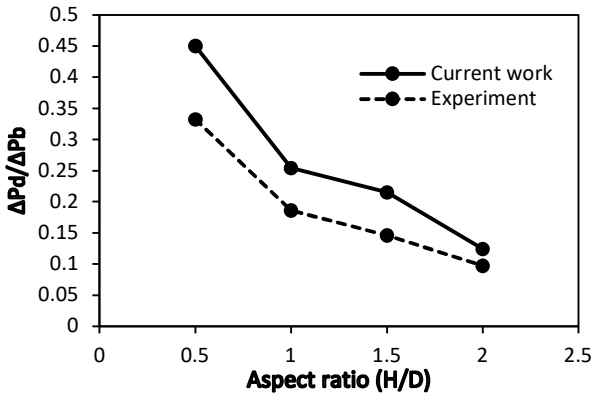

Fig. 4. Pressure drop versus bed H/D ratio

The model successfully imitates the Ghaly et al. solution (Figure 4) when the pressure drop is compared with the aspect ratio, albeit with some variations. The deviations could be attributed to the fact that it is difficult to replicate the exact conditions in which the experiment was conducted. Furthermore, the Ghaly et al. experiment falls short of carrying out an extensive study of the combustion properties of the designed reactor. Consequently, the reaction model is validated using computational combustion proposed by Magnussen [22]. The contours of CO_2 formation and O_2 depletion in the reactor are represented in Figures 6 and 7. The entire column is initially filled with oxygen, which is gradually consumed as combustion progresses. For simulation purposes, the bed section is patched with small concentrations of CO_2 and H_2O in other to initiate the chemical reaction.

A rich zone is created in the immediate vicinity of the fuel exit, and therefore, most of the combustion in the bed takes place in this region. The reactor temperature is compared with Magnussen's combustion model as highlighted in Figure 5.

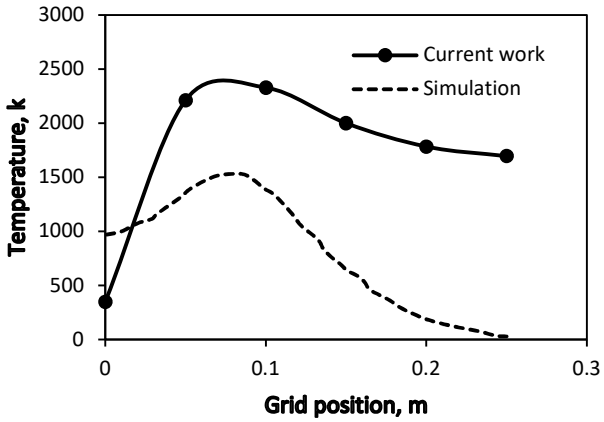

Fig. 5. Reactor temperature for different combustion models

The finite rate/eddy dissipation model predicts significantly higher values for the reactor temperature, which may not be desirable in fluidized beds. Selecting the appropriate set of reactor initial values and wall conditions is necessary to keep the combustion temperature as low as possible, to avoid ash

melting and fouling problems associated with biomass combustion. It is important to note that the Magnussen's model is based on the eddy dissipation concept, and hence differs from the finite rate/eddy dissipation model adopted in this study.

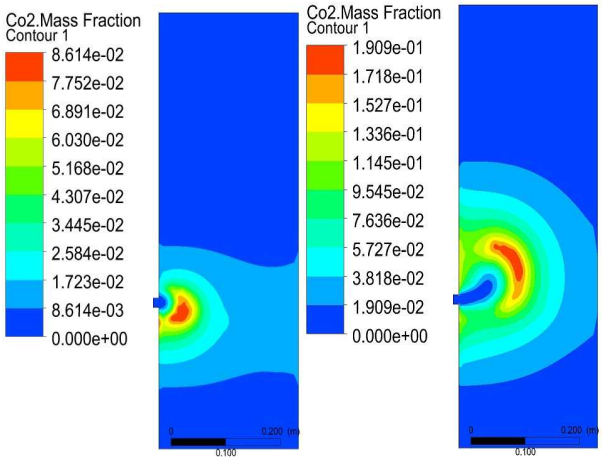

Fig. 6. Carbon dioxide specie formation in the reactor after 0.1s, at a bed aspect ratio of 1, and flow velocity of 7.35cm/s

CO is oxidized to CO_2 in the bed region, and the CO_2 concentration contour grows steadily within the reactor as the production of CO_2 is complemented by a corresponding decrease in oxygen concentration for various aspect ratios.

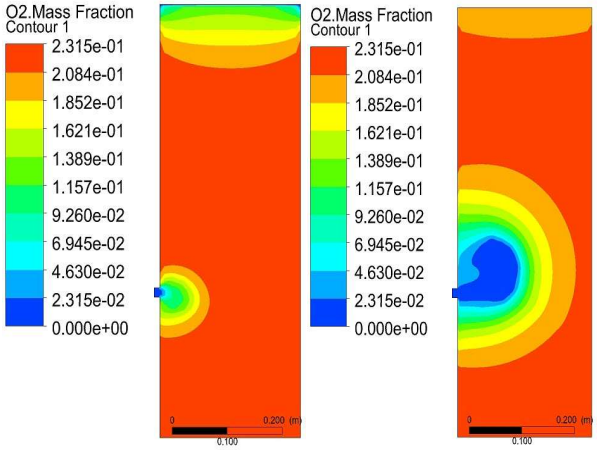

Fig. 7. Oxygen depletion at various times during combustion reactor after 0.1s, at an aspect ratio of 1, and flow velocity of 7.35cm/s

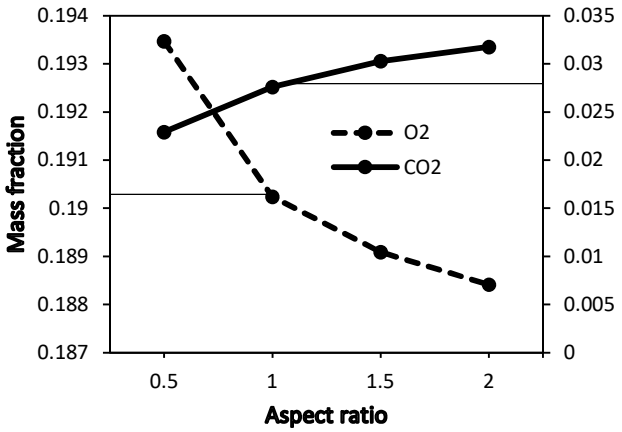

Fig. 8. Variation of CO_2 and O_2 concentrations with various aspect ratios

6. Conclusions and Perspectives

The combustion of biomass involves fluid flow, chemical reactions, heat and mass transfer which are very complex to predict simultaneously. Numerical solutions generally require a strong balance between model complexity and result accuracy. The current study indicates that it is possible to obtain a model for predicting the combustion characteristics of rice husk in fluidized bed reactors. However, better understanding of the underlying turbulent model, the reaction mechanisms that help predict NOx and soot formation, and the boundary conditions of the enclosing geometry is necessary in order to accurately emulate practical situations.

Nomenclature

A	Combustion model constant
ΔP, ΔP_B	Pressure drop
ε	Voidage
μ	Absolute viscosity
u	Velocity
ϕ	Sphericity
d, D	Diameter
H	Height
ρ	Density
$\dot{m}$	Mass flow rate
Y	Mass fraction
α	Volume fraction
K_{gs}	Drag
C_D	Discharge coefficient
$\hat{R}$	Molecular rate of creation/destruction of species
R, r	Reaction
υ'', υ'	Stoichiometric coefficients
k	Reaction rate constant
C	Molar concentration
η'', η'	Rate exponent
N	Number of chemical species
Da	Damkohler number
Ze	Zeldovich number
W	Molecular weight
$\bar{\bar{\tau}}$	Stress tensor

Subscripts

mf	*Minimum fluidization*
s	*Solid*
p	*Particle*
g	*Gas*
b	*Bubble, Backward*
k, l	*Phases*
i, j	*Specie*
f	*Fuel, Forward*
o	*Oxidizer*

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